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OBJECTIVE

Direct nanoHUB.org and the Center for Predictive Materials and Devices, and conduct nanoelectronic research, high performance computing, and software engineering.

EDUCATION

Ph.D., Electrical Engineering, Purdue University, GPA: 4.00/4.00 1994

Theoretical Thesis: Electron-Electron and Electron-Phonon Interactions in Quantum Transport.

Advisor: Professor Supriyo Datta

Dipl. Ing., Electrical Engineering, Ruhr University Bochum, Germany (equiv. M.S.E.E.) 1990

GPA: 5.97/6.00 (converted from German system), Class Rank 2/167

Experimental Thesis: Laser Noise Induced Intensity Fluctuations in an Optical Interferometer.

Advisor: Professor Daniel S. Elliott, Purdue (work conducted as an exchange student at Purdue).

Engineering Co-op program with Thyssen Mechanical Engineering, RWE, and Siemens AG.

APPOINTMENTS

Purdue University, Elmore Family School of Electrical and Computer Engineering

Elmore Chaired Professor, 12/22-present

Reilly Director of the Center for Predictive Materials and Devices (c-PRIMED) 10/13-present

Professor, Director Network for Computational Nanotechnology (NCN) 05/09-present

Professor, Network for Computational Nanotechnology Associate Director for Technology 12/03-04/09

- Transformation of www.nanoHUB.org - now recognized as NSF science gateways flagship
 - Growth from 500 annual users in 2003 to over 2,000,000 users (as of Dec. 2022)
 - Introduced fully interactive simulations, >22,000 annual users >1,000,000 simulations
 - Lead the analytics work to demonstrate nanoHUB impact in classrooms and research
 - Created a new type of publications now listed in Web of Science and Google Scholar: nanoHUB Scientific Apps used in teaching and duplication of research results.
- Lead the development of NEMO 3-D, OMEN, and NEMO5 development for atomistic, non-equilibrium quantum transport modeling of realistically scaled transistors and quantum dots. Demonstrated critical physics in Si-based transistors and explored alternatives in many other materials systems. Lead model development for quantum computing in Silicon. NEMO5 is now used at Intel to design transistors and commercialized through SILVACO.
- Lead ~15 professional nanoHUB staff members and up to 35 researchers in nanoelectronics.

NASA Jet Propulsion Laboratory, California Institute of Technology

Senior (02/98-9/01), Principal Member (9/01-6/15) of Technical Staff (academic part time 12/03 until 06/15)

Technical Group Supervisor, Applied Cluster Computing Technology Group 4/02-12/03

- Development of an atomistic nanoelectronic modeling and simulation tool NEMO3D, a genetic algorithm optimization and synthesis tool, Parallelization of Mars imaging software

Texas Instruments Incorporated, Corporate Research and Development 9/95-2/98

(transitioned to **Raytheon TI Systems**, Applied Research Laboratories 8/97).

Member of Technical Staff - Nanoelectronics Research Group

- Development and project management of the Nanoelectronic Modeling software (NEMO) (theory, algorithms, user-interface, implementation, verification, documentation and delivery)

University of Texas at Dallas, School of Engineering

Post-doctoral Research Associate - Supervisor: Professor William R. Frensley 2/94-9/95

- Prototype development of NEMO. Consultant to Texas Instruments,

SELECTED HONORS

- Fellow of IEEE, of the Institute of Physics (IOP), the American Physical Society (APS), Alexander von Humboldt Foundation, American Association for the Advancement of Science (AAAS)
- Awarded Proposal Author as PI and lead Co-PI exceeding \$116.3M – including 7 center level grants.
- Co/Author of 305 journal, 239 proceedings, 284 invited conferences, 520 contributed conferences
- h-index in Web of Science: 59, Scopus: 60, Google Scholar: 72
- Graduated 43 PhD and 16 Master Students, Supervised: 15 post docs, 5 research faculty, 59 undergraduates.
- 6 US Patents, 12 NASA software, NASA board, NASA Space Act, and NASA Tech Brief Awards

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PUBLICATION SUMMARY

Publication Type	total	Publication Type	total
- Peer reviewed Journals:	305	- Patents:	6
- Peer reviewed proceedings:	239	- Scientific Apps, Tools, Data:	42
- Invited Conference papers:	284	- Technical Reports:	36+
- Contributed conference papers:	520	- Technical Program Reviews:	98+
- Invited Seminars:	191	- Technical Briefings:	111+

Secondary Citations and h-index from Web of Science (WoS), Scopus (Sc), Google Scholar (GS)

Date	WoS Citations	Scopus Citations	GS Citations	WoS h-index	SC h-index	GS h-index	Years past PhD
1/16/2023	13,599	14,944	22,555	59	60	72	29

CAREER HIGHLIGHTS & IMPACT

Co-Lead (2003-2009) and Lead (2009-present) the vision and operation of nanoHUB.org

Grew nanoHUB use from 500 annual users to enable 160,000 nanoHUB users to run millions of simulations in the first scientific end-to-end cloud.

Created scientific Apps before Apple in the iPhone.

Over 13 million nanoHUB visitors viewed lectures and tutorials.

The US annually invests \$2B in nano research and lots of software and data are generated. But the broader audience cannot learn from these artifacts, because they are not accessible and usable. Therefore, Klimeck led the creation of Apps wrapped around scientific software packages that were previously inaccessible, very hard to use, and required specialized computing hardware. Before the iPhone introduced Apps Klimeck led efforts to package complex scientific software that ran in cluster computers into user friendly nanoHUB-hosted Apps in 2005. He helped to create the first scientific-end-to-end simulation cloud with a global research & education user base, before the cloud became popular. Klimeck morphed nanoHUB, operated by the Network for Computational Nanotechnology at Purdue, from a research network into a national and international Cyberinfrastructure with a global user base in 172 countries.

Over 160,000 users across the globe have run over 7 million simulations on nanoHUB (as on Dec. 2021). nanoHUB also developed into a MOOC with over 190 courses and a library of over 6,000 content items. Over 13 million visitors have utilized this nanoHUB content.

Demonstrate New Approaches in Interactive Education and Translational Research

Research software wrapped in easy-to-use Apps can be rapidly introduced into existing curriculum.

Research software wrapped in Apps can have translational success in adoption by other researchers such as experimentalists or researchers in adjacent fields

Around 1999/2000 the concept of scientific portals emerged with a vision to share scientific software and data that would execute “in the grid”. However, almost none of these portals grew to a critical mass of research users beyond their creators. By 2003/05 the community has begun to believe that such portals cannot be used to conduct research and certainly cannot be used in education. Klimeck had a vision to deliver scientific tools in a different way. The hard-to-install, hard-to-use, and computationally intensive software packages needed to be simplified such that experimentalists, educators, and students could use the software without reading massive manuals. The simplifications required the execution of the whole simulation flow including the set-up of the experiment, the execution and monitoring of the execution of the simulation, and the post-processing of the final data. Each of these 3 steps plus the software installation typically require expert knowledge. His NEMO1D and NEMO3D software packages already demonstrated easy-to-use and easy-to-build Graphical User Interfaces (GUIs) and I/O handling. They were indeed used by experimentalists. Klimeck hired Dr. Michael McLennan from Cadence and they created the envisioned specialized Apps. These Apps are geared towards the solution of specific sub-classes of problems that a general tool could handle and to make them easy to use in interactive user-interfaces. McLennan created Rappture inspired by Klimeck’s NEMO GUIs and his experience at Cadence. Using Rappture Klimeck created the first interactive tools. Today over 600 Rappture-based apps are running in nanoHUB. But the NSF evaluators stayed skeptical: Can these Apps be used in research or Education?

User Behavior Measurement & Analytics for Impact Studies

In the beginning of Klimeck’s nanoHUB involvement he immediately stated: “If we build an infrastructure, we need to measure if it works!”. Klimeck led the instrumentation of the apps for usage analytics and developed new impact assessment methodologies. By user-behavior clustering his team was able to show that 79,800+ students in 3,600+ classes at 185 institutions have used nanoHUB simulations in structured education (data as of Jan. 2022). They measured the median time between a specific tool publication and its first adoption in a classroom as less than 6 months, pointing to rather rapid curriculum innovation.

Measuring research impact requires a long-term view as the research and publication process requires a long time and is less predictable in its user behavior. Klimeck created a process to systematically track scientific publications that cite nanoHUB and to evaluate them carefully in various aspects. These aspects include the specific tool cited, the background of the users and the paper (experimental work, theoretical work,

benchmarking etc.), the institutions, and the resulting social network. As of Jan. 2022, nanoHUB is cited 2,553 times in the scientific literature.

In about 2008 when presented with the first 200 papers that cited nanoHUB the peer reviewers conceded that research may be possible but argued that it cannot be good research. Culture change requires patience and persistence. Klimeck proceeded to measure these citations through secondary citations and as of Jan 2021 identified over 53,000 secondary citations with an h-index of 105.

Learning and Research in The Cloud

“**Learning and research in the cloud**” published in *Nature Nanotechnology* [200] documents at a high level the dual use of tools education and research and demonstrates the classroom identification through usage analytics. Overall, the nanoHUB team overall has not spent a whole lot of time on writing research articles about the use and impact of nanoHUB but has focused on the usability of the tools and the site [72,80,98,110,119, 201, 202, 203,211]. There are also some initial published studies on how users “behave” inside individual tool sessions – do they methodically move through design spaces, or do they jump like wildcatters? [P225, P228] Also collective behaviors of classroom participants [P227] have been analyzed ultimately geared towards providing feedback to faculty members who utilize nanoHUB in their curriculum.

Creation of a new publication type

Web-of-Science and Google Scholar are listing nanoHUB Apps as proper publications since 2017

Early in the modernization of nanoHUB we began assigning DOIs to our nanoHUB Apps in 2005. Klimeck kept re-iterating in public presentations that these apps enable the duplication of scientific results and are in many ways “more important than the scientific paper” since many papers really cannot be duplicated. In 2016 Thompson-Reuters, the owner of Web of Science at the time, approached us if we are willing to list nanoHUB Apps as digital artifacts in the Web of Science.

Since 2017 the Web-of-Science is including nanoHUB Apps as their first scientific application in their publication index. Google Scholar followed suit a few months later. Web-of-Science and Google Scholar automatically polls nanoHUB publications.

In summary: nanoHUB demonstrated three distinct paradigm shifts

A paradigm shift is defined as “*a fundamental change in approach or underlying assumptions*” (Oxford Languages). nanoHUB has achieved that in three different aspects

nanoHUB Apps wrapped around research engines are be used in translational impactful research
(the community assumed that this was impossible).

nanoHUB Apps based on research codes are be used in systematic classroom-based education
(the community assumed that educational tools cannot be based on research grade software).

nanoHUB Apps are new publication types
a new approach – Apps formally listed in Web-of-Science and Google Scholar.

NEMO – Creating the Nano-Scaled Semiconductor Device Modeling Standard

Theory, Modeling, and Simulation have been key enablers to today's all-pervasive computing, data, network, and web technology. Without process, circuit, and device modeling tools this technology revolution would not have been possible. Moore's law device down-scaling has proceeded since 1965 and has reached device length scales that are counted in atoms and few nanometers. At that length scale carrier transport must be modeled fully quantum mechanically, out of equilibrium, and with a fundamental basis set that is explicitly including every atom in the active device. 30 years ago, the physical scaling end could have been predicted, but it was completely unknown what the right theory, modeling, and software framework might be needed to understand devices at such ultimate scaling limits.

30 years of fundamental and applied research by the Klimeck-led teams have resulted in the Nanoelectronic Modeling (NEMO) tool set that has set the standard for realistic nano-devices today. In graduate school Klimeck studied with advisor Supriyo Datta the esoteric Non-Equilibrium Green Function (NEGF) formalism and applied it to resonant tunneling diodes. At Texas Instruments (1994-1998) Klimeck built NEMO1D which established NEGF as the state-of-the-art standard for quantum transport theories and standard for room temperature quantum devices such as resonant tunneling diodes (RTDs). RTDs were the first quantum transport devices operating at room temperatures. The modeling of their critical layer thicknesses of about 5nm and extended contacts forecasted the needs for today's nano-transistors. He established the representation of the nanoscale materials in an atomistic tight-binding basis, rather than the widely accepted continuum models such as effective mass or $k \cdot p$. At NASA-JPL (1998-2003) Klimeck built the first multi-scale, multi-million atom electronic structure code NEMO3D. Also, at JPL he established the needed atomistic tight binding parameterizations for standard semiconductors (Si, Ge, SiGe, and AlGaIn/AsPSb) and their alloys). Since 2003 he has generalized these concepts at Purdue with OMEN and NEMO5. By 2004 most advanced modeling groups had adopted NEGF as a standard. By 2010 atomistic tight-binding, rather than continuum effective mass or $k \cdot p$ theory was accepted as the appropriate standard to represent the underlying materials.

Even by 2015 most commercial technical computer aided design tools (TCAD) for transistors do not even acknowledge the existence of atoms; everything is a continuum. Quantum mechanical effects such as tunneling or quantized bands are at best patched into semi-classical approaches that are based on a local equilibrium. NEMO5 establishes a completely different standard: atomistic device resolution, fully quantum mechanical, with full energy resolution to include non-equilibrium effects.

NEMO development and use impacted several distinct areas:

Industry Standard for nano-scaled transistor simulation

- 2013 and 2014 the International Technology Roadmap for Semiconductors (ITRS) adopted physics-based NEMO device models. NEMO replaced MASTAR a lump-system scaling model to provide meaningful device performance predictions looking forward 3 to 10 years.
- Intel integrated NEMO5 into their in-house TCAD tool chain to explore and design nano-scale transistors since 2015
- SILVACO commercializes NEMO5 as Victory Atomistic since 2018
- Samsung hired former NEMO team members to re-implement NEMO5

Modeling Standard in NEGF, Tight-Binding, and High-Performance-Computing

- NEGF is the accepted theoretical approach for nanoscale devices since about 2004. Many groups began to implement their own NEGF versions, typically in effective mass (single band).
- Tight-binding with experimentally accurate band structures is the atomistic basis standard since about 2010. Even today there are very few implementations that scale to realistically extended devices.
- Created implementations that run on single CPUs, small clusters, and the world's largest supercomputers. OMEN is one of the 5 codes that could run at the peta-scale in 2011 on the full Oak Ridge Supercomputer Jaguar at 220,000 cores. NEMO5 scales to the same level.
- Hundreds of user groups have downloaded and used NEMO3D and NEMO5 from nanoHUB.
- Over 20,000 Google citations to over 500 publications refer to results obtained with NEMO

Outreach and translational research via nanoHUB.org.

NEMO powers 9 Apps on nanoHUB that have served over 28,000 users in research and education. These tools are cited in research (>300 times) and used in formal classroom instructions.

The original NEMO1D and NEMO3D graphical user interfaces (GUI) and I/O handling guided the design of Rappture which is now the GUI for over 600 nanoHUB apps which served over 160,000 users with 7 million simulations. These nanoHUB Apps were cited over 2,500 times in the literature.

Quantum Computing in Silicon.

The electron wavefunctions in quantum dots or P-donors range over about 1-3 million atoms. NEMO is the only available modeling framework that can tackle realistically extended quantum dots and impurity systems for quantum computing in silicon. Specific achievements are listed in a dedicated section below.

End-of-Moore's-Law – The CMOS Transistor Replacement Search

Concept exploration tool. Specific achievements are listed in a dedicated section below.

- a) Tunneling transistors, Superlattice transistors, piezo-electric transistors, topological transistors
- b) 2D materials like graphene, TMDs or Phosphorene as well as standard SiGe, III-V, III-N etc.

NEMO enables the exploration and evaluation of these technology concepts and options on the same footing. The exploration is critically going beyond just the “essential” transport mechanisms like tunneling etc. The inclusion of electrostatics in realistically extended devices as well as non-idealities such as band tails and traps is critically needed. Ultimately, despite a lot of effort in the field virtually all these explored options can be **ruled out** as a CMOS replacement at the 5nm scale.

Towards the End-of-Moore's-Law – Nanoscale Transistors and Metals

NEMO provides a unified platform that enables material and design comparisons on equal footing. Comparison across different materials (Si, SiGe, III-V, III-N), geometries (standard 2D, double gate, nanowire, nanosheets), strains, doping, and transport mechanisms are critically needed for technology and design selections. NEMO5 enables such exploration for all these variations on the same footing. This universal ability ultimately enabled NEMO to be adopted as an industrial standard. I estimate that at least 130 (about 1/3) of my research publications since 2006 deal with these aspects.

Specific achievements are listed in the dedicated sections below.

Quantum Dot Modeling

NEMO3D is the only openly available multi-million atom, multi-scale simulation package for quantitative Quantum Dot design and analysis. This quantum dot modeling was a key driver for the development of strain dependent tight-binding parameters in Si&Ge and III-V materials. The interplay between long-range strain in self-assembled quantum dots and their confined electronic structure was clearly revealed.

The NEMO3D capabilities for quantum dots enabled all our work on Quantum Computing in Si.

Few specific achievements are listed in the impact section below.

Resonant Tunneling Diode (RTD) Modeling.

NEMO1D established the “gold standard” to quantitatively predict device performance. NEMO1D explained the fundamental limits of RTDs in terms of peak-to-valley ratios and the origin of valley currents. The critical RTD device dimensions are of the order of 5nm layer thicknesses with extended contacts. The 1994-98 development laid out clearly what will be needed for nano-scaled transistor modeling. Few specific achievements are listed in the impact section below.

Quantum Computing in Silicon

Klimeck formally began work on quantum computing gates in 2002 with a contract by NSA/ARDA entitled "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates". In the subsequent 17 years he partnered with three experimental groups:

- 1) Mark Eriksson (Wisconsin): electrically gated Si quantum dots in Si quantum wells on strained SiGe.
- 2) Michelle Simmons (Sydney, UNSW): single P impurity quantum dots in Si through STM lithography.
- 3) Andrea Morello & Andrew Dzurak (Sydney, UNSW): single P impurities in Si through implantation.

Answers to theoretical and experimental questions were obtained with the NEMO3D software in the Klimeck team. The key success was the ability to model realistically extended devices that included millions of atoms. These collaborations resulted in many highly visible articles such as *Nature Nano*, *Nature Physics*, *Nature Communications*, *Science* and even at *IEDM*. Some of the work is summarized in this highly cited review of modern physics article "Silicon Quantum Electronics" co-authored with 8 other leaders in the field.

Valley splitting (VS) in Si

Energetic proximity of quantum states fosters decoherence in quantum computing and it is desirable to separate the excited states as far as possible from the ground state. VS in Silicon stems from the 6-fold degeneracies of the Si conduction band. VS has been modeled with the standard effective mass theory for decades. However, detailed measurements for Si quantum wells on SiGe substrates could not be quantitatively explained. Our work is described in [176,142, 90, 79, 60, 57, 54, 47]

- VS results from interference of multiple states constituent of Bloch waves that are on the atomic scale. Spatial variations on the atomic scale modify the interference. These Bloch waves are not included in an envelope function approach such as effective mass.
- SiGe is a random alloy. A Si-SiGe interface is rather rough and disordered at the nanometer scale.
- SiGe is typically grown on a 2 degree slant, to achieve a smooth surface. The single atomic steps are disordered with specific patterns.
- A fully atomistic electronic structure model (NEMO) which can simulate systems of 1 million atoms can explain the observed experimental valley splitting.
- Valley-Orbit splitting subsequently emerged for qubits [150]

Single and dense P impurities in Si via STM

Prof. Michelle Simmons (Sydney) pioneered an STM-based lithography method to place P atoms on top of a Si surface. With this method she can create wire patterns that connect to single or multiple neighboring P impurities. Each individual P impurity acts as a quantum dot. Very densely placed P impurities create a semi-metallic wire that is just one atom tall embedded in Si. Our work is described in a series of publications including in *Science*, *Nature Nano*, *Nature Physics*, *Nature Materials*, *PRL*, and *IEDM*.

- **Single Atom Transistor:** Is it really a single P atom? Why can this single P atom stably hold 2 electrons? Can the charging energies in the Coulomb diamond be quantitatively explained? [215,174 in *Nature Nano*]
- **Ohm's law survives at the atomic scale:** Why is P-impurity based wire that is 1 atom tall and 4 atoms wide still conducting like a metal? What is its electronic structure? What is the impact of unavoidable spatial irregularities? Do they break the symmetry and destroy the conduction? [172 in *Science*, 197, 167,220]
- **Spin, Spin-Blockade, Exchange, Decoherence, All-Electrical Control, Transport in Chains:** determination of interactions that form the basic qubit building blocks in P-based Si quantum computing. [206 *Nature Materials*, 208 *Nature Nano*, 214 *PRL*, 279 *Nature Nano*, 252]
- **Quantum Simulation:** Hubbard Model in P-Impurities [245 *Nature Comm.*]

Single P impurities in MOS architectures

Profs. Morello and Dzurak implant individual P impurities into MOS-like geometries. Prof. Rogge analyzed accidental individual impurities in FinFETs.

- **Scalability issues for qubits:** spin-orbit interactions [287], long-distance qubit coupling [272, *Nature Comm.*], spin-qubit transport [252],
- **Qubit control:** controlling spin qubits [225 *Science Advances*], control nuclear spin in Si-29 [216 *PRL*]
- **Decoherence:** Spin-valley lifetime [196 *Nature Comm.*], lifetime enhancements [159 *PRL*]
- **Metrology:** non-invasive determination of experimental impurity placement and species [102 *Nature Nano*, 187 *Nano Lett.*, 152 *IEEE EDL*, 250 *Nature Nano*]
- **Orbital Control:** Orbital Stark Effects [122], g-factor control [121]

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End-of-Moore's-Law – The CMOS Transistor Replacement Search

Moore's law has been conceptually enabled by the power reduction in individual devices and the proportionally higher packing of ever smaller devices in the same area while maintaining the same total power consumption. Device sizes have continued to shrink albeit at a slower pace since 2010 yet the threshold voltage down-scaling has stalled since about 2010. The lowest CMOS threshold is determined by the thermionic limit of a MOSFET at 60mV/dec subthreshold slope (SS) and device noise margins. A new type of transistor would be the only hope to reduce the SS to below 60mV/dec and therefore reduce power consumption.

Various private-public partnerships emerged to create research centers to find the CMOS replacement switch starting around 2003 (NRI, SRC/DARPA, FCRP, STARnet). Klimeck was funded through various such research centers to help model and explore new concepts (MSD, MIND, FAME, LEAST). He partnered with several experimental groups to guide and predict experiments.

The following items highlight some of the device concepts explored with NEMO, their modeling challenges, and their ultimate failures. The transistor concepts typically rely on energetic filtering to prevent high energy electrons to leak through the device and therefore enable a sub 60mV/dec SS. In all of these devices a full-band atomistic model that can encompass realistically extended devices that includes realistic gating is needed to tackle the problems.

Graphene-based TFETs

Graphene is ideally 1 atom tall and need to be scaled to a few nanometers in lateral size to open a bandgap. The modeling challenges are the creation of a realistic basis set that can properly model edge states [153,210,P165] and perform a detailed electrostatic gating calculation over the whole extended device. Line edge roughness induced device-to-device fluctuations [P120,117], realistic ripples [193], strain [P197] as well as the very challenging electrostatics [251] point to practically extremely difficult manufacturing constraints. Few of these devices have been built in research labs that have decent performance characteristics.

Industrial manufacturing seems unfeasible at this stage. [302 *npj 2D*, 251, 210, 193,153,111,95]

TMD-based TFETs

TMD-based materials follow in principle the path of graphene except that the materials themselves have natural bandgaps and therefore do not rely on lateral lithographic precision. Electrostatics are just as crucial here as in graphene. The modeling challenge in TMD is the accurate electronic structure and atomistic representation of the material as well as the proper modeling of the band tails in the bandgap. Critical experimental challenges are doping, low mobility, material growth with high quality. A sequence of publications [226, 230, 233, 237, 239, 240, 276, 278, 286] builds up the modeling capabilities and introduces the concept of electrostatic doping. [255] culminates in a description of potential design rules. Vertical transport across multiple layers enables the modulation of bandgaps and offers performance enhancements [291]. Electrostatics [301] can be used to tune devices into PN-junctions, MOSFETs, and TFETs.

Even if the material challenges were to be overcome the electrostatic control and gate challenges at the nanometer scale appear to be rather stringent.

Much larger TMD-based transistors are currently considered for Back End Of Line (BEOL) processing on top of a normal Si device stack.

Phosphorine-based TFETs

Phosphorine encounters the same challenges as TMDs but adds the feature of an anisotropic effective mass and the potential choice of layer thickness. Design rules [256, 258, 275] and one patent [Pat5] point to potential designs. Applications are all pending the establishment of high-quality growth.

2D-device challenges

Graphene, TMD, and Phosphorine device concepts all are 2D materials that experience the same electrostatic gate control challenges. [283,290] Gate control must be much better than in standard MOSFETs to achieve better-than MOSFET performance.

III-V TFETs

Standard MOSFETs can in principle be doped such that they become TFETs. Si-Based TFETs cannot deliver enough ON-current due to their indirect bandgap [115,131,173] and III-V materials with narrow, direct bandgaps offer the best choice [243, 249]. III-V based TFETs involving InAs or InSb were heavily pursued by the MIND center at Notre Dame (2008-2013). III-V TFETs are also very sensitive to electrostatics and standard 2D MOS configurations will not outperform a MOSFET [115]. A double gate or gate-all-around

nanowire configuration would be needed. Leakage control concepts derived in OMEN/NEMO resulted in a patent [130, Pat3]. With these insights experimentalists began to explore various 3D geometries to control the active tunneling region in III-V TFETs [264,265] with the Rodwell group at UCSB [244], the Seabaugh and Xing groups at Notre Dame [243,P173]. Realistic band-tails in the band-gap [299], well as trap states [280] at the heterostructure interfaces, and tri-angular well notch states that determine current injection [274] point to possibly detrimental device performance degradation preventing III-V TFETs to really deliver sub 60mV/dec.

Intel started using OMEN and NEMO5 to pursue the exploration of III-V TFETs in about 2011. Intel re-directed research funding from III-V to III-N TFETs as the MIND research center reconfigured to become LEAST in 2013. Manufacturability and lack of overall performance gain seem to have stopped III-V TFETs.

III-N TFETs

GaN based TFETs were heavily pursued by the LEAST center at Notre Dame (2013-2018) as Intel had transferred III-V TFET concept exploration to be in-house and deemed that concept no longer pre-competitive. The built-in strong piezo-electric fields in GaN create effectively a narrow tunneling gap and relieve some of the electrostatic gate control challenges [227, P211]. However, the tunneling injection happens from quasi-bound confined states in the emitter that are filled due to incoherent scattering. NEMO5 was enhanced [274] to include the original NEMO1D model [19] to include thermalization in arbitrary contact potentials to model the proper current injection and devise optimized device designs [293]. The NEMO5 designs appeared feasible, but the experimental implementation attempts stopped with the end of LEAST. Experimental implementation appears to be as challenging and limited as the III-V devices.

Superlattice FETs

Superlattice TFETs utilize a man-made finite band of electron injection similar to a TFET. The Rodwell group at UCSB under NRI funding pursued this device concept. Critical ingredients are the scattering inside the source superlattice and the injection from such thermalized states [267,274] and the ability to represent a realistic 2D ultra-thin body geometry. We adopted the nanowire mode-space [281] capabilities to Ultra-thin body mode spaces to cover realistically large devices [304]. Realistic geometries and designs were derived for the Rodwell group [219, 270,305], however the experimental implementation faced significant challenges.

Piezo-Electric FETs

IBM Research heavily pursued Piezo-Electric devices to lower the SS. Around 2012 IBM approached Klimeck to identify a graduate student who could work with them to model their devices. Zhengping Jiang took a ½ year internship position at IBM research and worked with IBM for about 1.5 years on the design and modeling of these low subthreshold swing devices [190]. In the course of that work he demonstrated that adding “f” orbitals to the existing code is almost trivial and enabled us to include a suite of piezo-electric materials such as SmSe and SmTe into our portfolio.

While these devices do show low SS they ultimately have too large of a physical footprint (300nm) and their speed is too slow (~2GHz), and high line voltage (115V) to compete against nano-scaled CMOS transistors.

Topological Insulators and Superconductivity

NEMO5 can explore topological insulator materials in realistic extended devices [235,233]. The challenges of coupling surface states and bulk states can be explored [236]. Proximity-induced ferromagnetism and superconductivity in topological Bi₂Se₃ has also been explored [221,223].

Personal Conclusion – The CMOS Transistor Replacement Search

Since about 2002 “the whole field” of semiconductor device research has been searching for the replacement of the CMOS transistor. A large set of materials, geometries, and transport concepts were explored. I have observed repeatedly that “simple” estimates of the pure transport mechanism in a specific material, in absence of realistic geometries, gating potentials, contacts, or realistic material properties have lead the field to over-hyped promises of these concepts. When put together into a comprehensive simulation engine one can clearly see that most of these concepts cannot compete with a 5nm Si high performance transistor even if the huge material growth and quality challenges were to be overcome. Fortunately, or unfortunately the NEMO team did not have all the needed capabilities ready in 2003, but we were able to build these as we also worked on transistor scaling. I personally had great hope for the III-V tunneling transistor and apparently so did Intel. In summary, NEMO has proven to be extremely capable to explore complex device physics beyond the end of Moore's Law and it has become the modeling standard.

Towards the End-of-Moore's-Law - Transistor Scaling

NEMO provides a unified platform that enables material and design comparisons on equal footing. Most research groups have built specific solutions, customized to one specific class of materials and devices that result in research publications that explore some specific concepts. These solutions usually do not include extended contacts or extended electrostatic solutions. Such customizations make the comparison across different materials (Si, SiGe, III-V, III-N), geometries (standard 2D, double gate, nanowire, nanosheets), strains, doping, and transport mechanisms impossible. NEMO5 enables such exploration for all these variations on the same footing. I estimate that at least 130 (about 1/3) of my research publications since 2006 deal with these aspects. A partial list of explorations and conclusions is listed here.

International Technology Roadmap for Semiconductors (ITRS) uses NEMO5

Publication [213] in 2014 shows the breakdown of lumped system models previously used to project nano-scale device performance. The 2013 and 2014 roadmaps included physics-based device models to project future device trends.

Effective masses become design parameters

Effective mass and bandstructure are no longer a material constant. Instead confinement shape, crystal direction, and strain can be used to design specific effective masses and bandstructure. This opens a design space that has previously not been utilized [63, 93, P89, 100, 101, 180, 188, 189, 209, 222, 213, 228, 257].

Such exploration can ONLY be done with a comprehensive atomistic basis that is experimentally accurate at room temperature such as tight-binding. Effective mass models can be fitted a-posteriori to experiments or tight-binding, but by themselves they cannot predict the bandstructure of nano-scaled devices.

Framed slightly differently, although used by most researchers:

The standard effective mass model is not predictive at the nanoscale!

III-V-based transistors will not outperform silicon

III-V materials had been expected to outperform Si devices due to their smaller effective masses and higher electron velocities. However, in general transistors based on III-V materials such as InGaAs will not outperform strained Si transistors at the nanoscale. III-V systems are typically rather non-parabolic and under strong confinement the electron effective mass becomes heavy. Crystal orientation and strain can be used to make the Si effective masses comparable to InGaAs masses. A variety of design guidelines were published with NEMO5 [222,224] in part with industry partners GlobalFoundries.

Heavy masses are desirable in the sub 10nm transistor

For gate lengths of 7nm to 3nm electrostatic gate control becomes an enormous challenge even in nanowire or nanosheet designs. Direct tunneling under the gate potential becomes a critical leakage mechanism that can be reduced by a heavy transport mass. Since the transport is mostly ballistic in a quantum channel the carrier velocity is not a critical design parameter. [180, 181, 188, 189]

Interface roughness and alloy disorder dominate scattering

For gate lengths of 7nm to 3nm atomic arrangements at the wire edge strongly influence the elastic scattering in nanowires and ultra-thin body devices. [191]

Hole bandstructure can push carriers to the edges of wires

Hole bandstructure is highly anisotropic and HH, LH, and SO bands are highly mixed due to the breaking of crystal symmetry. Counter-intuitively holes may accumulate at the edges or perimeter for wires larger than 4nm in diameter. Crystal orientation, wire geometry, and strain are even more important here [109,128,191,228] compared to the electron bandstructure. Some of this work is published with our Intel colleagues [166].

Inelastic phonon scattering is critical in the source – not as much in the central device

The highly doped transistor source injects carriers into the gated central device region. Scattering in the source shapes the injection and gate potential profile in which electrons are injected. Scattering in the central device region occurs but backscattering into the source is relatively small [124 (c249)]. The smaller the nanowire diameter the more important the scattering is. Wires over 3nm diameter have less than a 35% current reduction due to scattering. This effect is conceptually similar to the first NEMO1D results of 1995 which demonstrated the scattering dominated contact source injection into resonant tunneling diodes. The empirical model to treat

scattering in the contacts was implemented in NEMO5 and shown to be critical to model Superlattice TFETs [267], Sb-based TFETs [243], and GaN TFETs [293]

Experimentally validated III-V transistors

We collaborated with several nationally recognized groups in the understanding and design of III-V and III-N nanotransistors. Jesus del Alamo in InGaAs [149], Suman Datta in Sb-Transistors [204], GlobalFoundries in InGaAs [224], Del Alamo in InGaAs [204]. We also worked with Tomas Palacios on the concept of a GaN based nanowire transistor [297].

All of these III-V transistor explorations refined the NEMO5 modeling capabilities, but ultimately these transistors cannot compete against a 5nm Si transistor.

Interface and bulk trap effects

Traps in electron transport and metrology have been analyzed [152, 157, 280] and incorporated into NEMO5. True transport with the inclusion of traps remains rather challenging to do in quantum transport. Recent work by Kubis with Büttiker probes has shown a general capability.

Phonon-dispersions, phonon transport, thermoelectric devices

Phonon dispersions have been designed for nanowires [172,168,164,163,157] and unfolded for general disordered large cells [212]. The Klimeck group advanced non-linear phonon models [139, 50] and simulated phonon transport with NEGF [262]. These advanced phonon models were also coupled to electron transport to model inelastic scattering and energy loss [124 (c249), 31 (c71), 266] and enabled model extractions for **Thermoelectric Devices** [168].

Personal Conclusion – Transistor Scaling – A tool set is now in industrial use

Since my PhD departure from Purdue in Jan. 1994 I have begun to work on modeling and simulation tool development with the goal to ultimately impact nano-scale transistors. It was clear to me in 1994 that a toolset would have to be built that just did not exist then. For the next 10 years I worked on Resonant Tunneling Diodes and Quantum Dots which exemplified quantum behaviors and allowed for the build-up of technology. Since my 2nd arrival at Purdue in Dec. 2003 I have worked concretely on transistor scaling issues. My group has systematically built up theoretical and algorithmic foundations to address the modeling needs of a sub-10nm transistor. Research publications along the way afforded the students to explore the device physics and validate the tool set. Most of these students are now in industry and NEMO is the industrial standard for quantum transport models in semiconductors.

Towards the End-of-Moore's-Law – Nano-scale metal contacts to any transistor

Transport in nano-scale metals with grain boundaries and interface roughness

Regardless of the choice of nano-scale transistor, electrons must be delivered through metals at that nanometer scale. NEMO5 was designed to be general enough to model transport through any system that can be described by a model Hamiltonian. The challenge in modeling transport through metals at the nanometer scale is like that of semiconductors; a sufficiently sophisticated atomic basis must be used to represent the electronic structure around the Fermi level and interactions due to voids and grain boundaries [207,205]. We modeled the structural details of grain boundaries through molecular dynamics in LAMPPS and imported the large atomic structure into NEMO5 to study the transport through grain boundaries and subject interface roughness [285, P220, P212], line edge roughness [P229] in collaboration with GlobalFoundries and thin copper films with Prof. Appenzeller at Purdue [303].

NEMO5 presents a breakthrough to model metals and semiconductors on the same footing

This is to my knowledge absolutely unique and has not been demonstrated by anyone else.

Two decades of Tight Binding development - Material Science for Engineering Problems

Electronic Device Designs Required Higher Accuracy than Typical DFT Delivered

In the past 25 years computational material science has made tremendous progress in refinements of Density Functional Theory (DFT). For electrical engineers DFT has enabled relatively recently the rapid exploration of bandstructure in novel material systems such as TMDs that are rather relevant to solid state devices. However there continue to be 4 fundamental challenges that limit the utility of DFT for device modeling: 1) highly accurate bandstructure models are limited to a few tens of atoms. DFT that can handle more atoms loose the needed accuracy in the conduction bands. 2) early DFT codes could not accurately predict fundamental bandgaps, 3) DFT remains a fundamentally zero-temperature theory and bandgaps depend strongly on temperature. 4) DFT is in principle an equilibrium theory. Even NEGF implementations of NEGF do not really incorporate inelastic scattering processes that incorporate energy loss. These limitations still persist today and limit the direct use of DFT for realistically extended devices.

Need to overcome shortcomings of existing Tight-Binding

In 1994 NEMO1D work on resonant tunneling diodes (RTDs) revealed the critical need to include an atomistic basis with bandstructure that is accurate in the conduction band to within about 20meV and effective that are accurate with in 1-2%. Empirical tight binding (ETB) offered the physical content of crystal symmetries and full bandstructure within the relevant valence and conduction band. The available ETB parameterizations, however, were tuned to overall bandstructure within a -20eV to 20eV spectrum and were not accurate enough in terms of bandgaps and effective masses. These available parameterizations were not at all suitable for transport in the conduction and valence bands. Furthermore accuracy of strain effects had not been carefully examined and in fact needed model refinements beyond parameterizations.

Analytical expressions and Genetic Algorithms for high-dimensional parameter fitting

Klimeck collaborated with Boykin to develop ETB representations for GaAs, AlAs, InGaAs, InAlAs, InAs, Si, and Ge that match in bulk experimental bandgaps and effective masses. Boykin derived analytical effective mass and bandgap expressions in terms of ETB parameters [17 (c74), 26(c36), 48 (c479)] (c=citation count) associated with material parameterizations. The early fitting process remained tedious at best and did not result in parameterizations exchangeable atomic representations. For example, “As” was note the same atomic representation in “GaAs” and “InAs”. Klimeck embraced Genetic Algorithms (GA) for multi-dimensional optimizations that also considered the analytical results for gaps and masses and advanced the ETB model for accurate treatment of strain [28 (c156), 29 (c137), 36 (c261), 37 (c298), 48 (c497)] with citation counts. This work in the time of 1995-2004 and the associated material parameters have been adopted widely by the field. The adoption can be somewhat measured by the large citation counts considering the field of tool builders is quite small.

GA-Framework used in several other fields (space flight, MEMs design, circuits)

As a side remark – Klimeck’s GA framework was general enough to be used for inverse designs of circuits [P22 (c32), P24 (c134)], space flight systems [60 (c16)], space craft trajectory planning [Seungwon Lee], and MEMs Gyroscopes. It won a “Human-Competitive awards in genetic and evolutionary programming” award in 2005.

Direct mapping from DFT to Tight-Binding

The GA-based tight-binding parameterization process was much more robust than pure manual fitting. However, the thorough fitting of a “new” material still required at least 4 weeks of work and careful attention. In addition, new materials such as TMD or Phosphorine had very limited experimental data and DFT had to be the base to describe these materials. As DFT bandgap and effective mass accuracy increased Klimeck’s group developed a generalized procedure to map DFT orbitals and bandstructure to ETB [184, 259] which was utilized for III-V, metals, TMD, Graphene, Phosphorine, topological insulators, MgO and new environmentally aware ETB Models. These methods now include a specific spatial resolution of the atomic basis, which was not present in the original ETB. Recently Kubis extended NEMO5 to incorporate Wannier function basis sets directly from DFT.

Passivation of surfaces

Practical usage of ETB in 3D geometries requires the termination of the simulation domain at real or computational surfaces for embedded structures. The usual approach of periodic boundary conditions is rather inappropriate for individual devices. An exposed ETB surface has dangling bonds which will result in localized

surface states with energies spanning the bandgap in semiconductors. Klimeck devised a method to passivate the surfaces in embedded structures [49 (c265)]. The high citation count reflects the wide adoption in the narrow field of tool builders. The method dated from 2004 was shown in 2016 to be equivalent to hydrogen passivation [260] and generalized to passivation with any surface element.

Tight-Binding naturally models Topological Insulators

Interestingly enough, the proper surface passivation reveals topological states in materials such as Bi_2Se_3 and Bi_2Te_3 without further adjustment. ETB contains all the physics needed to study surface and bulk effects of topological insulators [226]. Again, this is a huge advantage over typical effective mass models where researchers basically need to feed in artificial potentials or coefficients to “generate” the topological surface states.

Klimeck established Tight-Binding in the field of electronic device modeling as a standard

Klimeck established ETB in the field of electronic devices as a very practical compromise between ab-initio methods like DFT in the material science community and continuum effective mass theories in the electrical engineering community. ETB cannot model the total energy of a material and give insights over the stability of bonds. However, for semiconductor devices, we assume that the bonds and the overall Chemistry are stable.

Electronic device engineers can live with a less rigorous atomistic model. The ETB method balances physical content (symmetries, bonding, surfaces, exchangeable potentials) and close neighbor coupling to enable the modeling of realistically extended devices with millions of atoms. Significant existing shortcomings such as insufficient parameterizations, lack of accuracy in strain models, explicit representation of the 3D basis, and surface passivation were overcome in about 2 decades of work.

STRATEGIC HIGHLIGHTS & IMPACT AT PURDUE

- **09/2018 – 03/2019: Sabbatical and Remote work at University of Hamburg**, Center for Hybrid Nanotechnology. Established new collaboration on Hybrid Electronics
- **2016-19: Renewal of the Network for Computational Nanotechnology (NCN)** – development of strategic plan and proposal for a sustainable nanoHUB as a global platform. 5-year proposal worth \$14.5M from NSF, solely to be spent at Purdue on CI development and operation, assessment, and education research.
- **2017-19: LEDcentral, LLC** – co-founded start-up company with Prof. Tillmann Kubis to drive the commercialization of Light Emitting Diodes Simulation tools.
- **2013/--: Leadership in the Center for Predictive Materials and Devices (c-PRIMED)** – Develop strategies to connect Purdue to the Materials Genome Initiative, Named the Reilly Director of c-PRIMED
- **2011/12: Reconfiguration of the Network for Computational Nanotechnology (NCN)** – development of strategic plan and proposal for the next generation nanoHUB. 5-year proposal worth \$14.5M from NSF, solely to be spent at Purdue on CI development and operation, assessment and education research. Potential for renewal for another 5 years.
- **2012-2018: iCHEER - Institute for Continual Hub Enabled Education and Research** – director of newly formed center at Purdue to promote the use of nanoHUB for Purdue content. Purdue commitment exceeds \$5.7M for 5 years.
- **2012-2018: NEMOco, LLC** – founded start-up company to drive the commercialization of NEMO5 software. Start-up dissolved in 2018.
- **2006: Leadership at the Network for Computational Nanotechnology (NCN)** – development of strategic plan and follow-up proposal for years 6-10. Proposal worth \$18M from NSF and \$5M in cost-share. Annual reports and annual site visits for years 2-9 – annual center renewals.
- **2011: Programmatic Development of a ManufacturingHUB in support of small and medium enterprises** – Closely interacted with the Office of Science and Technology Policy / The White House on the development of a modeling and simulation HUB for small and medium manufacturing companies based on HUBzero technology. Engagement with the Purdue Technology Assistance Program and the school of Industrial Engineering.
- **2010-2012: Strategic Partnership between Purdue and the Country of Colombia** – Effort led by Profs. Arvind Raman and Jean Paul Allain. Developed strategy for Cyverinfrastructure enabled collaboration, research engagement, and economic development. Enabled development of a nanoHUB mirror in South America. Provided one-on-one briefings to the Colombian Minister of Education María Fernanda Campo (twice) and Secretary of economic development of the Bogota district, President of the science and technology council, Codiciti, Hernando Gomez. Effort leads to about 40 fully funded students from Colombia in nano and bio research areas per year for five years.
- **2009-2017: Industry Engagement** – Transferred OMEN and NEMO5 tool suite into the Intel TCAD and Strategic Research Groups. Collaborated with Intel on modeling capabilities and requirements. OMEN and NEMO5 are currently being used at Intel for the exploration of end-of-roadmap transistor devices. Transferred NEMO5 code to Global Foundries and Samsung. Engaged Global Foundries, Samsung, Lockheed-Martin as new industrial members of NCN, joining Intel and SRC.
- **2006/07: Conceptualizing the HUBzero.org framework** – In close collaboration with Dr. Michael McLennan conceptualize ideas for nanoHUB abstraction into HUBs for any other science and engineering area. HUBzero.org now supports over 40 other HUBs in many different fields of Science and Engineering. Developed the concept of a Purdue IT HUB infrastructure group that was led by Dr. McLennan until 2016. In 2020 the HUBzero group under the leadership of Dr. Michael Zentern transitioned to the San Diego Supercomputer Center.
- **Transformation of nanoHUB.org** - nanoHUB has operated a batch-oriented web-submission system that allows remote users to run nanotechnology simulations since 1996 [PUNCH – Purdue University Network Computing Hub]. Historically around 500 to 1,000 annual simulation users were served with such

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simulation services. As the NCN Technical Director Klimeck drove the deployment of the middleware that allowed interactive simulations. The nanoHUB team developed a new, stable, and fully operational middleware system that replaced PUNCH in April 2005. Since then the annual simulation user numbers have climbed above 21,000 with over 1 million simulation runs (data as of Dec. 2022). Over 700 interactive tools have been deployed. The key to this increase in user numbers is the usability of the HUB.

- **Interactive Simulation Concepts for nanoHUB.org**—most science gateways and portals do not enable true interactive simulation and data visualization. However, such interactivity is needed to inspire users to ask “what if?” questions rapidly. Based on the user interface concepts developed around NEMO1D (C-based automatic GUI generation), and NEMO3D (2 approaches: 1) tcl based automatic GUI generation, and 2) XML-based GUI generation using WIGLAF developed at NASA/JPL) created requirements for future nanoHUB simulations in 2004. Dr. Michael McLennan took these requirements and built Rappture for the nanoHUB environment in consultation and testing with Gerhard Klimeck. Rappture is now being employed in over 600 software projects, over 600 software tools on nanoHUB use it. (as of Dec. 2021)
- **Nanoelectronic Modeling Research** - Lead a research group of around 26 graduate and undergraduate students plus 3-4 post-doctoral researchers and research faculty in the development of nanoelectronic modeling tools. Initiate and guide the development of the next generation nanoelectronic modeling tools OMEN and NEMO5.

STRATEGIC HIGHLIGHTS AT JPL

- **Center for Evolutionary Computation and Automated Design at JPL** – Transformation of successful individual research projects in genetic algorithm development and use to a center level effort at JPL (Center is led by Dr. Richard Terrile at JPL).
- **Formation of a Nanoelectronic Modeling team at JPL** – Connect the High Performance Computing group at JPL to the Microdevices Laboratory at JPL through the creation of a modeling team with critical mass.

COMMUNITY IMPACT AT PURDUE

Deployment of interactive Simulation Tools on nanoHUB.org

Personally co-authored 42 simulation tools in terms of their development, user interface-redesign, and/or deployment. Over 85,000 users ran over 2.7 million simulations with these 42 tools (total count as of Feb. 2022).

Virtual Support of Remote Education via Simulation Tools on nanoHUB.org

Over 11,200 students in over 776 classes at 64 institutions used at least one one Klimeck’s simulation tools in formalized teaching environments (homeworks or projects, data as of Aug. 2018).

Nanotechnology Tutorials, Seminars, and Course on nanoHUB.org

Published 350 on-line contributions in forms of interactive Breeze presentations, pdf presentations, and/or Pod-Casts (on iTunes). All “nanoHUB and more” content items have been used by over 596,000 users. (Data as of Aug. 2018)

TOOL DEVELOPMENT HIGHLIGHTS

NEMO5–Strain, Phonons, Quantum Transport, Electronic Structure with atomistic resolution

Envisioned a peta-scale transport simulation tool and received NSF and industrial funding. Guided and advised a team of post-doctoral researchers and research faculty in the construction of a general tool framework (Michael Povolotsy, Hong-Hyon Park, Sebastian Steiger, and Tillmann Kubis). Code combines features and capabilities of NEMO1D, NEMO3D, NEMO3D-peta, and OMEN in a modular structure in which also students can contribute modules. Demonstrated and validated strain, phonon, electronic states, and transport simulations against the predecessor codes. Demonstrated scaling to 100,000 cores. Device physics-oriented studies using NEMO5 are under way.

OMEN–Quantum Transport with atomistic resolution running at the Peta-Scale

Envisioned a peta-scale transport simulation tool and received NSF and industrial funding. Guided and advised the principal developer of OMEN, Dr. Mathieu Luisier towards the construction of a peta-scale simulation engine, which embodies 3D, 2D, and 1D device resolutions. Almost perfect parallel scaling to over 222,000 processors delivering a sustained 1.4PFLOP was demonstrated utilizing a 4-level parallelism. Utilize OMEN to study band-to-band-tunneling transistors, advanced high mobility transistors, interface roughness in si nanowires, and line edge roughness in Graphene transistors. OMEN has also been extended to include incoherent scattering from structurally influenced phonon spectra.

NEMO 3-D-peta-Electronic Structure towards Peta-scale Computing

Guided the re-write of NEMO3D with 2 graduate students at Purdue: Hoon Ryu and Sunhee Lee. Incorporated full 1D, 2D, and 3D spatial decomposition of arbitrary device geometries. Demonstrated scaling of the code to over 32,000 processors utilizing a generalized parallelism structure of multiple parallel groups. Improved the NEMO3D Lanczos eigensolvers for controlled convergence onto interior spectrum eigenvalues. Applied code for electronic structure calculations of single and dense impurity systems.

NEMO 3-D - Development of atomistic Nanoelectronic Modeling in 3-D

Principal designer and developer of a bottom-up nanoelectronic modeling tool for the analysis of the electronic structure in a nano-scale system based on the representation of each individual atom in the structure. The simulator enables the analysis of electronic structure and optical response in a variety of crystal structures and semiconductor material systems. Demonstrated the simulation of a system as large as 52/64 million atoms for electronic structure / strain simulations, respectively. Parallelized the simulator on a Linux-based Beowulf system and later demonstrated scaling up to 8,192 processors. Scientific impact of the tool is highlighted below.

NEMO 1-D – Comprehensive Quantum Electron Transport

Principal designer and developer of the NEMO software. NEMO is the world's first comprehensive 1-D quantum electron transport simulator including effects due to charging, multiple bands and scattering. Fundamentally based on the non-equilibrium Green function formalism (NEGF), a general purpose quantum statistical method. Code consists of about 250,000 lines of C/F90 code and is documented with over 3,000 pages. Tool was used for quantitative device design and analysis at Texas Instruments.

Tool was parallelized on three hierarchical levels to enable massive scaling and user flexibility. Demonstrated scaling NEMO 1-D to 23,000 processors on a Cray XT3/4 at Oak Ridge National Lab.

Parallelization of Mars Imaging Software

Converted existing serial Mars imaging software (e.g. mosaic generation from many images, left/right eye correlation for two images) to efficient parallel code. Hardware: COTS Linux-based Pentium III cluster (Beowulf) using MPI. Achieved time reductions from original baseline of 90 minutes to 3 minutes (mosaic software) and 90 minutes to 6 minutes (correlator). This acceleration enables fast feedback (near real-time) to mars rover control [P27, P30].

Genetic Algorithm-Based Optimization and Synthesis

Developed an optimization and synthesis tool based on a massively parallel genetic algorithm (GA) and incorporated various high-level simulation tools into the toolbox. Developed for device design and metrology. Also applied to materials, circuit, and optical filter design.

SCIENCE AND ENGINEERING HIGHLIGHTS

Impacting the Global Semiconductor Industry Roadmap (ITRS)

Introduced quantitative, physics-based modeling into the the ITRS roadmap – replacing a non-physics, lumped system model used for 30 years in device scaling by physics based models. Demonstrated that the lumped system model provides wrong trends and provided guidelines for future improvements based on NEMO modeling results. Results adopted into the 2014 ITRS roadmap document.

Single Impurity Physics

Demonstrated the capability to model *single Phosphor atom transistors* in Silicon with NEMO 3-D-peta in close collaboration with Australian experimentalist team around Michelle Simmons. Agreement between

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modeling and experiment achieved without fitting parameter through multi-million atom simulations. Results published in *Nature Nanotechnology*.

Dense Impurity Physics

Demonstrated the capability to model dense Phosphor impurity sheets and wires with NEMO 3-D-peta in close collaboration with Australian experimentalist team around Michelle Simmons. Demonstrated capabilities beyond the usual Density Functional Theory limits of a few atom, ideal cells. Results published in *Science*.

Full 3D Atomistic Carrier Transport

Demonstrated capability to model on an atomistic basis: strained InAs/InGaAs/InAlAs HFETS, band-to-band tunneling transistors, interface roughness in nanowires, line edge roughness in Graphene transistors, patent generated for improved BTBT transistor. Demonstrated incoherent scattering calculation in nanowires with atomistically represented phonons.

Multi-million atom electronic structure with NEMO 3-D

Demonstrated control of electronic states on single impurities in Silicon [89] and experimental / theoretical metrology of single impurities in FinFET transistors (published in *Nature Physics* and IEDM) [101]. Matched optical emission wavelength of an experimental sequence of different quantum dot structures without any parameter adjustments [114, P93]. Provided critical insight into the Valley Splitting in strained Si quantum wells for Quantum Computing [79] matching experiment. Studied effects due to atomic alloy disorder and interface interdiffusion in quantum dots [33, 36, 39, I21-I31]. Optimized material parameters resulted in good experimental agreement for optical transitions in colloidal quantum dots [33, 38]

Quantitative High Bias Quantum Transport in 1D heterostructures

NEMO 1-D is now considered the “gold Standard” in Resonant Tunneling Diode simulation. NEMO 1-D has shown predictive capabilities for devices design and analysis. The world’s first high-bias quantum mechanical, simulations of scattering enhanced charging and charge self-consistency of holes and electrons [9-24,P4-P17] for RTDs were generated. Unintuitive quantum transport phenomena [30, 31, 32, 34, 40] were resolved.

Material Science – Tight Binding Parameterization

Performed parameterization of tight banding bandstructure models to achieve the proper representation of basic material properties such as bandgaps and effective masses. NEMO+GA [28, 29, 36, 37]. This synthesis enabled quantitative multi-million atom device analysis.

Electron device synthesis – Inverse Design:

Solved the inverse resonant tunneling diode design problem: what is the structure that will generate a particular current-voltage characteristic? NEMO+GA [P18, P20].

Circuit synthesis:

Enabled a GA based circuit configuration on an FPGA to achieve a Gaussian pulse response. SPICE + GA [P22, P23].

Optical filter synthesis:

Optimized a pattern on a frequency selective surface to achieve optimal transmission and reflection. [P22, P23].

Tight-Binding Model Theory

Collaborated with Prof. Tim Boykin on the fundamental understanding of tight binding models and their applications to quantum transport simulations [25-29].

GRADUATE RESEARCH

- **High Bias Coulomb Blockade** : Initiated analysis of high bias transport in quantum dots. Key investigator of Coulomb blockade at Purdue University [8,P1].
- **Linear Response of Coupled Quantum Dots:** Proposed experiment on conductance spectroscopy in coupled quantum dots and analyzed experimental feasibility [6,7]. This work is cited over 70 times.

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- **Scattering and Incoherent Transport:** Studied and explained the scattering enhanced valley current in RTDs [4,5,9-24,P4-P17].
- **2-D Linear Response:** Analyzed anomalous Quantum Hall Effect in 2-D electron gas system. [3].
- **Laser Noise Experiments:** Implemented high frequency (200MHz) laser amplitude modulation circuitry. Developed laser stability controller (15 kHz) using an external resonance cavity. Measured the propagation of laser noise through optical systems. Calculated and measured higher order, non-linear laser noise fluctuations [1,2].
- **Thin Film Deposition:** Analyzed the experimental feasibility of a novel fast thin film deposition process. Fabricated first clean metallic films (senior project).

SOFTWARE DEVELOPMENT EXPERIENCE

- **Software Project Management**
NEMO1D and NEMO3D are simulation tools consisting of about 250,000 lines of code each. Personally wrote about 80,000 lines of NEMO1D code and 40,000 lines of NEMO3D code. Tackled issues of software design, documentation, release, graphical user interface design, and maintenance.
- **Hybrid Language Design**
Developed hybrid C, F77 and F90 code which allows the utilization of the flexibility of object oriented C data structures and vectorization capabilities of F77 and F90.
- **Software Documentation**
Invented a software documentation tool that allows for a close connection of the development software and its structural documentation. Pseudo code and code are kept in one file but can be presented in a user friendly, interactive form. A similar methodology is now common place with another open source package entitled Doxygen.
- **Numerical Methods**
Solutions of large, sparse systems of equations, Eigen-value and Eigen-vector analysis of large systems, program vectorization.
- **Software Release**
Released NEMO code at Raytheon with 3,000 pages of documentation, consisting of User's Guide, Theory Guide and Developer's Guide. At Purdue co-authored and released 2 Purdue University simulation packages: SQUALID-2D and QUEST. Developed QUEST User's Manual and Tutorial [T1,T2].
- **Operating Systems Experience**
Linux, HP-9000, SUN, IBM-RISC, SGI, IBM SP2, Ardent, and GOULD, MAC, MS.

TEACHING

- I created 14 of the top 20 nanoHUB tools as ranked by annual number of users (data Feb. 2022). These tools are easily integrated by faculty members into existing curricula. These tools have been used by approximately 30,000 students across the globe. These tools offer a unique way to explore semiconductor device physics.
 - My 42 nanoHUB tool contributions have been used by 85,965 users (as of Feb. 2022) who ran over 2.7 million simulations.
 - My 342 lectures, tutorials, and classes in nanoHUB have served over 1.04 million visitors in total.
- [F09][S10][F10][S11][F11][S12][F12][S13][F13][S14][F14][S15][F15][S16][F16][S17][F17][S17][F17][S18][F19][S20][F20][S21][F21][S22][F22][S23] "ECE 694 - Graduate Student Seminar Course", Mandatory Course for all ECE graduate Students. Purdue University. Instructor Goal: A Professional Development Course instead of arbitrary research seminars. ½ the seminars are Purdue internal presentations the other ½ presentations by alumni on professional aspects of life after graduate school. Covered topics are resumes, paper writing, career planning, interview skills, financial planning. Developed a new syllabus, which includes a massive peer review where students evaluate a complete stack of their 60-100 peers in 45 minutes to enforce them with a view of a hiring manager.
- [S10][S12][F12][F20][S21][F21][S22][F22][S23] "ECE 606–Fundamentals of Semiconductor Devices", (S10: co-taught with Prof. Mark Lundstrom, S12: co-taught with Prof. David Janes, and Jim Cooper), Core course in the micro-nano area in ECE. Developed associated crystal structure, bandstructure and quantum transport simulation tools to integrate nanoHUB into the course curriculum.
Deployed a new version of the course into edX in the summer of 2020.
Modified course in Fall 2021 to include projects on quantum dot and nanowire designs instead of midterms.
- [F09] "Nanoelectronic Modeling: From Quantum Mechanics and Atoms to Realistic Devices" Ph.D. Short Course, University of Pisa, Oct. 5-9 2009, Host: Prof. Gianluca Fiori. 20 participants from Italy and Europe overall, 41 individual lecture elements - approximately 16 hours of lectures.
- [F96] "UTD - Advanced Semiconductor Device Theory" University of Texas at Dallas. 18 Ph.D. and Master students, evening course Text book primarily used: S. Datta, Quantum Phenomena.
- Lead a research group of 25 graduate students at Purdue. Mentor Post-Doctoral Researchers and summer students (see professional services section).
 - National Research Council Advisor – 1998-2003.
 - Conducted user training sessions for the NEMO software – 1996-1997
 - Instructor of the Purdue Jido Kwan Tae Kwon Do club (1991-1994).

PERSONAL / ACADEMIC ACHIEVEMENTS / SCHOLARSHIPS / AWARDS**Personal / Academic Achievements**

- 10/1987 Best in Prediploma Class in Electrical Engineering at the Ruhr University Bochum. (Resulted in a full ride fellowship into an exchange program at Purdue, and full ride Fellowships with Friedrich Ebert Stiftung and Studienstiftung des Deutschen Volkes))
- 10/1990 Second Best in Diploma Class in Electrical Engineering at the Ruhr University Bochum. (Resulted in a German award by a Foundation for German Science)
- 01/1994 Defended Ph.D. thesis at Purdue University with GPA of 4.00/4.00.
- 03/1992 1st degree black belt, World Tae Kwon Do Federation, South Korea.
- 05/1993 2nd degree black belt, World Tae Kwon Do Federation, South Korea.

Scholarships

- 04/1987-09/1990 Friedrich Ebert Stiftung, Begabtenförderung, Germany
Full ride scholarship for gifted students providing monthly living stipend and book expenses (there is no tuition at public German Universities).
- 04/1987 RWE Industrial Scholarship
Three-year scholarship providing stipend for students selected by the Institute of Power Electronics at the University of Bochum (declined receipt due to other received fellowship).
- 02/1988-09/1990 Studienstiftung des Deutschen Volkes, Begabtenförderung
Most prestigious German scholarship for gifted students from the equivalent of the US National Science Foundation. –
alternative formulation: He is a member of the “Studienstiftung des Deutschen Volkes”, an elite organization sponsoring the 0.5 percent best German students.
- 08/1988-05/1989 Deutscher Akademischer Austauschdienst (DAAD), Integriertes Auslandsstudium
German Academic Exchange Service Scholarship for support of exchange program participation between Bochum and Purdue, providing travel expenses, living-abroad supplement, and US health insurance.
- 08/1988-05/1989 Purdue University Fee Remission Award.
- 08/1989-09/1990 Friedrich Ebert Stiftung, Begabtenförderung
Scholarship expansion for tuition and additional living-abroad supplement.

Awards / Recognitions

- 10/1987 Siemens circle of selected, highly qualified students in Engineering and Sciences. Support for a one-week seminar, science books, selected internships and senior and thesis projects.
- 12/1988 Purdue dean's list.
- 1989 HKN - Electrical engineering honor society.
- 1989 TBP - Engineering honor society.
- 02/1990 Permanent Member of the most prestigious German Science Foundation, Permanentes Mitglied der Studienstiftung des Deutschen Volkes.
- 03/1991 Foundation for German Science, Prize for the especially fast and very successful completion of studies.
Stifterverband für die Deutsche Wissenschaft, Preis für ein in besonders kurzer Zeit sehr erfolgreich abgeschlossenes Studium.
- 1992 Best student presentation in Purdue EE Industry Initiative Workshop.
- 07/1995 Recognition of my US PhD degree within the German official title system by the Department of Science and Research.
Ministerium für Wissenschaft und Forschung des Landes NRW: Zustimmung zur Führung eines ausländischen Grades: Ph.D. (USA) oder Dr. (USA).

- 10/1996 Texas Instruments Award, Citation: Gerhard Klimeck is recognized for outstanding achievement in the development and demonstration of quantum device design tools. His leadership in developing computer code and documentation for NEMO, a world class device modeling program exceeded customer requirements and helped win follow-on contract. Due to this effort, TI has strengthened its competitive position in nanoelectronics and is viewed by our customers as the industry leader in the development of quantum design tools.
- 1997 DARPA, Ultra Dense, Ultra Fast Computing Components, Award to Raytheon-TI Systems: Sustained Excellence by a Performer in Fiscal Year 1997.
- 2002 JPL, Dr. Edward Stone Award for Outstanding Research Publication, Citation: This paper represents a milestone publication for JPL's entry into the field of nanoelectronic device modeling and simulation for future NASA missions. It is also of value to the international semiconductor industry community. (\$4,000)
- 2003 NASA Space Act Award: NPO no. 30520, "Nanoelectronic Modeling 3-D (NEMO 3-D) Upgrade", \$600
- 2004 NASA Tech Brief Award: NTR no 30842: "WIGLAF (A Web Interface Generator and Legacy Application Façade)", \$350
- 2004 NASA Tech Brief Award: NTR no 30843: "Nanoelectronic Modeling (NEMO 3-D) upgrade to no license restrictions", \$350
- 2004 NASA Tech Brief Award: NTR no 30844: "XML-based C++ Code Generation for User Interface Integration", \$350
- 2004 NASA Tech Brief Award: NTR no 30834: "Parallel Complex Hermitian Sparse Matrix Eigensolvers.", \$350
- 2004 NASA Software Award: NTR no 30630: "Parallel Algorithms for Near-Realtime Mosaic Generation", \$500
- 2004 NASA Tech Brief Award: NTR no 30631: "Parallel Algorithms for Near-Realtime Image Correlation", \$350
- 2004 NASA Tech Brief Award: NTR no 30632: "Quality Control of Tiepoints Computed from Image Correlation", \$350
- 2004 NASA Software Award "Quality Control of Tiepoints Computed from Image Correlation", \$500
- 2004 NASA Tech Brief Award: NTR no 30835: "Structure Based input using tcl/tk", \$350
- 2004 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- 02/2005 NASA Board Award for NTR no. 30630_30632: Parallel Algorithms for Near-Realtime Image Processing in Commodity Cluster Computers, \$2,000
- 2005 listing in AcademicKeys Who's Who in Engineering Education (WWE): [http://engineering.academickeys.com/whoswho.php?dothis=display&folk\[IDX\]=281441](http://engineering.academickeys.com/whoswho.php?dothis=display&folk[IDX]=281441)
<http://Engineering.academickeys.com/index.php>
- 08/2005 Human-Competitive awards in genetic and evolutionary programming– the "HUMIES", \$1,000 shared with Richard J. Terrile, Hrand Aghazarian, Michael I. Ferguson, Wolfgang Fink, Terry Huntsberger, Didier Keymeulen, Gerhard Klimeck, Mark Kordon, Seungwon Lee, Boris Oks, Chris Peay, Anastassios Petropoulos, Paul von Allmen. Karl Yee, Jet Propulsion Laboratory, paper titles: "Evolutionary Computation Technologies for the Automatic Design of Space Systems", "Evolutionary Computation applied to the Tuning of MEMS gyroscopes", "Multi-Objective Evolutionary Algorithms for Low-Thrust Orbit Transfer Optimization", <http://www.genetic-programming.org/hc2005/cfe2005.html>
- 2005 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- 06/2006 NASA Tech Brief Award for NTR no 41155: "Efficient boundary condition for embedded semiconductor nanostructure modeling", \$350
- 2006 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M

- 08/2007 NASA Board Award for NTR no. 41155: “Efficient boundary condition for embedded semiconductor nanostructure modeling.” \$500
- 2007 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- 12/2007 NASA Tech Brief Award for NTR no 30630: “Parallel Algorithms for Near-Realtime Mosaic Generation”, \$350
- 2008 Purdue Engineering Team Award shared with Mark S. Lundstrom and Michael McLennan. \$1,000 award per awardee and a \$10,000 research funding award. Citation: “For his role in the creation of nanoHUB and its impact on the cyberinfrastructure for the national nanotechnology initiative leading a cultural change in research and education.
- 2008 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- 2009 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- 2010 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- 2011 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- May 2011, Elected Fellow Institute of Physics, citation: “For the development, application, and dissemination of atomistic quantum simulation tools for nanoelectronic devices.”

<https://engineering.purdue.edu/ECE/News/2011/professor-gerhard-klimeck-elected-fellow-of-american-physical-society>

- 2011 Campus Technology Innovators Award - Category: IT Infrastructure and Systems, “HUBzero Platform for Scientific Collaboration”, Michael McLennan, George B. Adams III., Mark Lundstrom, Gerhard Klimeck;
10 winners were selected in six categories, out of 393 nominations submitted from higher education institutions around the globe. Entries were reviewed by our Innovators Judging Committee, a group of higher ed tech leaders, many of whom are former Campus Technology Innovators award winners. Final winners were chosen by our expert team of editors.
- 2011 Best Student Poster award. Seung Hyun Park wins a best poster award at the IEEE NMDC conference on Jeju Isand, Korea. The title of the poster is "Contact Modeling and Analysis of InAs HEMT Transistors". Co-authors and award winners are Hong-Hyun Park, Mehdi Salmani-Jelodar, Sebastian Steiger, Michael Povolotsky, Tillmann Kubis, and Gerhard Klimeck. There were 12 awards out of about 170 posters at IEEE NMDC.
- 2011 Gordon Bell Prize Competition Finalist, Received Honorable Mention: Mathieu Luisier, Timothy B. Boykin, Gerhard Klimeck, Wolfgang Fichtner, “Atomistic nanoelectronic device engineering with sustained performances up to 1.44 PFlop/s”, IEEE and ACM Supercomputing 2011, Nov 12-18, 2011.
- Nov. 2011, Elected Fellow of the American Physical Society, citation: “For the development, application, and dissemination of atomistic quantum simulation tools for nanoelectronic devices.”
<https://www.aps.org/programs/honors/fellowships/archive-all.cfm?initial=K>
- 2012 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- Dec. 2012, Elected Fellow of the IEEE, citation: “for his contributions to atomistic quantum simulation tools for nanoelectronic devices” <https://ieeenano.org/about/ieee-fellows-of-the-nanotechnology-council>
- 2013 Intel award for contributions to the NEMO5 simulation software tool
- 2019 Purdue Seeds of Success Acorn given by Vice Provost for Research, research award exceeding \$1M
- 2019 Humboldt Foundation Research Prize, at Charlottenburg Palace in Berlin, Germany. Attending the ceremonies were Germany’s Chancellor Angela Merkel and President Frank-Walter Steinmeier. The international Humboldt Research Award is one of the most prestigious awards in science and is given each year to researchers from all academic disciplines by Germany’s Alexander von Humboldt Foundation. The award recognizes researchers who have made significant discoveries that have influenced their fields, and who are expected to continue producing such advances in the future.

Citation: Professor Klimeck is a leading expert in the modeling of nanoelectronics devices. He is well known internationally for building and defining the state-of-the-art in atomistic modeling theory and simulation tools for today's most advanced transistor devices. He also guides the technical developments and strategies of the site nanoHUB.org, which annually serves over 1.5 million users worldwide with online simulations, tutorials, and seminars. In Germany, he continues his research on atomic-scale semiconductor devices to explore new concepts in hybrid nanostructures.

https://service.humboldt-foundation.de/pls/web/pub_auswahlergebnisse.main?p_lang=de&p_bereich=&p_pattern=&p_humboldt_nation=&p_address_country=&p_address_region=&p_address_city=&p_address_uni=&p_host_country=&p_host_region=&p_host_city=&p_host_uni=&p_fgb1=&p_fgb2=&p_fgb3=&p_order_by=N&p_button_search=&p_page=18

- Sept 2020: R&D 100 award winner in Software and Services category. “Making simulation and data pervasive”, “nanoHUB: Democratizing Learning and Research”. Award winners: Gerhard Klimeck, Alejandro Strachan, Lynn Zentner, Michael Zentner. <https://www.rdworldonline.com/rd-100-2020-winner/nanohub-making-simulation-and-data-pervasive/> <https://www.rdworldonline.com/rd-100-winner-of-the-day-nanohub-making-simulation-and-data-pervasive/>
- Oct. 2020 Elected Fellow of American Association for the Advancement of Science (AAAS), “For the quantum mechanical modeling theory and simulation tools to design today's nanotransistors and for leadership of the global nanotechnology community as Director of nanoHUB.”
<https://www.aaas.org/news/aaas-announces-leading-scientists-elected-2020-fellows>
- Dec. 2020, Purdue Bravo Award.
- April 2021, Purdue College of Engineering Faculty Excellence Award for Impact on Industry.
- Dec. 2021, Purdue Bravo Award.

Research Funding Summary (\$116M):

	Total Funding
Total Funding:	\$116,500,000
Funding generated before Purdue:	\$6,071,000
NCN years 1-5: 13.8 NSF +6.9 Purdue =	\$20,700,000
NCN years 6-10: 18.241 NSF +7.2 Purdue =	\$25,441,000
NCN years 11-15: NSF	\$16,500,000
NCN iCHEER (2012-2017) (committed by Purdue):	\$5,700,000
NCN supplelement year 15:	\$2,000,000
NCN years 16-21: NSF	\$13,250,000
NCN_total=	\$83,341,000
Cyber Center	\$2,500,000
c-PRIMED (2013-2018) (committed by Purdue):	\$2,803,458
Total Centers and pre-Purdue	\$94,965,458
Klimeck controlled research Funding at Purdue	\$21,459,236
NSF Funding for NCN	\$63,791,000

RESEARCH PROPOSAL AWARDS (PI OR PRIMARY CONTRIBUTOR)**Research Proposal Awards at JPL**

- 1) 1999, SBIR Phase I Award, ONR, \$100k, 6 months, "An Advanced CAD Tool for Quantum Device Simulation", PI: Phillip Stout, CRFDR Corporation, Co-I Gerhard Klimeck (JPL). \$100k
- 2) 12/2001, JPL Directors Research and Discretionary Fund (DRDF), \$100k, 18 months, "Nanoelectronic and Nanomagnetic Devices for Revolutionary Computing and Sensor Applications", PI: Gerhard Klimeck, participating: Fabiano Oyafuso (JPL) \$200k
- 3) 03/2002, JPL Internal Research and Development (phase 1), \$343k, 6 months, "Evolutionary Computing Technologies for Space Systems", PI: Richard Terrile, Co-PI: Gerhard Klimeck, and others. \$543k
- 4) 10/2002, JPL Internal Research and Development (phase 2), \$624k, 12 months, "Evolutionary Computing Technologies for Space Systems", PI: Richard Terrile, Co-PI: Gerhard Klimeck, and others. \$1,167k
- 5) 03/2002, NSA/ARDA, \$900k, 3 years, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", PI: Gerhard Klimeck, participating: Fabiano Oyafuso (JPL), Timothy Boykin (U. Alabama Huntsville). \$2,067k
- 6) 07/2002, ONR, \$680k, 3 years, "Atomistic 3-D Nanoelectronic Modeling (NEMO) for Electron Transport in Realistic Nano-Scale Devices", PI: Gerhard Klimeck, participating: Fabiano Oyafuso (JPL), Supriyo Datta (Purdue Univ.). \$2,747k
- 7) 10/2002, JPL Internal Research and Development, \$624k, 12 months, "Evolutionary Computing Technologies for Space Systems (phase 3)", PI: Richard Terrile, Co-PI: G Klimeck, and others. \$3,371k
- 8) 03/2003, JPL IRTD, \$2.7M, 36 months, "Evolutionary Computation Technologies for Space Systems: Revolutionary Tools for Complex Systems", PI: Rich Terrile, Co-PI: Chris Adami, Savio Chau, Ian Ferguson, Wolfgang Fink, Terry Huntsberger, Gerhard Klimeck, Mark Kordon. \$6,071k

Research Proposal Awards at Purdue

- 9) 09/2002, NSF Network for Computational Nanotechnology, \$11,300k over 5 years proposed (\$13.8M actual + \$6.9M cost-share), individual awards listed below on an annual basis, (JPL is government collaborator – no funds exchanged with JPL), PI: Mark Lundstrom (Purdue University). \$26,771k
- 10) 01/2004, NSF Teragrid, friendly user account, 50,000 SUs, "NEMO 3-D on Teragrid", PI: James Bottum, Co- PI: Gerhard Klimeck, Sebastien Goasguen.

- 11) 03/2004, IBM SUR Grant, \$1.3M, PI: Mark Lundstrom, Co-PIs: Sebastien Goasgien and Gerhard Klimeck, Hardware donation to the NCN for IBM Regatta HPC machine. \$28,071k
- 12) 05/2004, NSF NMI, \$3M, 36 months, "NMI Deployment (ENG): nanoHUB", PI: Sebastien Goasguen, Co-PI: Gerhard Klimeck, Dongyan Xu (Purdue), Alain Roy (U. of Wisconsin), Renato Figueiredo (U. of Florida). \$31,071k
- 13) 06/2004, Semiconductor Research Corporation, \$75k, 12 months, "Atomistic Nanoelectronic Modeling (NEMO) for Nano-Scale Wires", NCN industrial Membership, PI: Gerhard Klimeck. \$31,146k
- 14) 07/2004, Intel Equipment Grant, \$78k, PI: Gerhard Klimeck, Hardware donation to NCN for In-Vigo computation on nanoHUB. \$31,224k
- 15) 07/2004, NSF NRAC, 200,000 Service Units on Teragrid, "NSF Network for Computational Nanotechnology (NCN) TeraGrid Allocation Proposal", PI: Gerhard Klimeck, Co-PI: George Schatz, Mark Ratner, Susan Sinnott, Renato Figueiredo, Jose Fortes Umberto, Ravaioli, Sebastien Goasguen, Jean Pierre Leburton – no cash value
- 16) 9/15/04 – 9/14/05, \$2,648,333, 1 year, National Science Foundation, "Network for Computational Nanotechnology," (M.S. Lundstrom, A.H. Sameh, A.Y. Grama, D.S. Ebert, J.F. Pekny, J.R. Bottum, J.Y. Murthy, K. Roy, N.A. Bulger, Gerhard Klimeck, and S. Datta. (already in the total)
- 17) 04/2005, ARO, \$300k, 36 months, "Add on proposal for QCTM-QCCM: The case for NEMO", PI: Robert Clark, Australian Center for Quantum Computing Technologies", Co-PI: G Klimeck. \$31,524k
- 18) 04/2005, ARO, \$300, 36 months, "Realistic SiGe Quantum Dot Qubit Design", PI: Mark A. Eriksson, U Wisconsin, Madison, Co-PI: Gerhard Klimeck. \$31,824k
- 19) 9/15/05–9/14/06, \$3,148,333, 1 year, National Science Foundation, "Network for Computational Nanotechnology," (M.S. Lundstrom, A.H. Sameh, A.Y. Grama, D.S. Ebert, J.R. Bottum, J.Y. Murthy, K. Roy, N.A. Bulger, Gerhard Klimeck and S. Datta. (already in total)
- 20) 10/2005, NIH, \$1,461,911 (year 1), \$6,476,476 (5 years), Purdue part \$89,930 (year 1), \$420,518 (5 years) "National Center for Design of Biomimetic Nanoconductors" PI: Erik Jakobson (UIUC), Co-PI at Purdue: Michael McLennan and Gerhard Klimeck – just count the Purdue Portion \$32,244k
- 21) 09/05 – 08/06, \$75,000, Intel Corporation, "Membership in the Network for Computational Nanotechnology," PI's Mark Lundstrom and Gerhard Klimeck. \$32,319k
- 22) 11/05 – 10/06, \$75,000, Semiconductor Research Corporation, "Membership in the Network for Computational Nanotechnology," November 1, 2004 – October 31, 2005, \$75,000 \$32,394k
- 23) 10/05-9/08, \$2.5M, 3 years, Purdue Discovery Park, "Purdue Cyber Center", PI: Ahmed Emargarmid, Co-PIs: Elisa Bertino, Gary Bertoline, James Bottum, Scott Brandt, Jim Caruthers, Alok Chaturvedi, Ed Coyle, Melissa J. Dark, Jo Davisson, Ahmed K. Elmagarmid, Arif Ghafoor, Chris Hoffmann, Matthew Huber, Reza Kamali, Gerhard Klimeck, Mourad Ouzzani, and Jeffrey S. Vitter \$34,894k
- 24) 10/02/2006-12/31/2008, \$480k, Semiconductor research corporation, "Full 3D quantum transport modeling of realistically extended devices", Gerhard Klimeck, Mark Lundstrom, Cheng-Kok Koh, R. Balakrishnan, Timothy B. Boykin. \$35,374k
- 25) 9/15/06-9/14/07, \$3,648,333, 1 year, National Science Foundation, "Network for Computational Nanotechnology," (M.S. Lundstrom, D.S. Ebert, J.Y. Murthy, K. Roy, G Klimeck and S. Datta)
- 26) 9/15/06-9/14/07, \$100k, 1 year, MARCO/MSD, "Software Customization and Deployment on the nanoHUB", PI.: Gerhard Klimeck \$35,474k
- 27) 11/1/06–10/31/07, \$75,000, 1 year, Semiconductor Research Corporation, "Membership in the Network for Computational Nanotechnology". \$35,549k
- 28) 11/1/06–10/31/07, \$75,000, 1 year, Intel Corporation, "Membership in the Network for Computational Nanotechnology". \$35,624k
- 29) 4/15/07-4/14/10, \$300,000, 3 years, National Science Foundation, "Contact Block Reduction Method for transport in Multimillion Atom Systems", Dragica Vasileska (PI, Arizona State University), Gerhard Klimeck (Co-PI, Purdue share \$135k). \$35,924k

- 30) 8/20/07-8/19/08, \$25,000 (basic full time student funding), Purdue Computing Research Institute (CRI), “Reaching Peta-Scale Computing with a widely known, Purdue-Centered Simulation code in Nanoelectronics for Applications in Solid-state Lighting”, PI: G Klimeck, Co-PI: E Garcia \$35,949k
- 31) 8/20/07-8/19/08, \$25,000 (basic full time student funding), Purdue Computing Research Institute (CRI), “Predictive modeling of the atomic level structure and electronic properties of semiconductor nanostructures”, PI: Alejandro Strachan, Co-PI: Gerhard Klimeck \$35,974k
- 32) 9/15/07-9/14/12 National Science Foundation, “Network for Computational Nanotechnology,” (PI’s: M.S. Lundstrom, G Klimeck and Michael McLennan) – total funding \$18,241M NSF and \$6,9M Purdue cost share. 9/15/07-9/14/08, \$3,648,333, year 1. \$61,115k
- 33) 9/15/07-9/14/11, \$1,600,000, 4 years, National Science Foundation, “Accelerating Nano-scale Transistor Innovation through Petascale Simulation”, PI: Gerhard Klimeck, Co-PI’s: Thomas Hacker (Purdue), Dongyan Xu (Purdue), Saroj Nayak (RPI). \$62,715k
- 34) 9/15/07-9/14/10, \$1,599,205, 3 years, National Science Foundation, “SDCI NMI Improvement: nanoHUB Middleware”, PI: Michael McLennan, Co-PI’s: Gerhard Klimeck, Dongyan Xu. \$64,314k
- 35) 9/15/07-9/14/08, \$100k, 1 year, MARCO/MSD, “Software Customization and Deployment on the nanoHUB”, PI.: Gerhard Klimeck \$64,414k
- 36) 11/1/07–10/31/08, \$75,000, 1 year, Semiconductor Research Corporation, “Membership in the Network for Computational Nanotechnology”. \$64,489k
- 37) 11/1/07–10/31/08, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”. \$64,564k
- 38) 12/1/07, \$20,000, AMD hardware donation to Network for Computational Nanotechnology. \$64,584k
- 39) 4/1/08-3/31/11, \$3,100,000, NRI funded center at Notre Dame, MIND – Midwest Institute for Nanoelectronics Discovery. PI. Alan Seabaugh, Lead at Purdue: G. Klimeck, Purdue Portion \$910k. Purdue Cost share \$360k. Count Purdue funds only. \$65,854k
- 40) 9/15/08-9/14/09, \$3,648,333, 1 year, National Science Foundation, “Network for Computational Nanotechnology,” (PI’s: M.S. Lundstrom, Gerhard Klimeck and Michael McLennan), \$ amount already counted in the full grant. \$65,854k
- 41) 9/15/08-9/14/09, \$100k, 1 year, MARCO/MSD, “Software Customization and Deployment on the nanoHUB”, PI.: Gerhard Klimeck \$65,954k
- 42) 11/1/08–10/31/09, \$75,000, 1 year, Semiconductor Research Corporation, “Membership in the Network for Computational Nanotechnology”. \$66,029k
- 43) 11/1/08–10/31/09, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”. \$66,104k
- 44) 10/1/08-9/30/12, \$100,000 Klimeck portion, 4 year, Army Research office, subcontract to University of Wisconsin, Madison, “Solid State Quantum Computing using Spin Qubits in Si/SiGe Quantum Dots”, PI: Mark Eriksson, Wisconsin, Co-PI: Gerhard Klimeck. \$66,204k
- 45) 10/1/08-9/30/12, \$4,463,000 total, \$400,000 Klimeck portion, 4 year, Army Research office, subcontract to University of New South Wales, “Solid State Quantum Computing in Silicon”, PI: Robert Clark, UNSW, Co-PI: Gerhard Klimeck. \$66,604k
- 46) 12/1/08-11/30/10, \$160,000, Sandia National Laboratory, “Nanoelectronic Modeling for Semiconductor Qubits”, PI: Gerhard Klimeck. \$66,764k
- 47) 7/15/08-7/14/11, \$657,479.00, 2 years, National Science Foundation, “A TeraGrid MATLAB Cluster – Exploring New Services for an XD Future”, PI.: David Lifka, Cornell, Co-PIs: Gerhard Klimeck, Michael McLennan, Purdue. Purdue portion of funding \$313,715. \$67,078k
- 48) 9/1/09-8/31/11, \$1,412,406.53, 2 years, National Science Foundation, “Instant-On Simulation Delivery: Helping TeraGrid Achieve Its Wide and Open Strategic Goals”, PI: Gerhard Klimeck, Co-PIs: George B. Adams III, and Michael J. McLennan. \$68,490k

- 49) 9/15/09-9/14/10, \$3,648,333, 1 year, National Science Foundation, “Network for Computational Nanotechnology,” (PI’s: M.S. Lundstrom, Gerhard Klimeck and Michael McLennan), \$ amount already counted in the full grant. \$68,490k
- 50) 11/1/09–10/31/10, \$75,000, 1 year, Semiconductor Research Corporation, “Membership in the Network for Computational Nanotechnology”. \$68,565k
- 51) 11/1/09–10/31/10, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”. \$68,640k
- 52) 11/01/09-10/31/10, \$693,488, Theory, Modeling, and Simulation of Nanotransistors, Massachusetts Institute of Technology, MSD, FCRP, PI: M. S. Lundstrom, Co-PI: G. Klimeck, A. Strachan, Klimeck Portion: \$85,000 \$68,725k
- 53) 06/01/2010-09/30/2011, \$16,795, Purdue Research Foundation: Xr Grant Midwest Academy For Nanoelectronics & Architectures Mana, Klimeck Portion: \$16,795 \$68,742k
- 54) 06/01/2010-09/30/2011, \$16,750, Purdue Research Foundation: Xr Grant Midwest Academy For Nanoelectronics & Architectures Mana, Klimeck Portion: \$16,750 \$68,759k
- 55) 09/01/2009-08/31/2011, Src Education Alliance, Src Education Alliance Master's Scholarship Program, \$58,435, Klimeck Portion: \$58,435 \$68,817k
- 56) 9/15/10-9/14/11, \$3,857,333, 1 year, National Science Foundation, “Network for Computational Nanotechnology,” (PI’s: M.S. Lundstrom, Gerhard Klimeck and Michael McLennan).
- 57) 09/01/2010-08/31/2011, \$100,000, 1 year, National Science Foundation, Network for Computational Nanotechnology Education Research Group, PI’s Gerhard Klimeck and Krishna Madhavan, Klimeck Portion: \$50,000. \$68,867k
- 58) 05/01/10-12/31/10, \$50,000, Lockheed Martin, “Direct mapping from First Principles to Empirical Tight Binding”, PI: Klimeck, Klimeck Portion: \$50,000 \$68,917k
- 59) 09/01/2010-08/31/2013, \$498,431, National Science Foundation, Iii:Small: Information Recommendation for Online Scientific Communities, PI: Luo Si, Co-PI: Klimeck, Klimeck Portion \$150,000. \$69,067k
- 60) 11/1/10–10/31/11, \$75,000, 1 year, Semiconductor Research Corporation, “Membership in the Network for Computational Nanotechnology”. \$69,142k
- 61) 11/1/10–10/31/11, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”. \$69,217k
- 62) 11/01/2010-10/31/2012, Massachusetts Institute Of Technology, “Theory, Modeling, And Simulation Of Nanotransistors”, \$535,983, PI: Mark Lundstrom, Co-PI: G. Klimeck, A. Strachan, Klimeck Portion: \$85,000 \$69,302k
- 63) 01/01/2011-12/31/2011, \$150,00, 1 year, Intel Corporation, Topological Insulator Based Field Effect Transistors, PI: Yong Chen, Co-PI Klimeck, Klimeck Portion: \$50,000 \$69,352k
- 64) 02/01/2011-01/31/2013. \$160,000, 2 years, NRI, University Of Notre Dame Midwest Institute For Nanoelectronics Discovery (MIND), Klimeck Portion: \$160,000 \$69,512k
- 65) 9/15/09-9/14/10, \$109,000 1 year, National Science Foundation, “Network for Computational Nanotechnology,” Node Expansion to MIT (PI’s: M.S. Lundstrom, Gerhard Klimeck and Michael McLennan). \$69,621k
- 66) 9/15/10-9/14/11, \$3,648,333, 1 year, National Science Foundation, “Network for Computational Nanotechnology,” (PI’s: M.S. Lundstrom, Gerhard Klimeck and Michael McLennan). \$69,621k
- 67) 05/01/11-12/31/12, \$75,000, Lockheed Martin, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$69,696k
- 68) 11/1/11–10/31/12, \$30,000, 1 year, Semiconductor Research Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$69,726k
- 69) 11/1/11–10/31/12, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$69,801k

- 70) 11/1/11–10/31/12, \$75,000, 1 year, Samsung, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$69,876k
- 71) 11/1/11–10/31/12, \$75,000, 1 year, Global Foundries, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$69,951k
- 72) 1/1/11–12/31/13, \$300,000, 3 years, Semiconductor Research Corporation, Custom Research sponsored by Intel, “Advanced Quantum Device Simulation Using NEMO5”, PI: Klimeck \$70,251k
- 73) 5/1/11–4/30/13, \$120,000, 2 years, Hamamatsu, Japan, “Design and Modeling of Terahertz Quantum Cascade Lasers”, PI: Klimeck, Co-PI Tillmann Kubis. \$70,371k
- 74) 8/1/11–7/31/15, \$40,163, Travel funds for NSF PRAC- Accelerating Nano-Scale Transistor Innovation. PI Klimeck \$70,411k
- 75) 8/1/11–6/30/12, \$80,000, ARO, Wyle Lab, “Modeling Current Collapse in GaN HEMTs”, PI Klimeck \$70,491k
- 76) 06/1/11–05/31/14, \$121,500, NSF Graduate Research Fellowship for Matthias Yui Hong Tan. \$70,613k
- 77) 5/1/11–4/30/12, \$299,982, NSF Supplement to Network for Computational Nanotechnology, manufacturingHUB, PI Klimeck \$70,913k
- 78) 11/1/12–8/31/17, \$14,500,000, NCN Reconfigurations \$85,413k
- 79) Purdue: 8/1/12–7/31/17, \$5,700,000, iCHEER \$91,113k
- 80) 11/1/12–10/31/13, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$91,188k
- 81) 11/1/12–10/31/13, \$75,000, 1 year, Samsung, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$91,263k
- 82) 11/1/12–10/31/13, \$75,000, 1 year, Global Foundries, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$91,338k
- 83) 11/1/12–10/31/16, \$440,000, 4 years, ARO, subcontract from Univ. of Wisconsin, “Solid State Quantum Computing Using Spin Qubits in Silicon Quantum Dots”, PI: Klimeck \$91,778k
- 84) 2/15/13–12/31/18, \$3,559,683.00, 5 years FCRP – LEAST, Notre Dame: Total Proposal: 3,559,683.00 Klimeck Portion of Budget: \$639k \$92,417k
- 85) 1/15/13–12/31/18, \$3,559,683.00, 5 years FCRP – FAME, UCLA, Purdue Portion: 905,000.00: Klimeck Portion of Budget: \$275k \$92,692k
- 86) 1/1/13–12/31/13, \$75,000, 1 year, Philips Lumileds, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$92,767k
- 87) 12/21/12–12/20/16, \$509,992, 4 years, ARO, subcontract from Univ. of New South Wales, “Solid State Quantum Computer in Silicon”, PI: Klimeck \$93,277k
- 88) 06/01/13–05/31/14, \$100,000, 1 year, SRC, “Incoherent Scattering in Non-equilibrium Green’s Functions in Realistic III-V Devices”, PI: Klimeck \$93,377
- 89) Purdue: 06/12/13–06/30/2018, \$2,803,458.00, 5 years, c-PRIMED \$96,180k
- 90) 07/01/13–06/30/14, \$75,000, 1 year, AFRL, subcontract from Alion, “Nanoelectronic Modeling for Sub-Monolayer Quantum Dot Stacks”, PI: Klimeck. \$96,255k
- 91) 10/01/13–09/30/14, \$126,000, 1 year, Intel Corporation, “iNEMO Discretionary”, PI: Klimeck \$96,381k
- 92) 11/1/13–10/31/14, \$75,000, 1 year, Global Foundries, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$96,456k
- 93) 11/1/13–10/31/14, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$96,531k
- 94) 1/1/14–12/31/14, \$75,000, 1 year, Philips Lumileds, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$96,606k

- 95) 11/1/13–10/31/14, \$75,000, 1 year, Samsung, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$96,681k
- 96) 11/1/13–10/31/14, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$96,756k
- 97) 1/1/14–12/31/14, \$75,000, 1 year, TSMC, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$96,831k
- 98) 12/1/14–11/30/17, \$199,392, 3 years, NSF, “Network for Computational Nanotechnology”, Data Supplement, PI: Klimeck \$97,031k
- 99) 12/1/15–11/30/17, \$580,000, 2 years, NSF, “Network for Computational Nanotechnology”, Engineering Observatory Supplement, PI: Klimeck, Total Proposal: \$580,000, Klimeck Portion: \$275,706 \$97,306k
- 100) 11/1/14–10/31/15, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$97,381k
- 101) 1/1/15–12/31/15, \$75,000, 1 year, Philips Lumileds, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$97,456k
- 102) 1/1/15–12/31/15, \$75,000, 1 year, TSMC, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$97,531k
- 103) 06/01/14–05/31/15, \$100,000, 1 year, SRC, “Incoherent Scattering in Non-equilibrium Green’s Functions in Realistic III-V Devices”, PI: Klimeck \$97,631k
- 104) 9/1/15–8/31/18, \$450,000, 3 years, Intel, “NEMO5 Development Plan”, PI: Klimeck \$98,081k
- 105) 10/01/14–09/30/15, \$126,000, 1 year, Intel Corporation, “iNEMO Discretionary”, PI: Klimeck \$98,207k
- 106) 9/1/11–8/31/15, \$1,280,000, 4 years, NSF, “NEB: Superlattice-FETs, Gamma-L-FETs, and Tunnel-FETs: Materials, Devices and Circuits for Fast Ultra-Lower-Power ICs” University of California – Santa Barbara: Total Proposal: \$1,280,000, Povolotskyi/Klimeck portion: \$371,410 \$98,579k
- 107) 9/15/15–8/31/18, \$240,000, 3 years, NSF, “nm Electron Wave Devices for Low-Power VLSI Electronics”, PI: Povolotskyi, co-PI: Klimeck \$98,819k
- 108) 10/01/15–09/30/16, \$126,000, 1 year, Intel Corporation, “iNEMO Discretionary”, PI: Klimeck \$99,945k
- 109) 1/1/16–12/31/16, \$75,000, 1 year, Philips Lumileds, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$99,020k
- 110) 1/1/16–12/31/16, \$75,000, 1 year, TSMC, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$99,095k
- 111) 1/1/16–12/31/18, \$300,000, 3 years, SRC, “NEMO5: Engineering Band Tails and Band to Band Tunneling in III-V Semiconductors”, PI: Kubis, co-PI: Klimeck \$99,395k
- 112) 9/2016, \$27,000, 4 Years, “The Nanotechnology Applications and Career Knowledge (NACK) National Support Center”, PI: Klimeck \$99,422k
- 113) 11/2016, \$12,710, 1 year, NSF, “PRAC Travel – atomistic simulations”, PI: Klimeck \$99,435k
- 114) 11/1/16–10/31/17, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$99,510k
- 115) 10/01/16–09/30/17, \$100,000, 1 year, Intel Corporation, “iNEMO Discretionary”, PI: Klimeck \$99,610k
- 116) 1/1/17–12/31/17, \$75,000, 1 year, Philips Lumileds, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$99,685k
- 117) 1/1/17–12/31/17, \$75,000, 1 year, TSMC, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$99,760k
- 118) 8/1/17–12/31/18, \$2,000,000, 18 months, NSF, Supplement for Network for Computational Nanotechnology, PI: Klimeck \$101,760k
- 119) 6/1/17–03/01/2018, \$100,000, 9 months, NSF, NSF Grantee’s Meeting, PI: Klimeck \$101,860k

- 120) 11/1/17-10/31/18, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$101,935k
- 121) 1/1/18-6/30/18, \$50,000, 6 months, I-Corps nanoHUB: cyber platform for STEM research, education, and collaboration, PI: Klimeck \$101,985k
- 122) 5/2018-5/2019, \$50,000, 1 year, NSF, PARADIM support through nanoHUB, PI Klimeck \$102,035k
- 123) 5/2018-5/2021, \$450,000, 3 years, CRANE, “ASSURE”, PI Klimeck \$102,485k
- 124) 1/1/18–12/31/18, paid on 8/2018 , \$75,000, 1 year, TSMC, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$102,560k
- 125) 11/2018-11/2023, \$13,250,000, 5 years, NSF, “Network for Computational Nanotechnology – Cyber Platform” \$115,810k
- 126) 11/1/18-10/31/19, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$115,885k
- 127) 1/2019, \$15,000, 6 months, MIT Lincoln Labs, “Computational Assessment of Ferroelectric FETS for low-power Digital Applications”, \$115,900k
- 128) 9/2019, \$300,000, 3 years, NSF, Harvard University, “QII-TAQS: Majorana Nanomanipulation for Topological Quantum Computing” \$116,200k
- 129) 11/1/19-10/31/20, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$116,275k
- 130) 11/1/20-10/31/21, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$116,350k
- 131) 11/1/21-10/31/22, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$116,425k
- 132) 11/1/22-10/31/23, \$75,000, 1 year, Intel Corporation, “Membership in the Network for Computational Nanotechnology”, PI: Klimeck \$116,500k

RESEARCH PROPOSAL AWARDS (PERIPHERAL CONTRIBUTOR)

- 1) 07/2002, SRC, \$468k, 3 years, (JPL collaborator only - no funds exchanged with JPL), "Study of Mobility Degradation and Detailed Structure of Si/high-k Interfaces including Dopant Segregation Using AIDA-TEM (Ab-initio Interface Defect detection by Analytic Transmission Electron Microscopy)", PI: Wolfgang Windl (Ohio State U), Co-PIs: Gerd Duscher (North Carolina State U), Maria Merlyne De Souza (De Montfort U).
- 2) 04/2003, JPL Internal R&TD, \$30k, 3 months, "Simulation of hydrogen sensors with Pd nanowires", PI: Paul von Allmen, Co-I: Seungwon Lee and Gerhard Klimeck.
- 3) 03/2003, JPL IRTD, \$2.185M, 36 months, "Computational Architecture and Coupled Modeling Environment for Solid Earth Science", PI: Ronald Blom, Co-PI: William Bosl (Architecture), Eric DeJong (Scientific Visualization), Erik Ivins (Gravity, Model codes), Jeffrey Jewell (Gravity modeling), Dan Katz (Process flow) Gerhard Klimeck 3816 (Parallel cluster computing), Carol Raymond (Joint Gravity/Magnetics), Paul Rosen (InSAR), Mike Watkins (GRACE/GRACE Follow-on), Frank Webb 335 (GPS earthquake predef modeling), Xiaoping Wu (Gravity Inversion).
- 4) 03/2003, JPL IRTD, \$450k, 36 months, "Evolving Spintronic Circuits for Fast, Low-Power, Radiation Tolerant Hardware", PI: Colin Williams, Co-PI: Gerhard Klimeck, Farrokh Vatan, Amir Fijany.

SERVICE – EDITORIAL AND CONFERENCE ROLES**Journal Editor**

- Editorial Board, Nature Computational Materials, Nature Publishing Group, Nov 2016-August 2018
- Editorial Board, Journal of Computational Electronics, Springer Verlag, Editors David Ferry, Karl Hess (until 2015), Massimo Fischetti editor since 2015, 2010-November 2019
- Editorial Board, Nanoscale Systems:Mathematical Modeling Theory and Applications, Open Access Journal, Versita.com. Editor Roderick Melnick, 2012-present

Special Issues Editor

- Proceedings of the 10th International Workshop on Computational Electronics, Journal of Computational Electronics, Springer, ISSN 1569-8025 (Print) 1572-8137 (Online), IssueVolume 3, Numbers 3-4 / October, 2004
- Extending Moore's Law with Advanced Channel Materials, edited by S. Chakravarthi, R. Arghavani, G. Klimeck (Mater. Res. Soc. Symp. Proc. Volume 995E, Warrendale, PA, 2007).
- Guest Editor: Journal of Computational Electronics, from 14th International Workshop for Computational Electronics, Oct. 24-27, 2004. Springer Verlag, 2005.
- Guest Editor, Proceedings of the International Workshop for Computational Electronics, Sep. 2-4, 2015, Purdue University.

Program Committee, Conference Preparation, Conference / Session Chair

1. Program Committee, 27th international Symposium on Compound Semiconductors (ISCS), IEEE, (2000), Monterey, CA, Oct 2-5, 2000.
2. Session Moderator, Quantum Transport, Advanced Research Workshop on Quantum Transport in Semiconductors, Maratea, Italy, June 17-22, 2001.
3. Program Committee, Session Chair, Nanoelectronics Session, Nanospace 2002, Galveston, TX, June 24-28, 2002.
4. Session Chair, Superlattices and Resonant Tunneling Structures, March Meeting of American Physical Society, March 16-21, Austin, TX (2003).
5. Program Committee, 2nd International Workshop on Quantum Dots for Quantum Computing and Classical Size Effect Circuits, University of Notre Dame, August 7-9, 2003.
6. Session Chair, Computational Approaches Toward the Electronic Properties of Quantum Dots Workshop, Chicago, September 22-24, 2003, sponsored by DARPA.
7. Session Chair, "Advanced MOS Devices", 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona, Spain. October 16-17 2003.
8. Program Committee, IEEE Nano 2004, Munich, Germany, August 16-19, 2004.
9. Session Chair, IEEE Nano 2004, Session Nanoelectronics 1, Munich, Germany, August 16-19, 2004.
10. Conference Chair, International Workshop for Computational Electronics, Purdue University, October 24-27, 2004.
11. Program Committee, 15th Workshop on Modelling and Simulation of Electron Devices (MSED) 4-5 July 2005, Pisa, Italy.
12. Program Committee, 14th International Conference on Nonequilibrium Carrier Dynamics in Semiconductors (HCIS-14), Chicago, Illinois, July 24-29, 2005.
13. Program Committee, IEEE Nano 2005, Nagoya, Japan, August 11-15, 2005.
14. IEEE IEDM Modeling and Simulation Program and Selection Committee, Vancouver, Canada, August 1st, 2005.

15. Supercomputing 2005, Session chair, Education Program to Middle School and High School Teachers, Introduction to the Integration of High Performance Computing: Nanotechnology. Physics, Chemistry, Chemical Engineering, Nov 12-18, 2005, Seattle, WA.
16. Program committee: HPCNano2005 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2005, Nov 12-18, 2005, Seattle, WA.
17. Session Chair, IEEE IEDM Modeling and Simulation, Nanowires, Washington DC, Dec. 6th, 2005
18. International Advisory Board, IEEE International Workshop for Computational Electronics, Technical University Vienna, May 25-27, 2006.
19. "nanoHUB - a community website for online simulation and more", Short Course at IEEE-NMDC, IEEE Nanotechnology Materials and Devices Conference, October 22-25, 2006, www.ieee-nmdc.org
20. Program committee: HPCNano2006 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2006, Nov 12-17, 2006, Tampa, FL.
21. "nanoHUB tutorial - overview, usage scenarios, vision", The 2nd Annual IEEE International Conference on Nano/Micro Engineered and Molecular Systems (IEEE NEMs) Jan 16-19, 2007, Bangkok Thailand.
22. Program Committee, MRS 2007 Spring Meeting, Session G, Extending Moore's Law with Advanced Channel Materials.
23. Session chair (2 sessions), MRS 2007 Spring Meeting, San Francisco, CA, April 10, 2007, Advanced Channel Materials I: (110) Si, Ge, Advanced Channel Materials II
24. NSF workshop organizer, jointly with Prof. Jonathan Dowling (LSU) and Paul Werbos (NSF), Quantum, Molecular and High Performance Modeling and Simulation for Devices and Systems (QMHP), April 16, 17, 2007
25. International Advisory Board, IEEE International Workshop for Computational Electronics, University of Mass Amherst, Oct. 8-10, 2007.
26. Workshop Co-Chair: HPCNano2007, Nov. 16, 2007 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2007, Reno, NV.
27. Session Chair - "nanoHUB tutorial", IEEE Nano conference, Arlington, TX, August 18, 2008.
28. Workshop Advisory Committee: HPCNano2008, Nov. 21, 2008 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2008, Austin TX.
29. International Advisory Board, IEEE International Workshop for Computational Electronics, Tsinghua University, Beijing, China, May 27-29, 2009.
30. Workshop Advisory Committee: HPCNano2009, Nov. 15, 2009 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2009, Portland OR.
31. International Advisory Board, IEEE International Workshop for Computational Electronics, University of Pisa, Italy, Oct. 27-29, 2010.
32. General Chair National Science Foundation Nano Grantees Conference, Arlington VA, Dec. 6-8, 2010.
33. IEEE Nanotechnology Materials and Devices Conference (NMDC) 2011, Jeju Island, South Korea, Oct 18-21, Session Chair, Characterization and Simulation of Nanomaterials and Nanostructures.
34. Member of the program committee (PC) for the IEEE International Parallel and Distributed Processing (IPDPS), May 21 - May 25, 2012 in Shanghai, China. Technical committee member, Symposium IEEE International Parallel and Distributed Processing (IPDPS 2012) in the area of applications. Formalized paper evaluation. Oct-Nov. 2011
35. International Advisory Board, IEEE International Workshop for Computational Electronics, University of Wisconsin, May 22-25, 2012.

36. International Advisory Board, IEEE International Workshop for Computational Electronics, Nara, Japan, June. 4-7, 2013.
37. General Chair of nanoHUB user conference, Arizona State University, April 9-11, 2014
38. International Advisory Board, IEEE International Workshop for Computational Electronics, Paris, France, Sept. 9-11, 2014.
39. General Chair of nanoHUB user conference, Purdue University, August 31-Sept 1st. 2015
40. General Chair of International Conference for Computational Electronics (IWCE), Purdue University, Sept 2-4, 2015
41. International Advisory Committee of International Conference for Computational Nanotechnology (IWCE), Leeds, UK, June 5-9, 2017
42. General Chair National Science Foundation Nano Grantees Conference, Arlington VA, Dec. 12-13, 2017
43. International Advisory Committee of 2018 IEEE Nanotechnology Materials and Devices Conference (NMDC), Portland OR, Oct. 14-17, 2018.
44. International Advisory Committee of International Conference for Computational Nanotechnology, Evanston, IL, May 2019
45. International Advisory Committee of 2019 IEEE Nanotechnology Materials and Devices Conference (NMDC), Stockholm, Sweden, Oct. 27-30, 2019.
46. Leading Member of Steering Committee, NSF-directed effort: “Summit on Big Data and Cyberinfrastructure in Materials Research”, Planned and executed multiple meetings that culminated in the summit attended by ~100 researchers at the Big 10 center in Chicago in Nov. 21-22, 2019.
47. Gerhard Klimeck, “The nanoHUB Platform”, 2021 NNI Strategic Planning Stakeholder Workshop, January 11-13, 2021, National Nanotechnology Coordination Office
48. Gerhard Klimeck, “The nanoHUB Platform”, NITRD Big Data Interagency Virtual Workshop on Pioneering the Future of Federally Supported Data Repositories Wednesday Jan 13th - Friday Jan 15th, 2021 <https://www.orau.gov/bdworkshop21>
49. International Advisory Committee of International Conference for Computational Nanotechnology (IWCN), Seoul Korea, May, 2021
50. Session Chair, SiNano Summer School, July 12-16, 2022, Glasgow, UK
51. Session Chair, International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Sept. 5-9, 2022, Granada, Spain

SERVICE – REVIEW PANELS, ADVISORY BOARDS, COMMITTEES

National Review Panel Service

- National Academy of Sciences, National Nanotechnology Initiative (NNI) Triennial Review Committee Member. Jan. 2015 – Sept 2016, Report published at: <https://www.nap.edu/catalog/23603/triennial-review-of-the-national-nanotechnology-initiative>
- IEEE NTC (Nanotechnology Council) Fellow Evaluation Committee Member. Starting August 2021 to present.

External Review Panel Service

1. National Science Foundation, Jan 13-14, 2005, Review panel on Electronic Devices, Washington DC.
2. National Science Foundation, Oct 31-Nov 1, 2006, Review panel on Electronic Devices, Washington DC.
3. National Science Foundation, Feb 28-March 1, 2012, Nano Engineering Research Center, Los Angeles.

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4. National Science Foundation, Sept 23-24, 2013, EPSCOR center review, Washington DC
5. National Science Foundation, Oct. 14, 2015, Review Panel on Personalized & Low –Cost Manufacturing
6. National Science Foundation, Nov. 5-6, 2015, Software Institutes Implementation Proposals in Chemistry and Materials Research
7. Site visit reviewer, Trinity College Dublin, Ireland, “Atom Level Engineering of Material-on-Insulator Devices and Sensors”, January 21-22, 2016
8. PhD Candidate Examiner / Opponent, Lund University Sweden, May 13, 2016
9. National Science Foundation, July 13, 2017, Review Panelist
10. Florida Center for Cybersecurity, Nov. 2018, External Reviewer
11. National Science Foundation, Feb. 22, 2019, Review Panelist
12. PhD Candidate Examiner, March 2019, PDPM-IIITDM Jabalpur, India
13. US Department of Energy – Proposal reviewer, Jan 2020.
14. European Research Council (ERC) – External reviewer for ERC 2020 Starting, Consolidator, Advanced and Synergy Grant Calls. Jan. 2021
15. National Science Foundation, June 28-29, 2021, Review Panelist
16. National Science Foundation, June 22-24, 2022, Review Panelist
17. National Science Foundation, Feb. 24, 2023, Review Panelist

US Nationwide Advisory Board Service

- Scientific Expert recruited by UChicago Argonne LLC for the sponsored review of Argonne National Laboratory’s Computing, Environment and Life Sciences Directorate (CELS) scheduled for September 9-11, 2014.
- Triennial Review of the National Nanotechnology Initiative (NNI), Committee Member, Focal Point Infrastructure and Management, Federally mandated review for an annual budget of the National Nano Research of about \$2B. January 2015-Feb. 2016

International Advisory Board Service

1. Advisory Board Meeting, “Meeting the Materials Challenges of nano-CMOS Electronics”, University College London, Oct. 22, 2007, Hosts Alex Shluger, University College London and Asen Asenov, University of Glasgow.
2. Advisory Board Meeting, “NanoCMOS – e-Science - EPSRC”, Oct 24, 2007, Host Asen Asenov, University of Glasgow.
3. Advisory Board Meeting, “NanoCMOS – e-Science - EPSRC”, Nov. 12, 2008, Host Asen Asenov, University of Southampton.
4. Advisory Board Meeting, “NanoCMOS – e-Science - EPSRC”, Nov. 14, 2009, Host Asen Asenov, University of York.
5. KIM Governance Committee, “KIM – Knowledgebase of Interatomic Models”, Workshop, San Diego, Feb. 26-27, 2011
6. Advisory Board Meeting, “NanoCMOS – e-Science - EPSRC”, March 23, 2011, Host Asen Asenov, University of Southampton.
7. Advisory Board ARCHIE-WeSt High Performance Computer Centre, Glasgow, funded by EPSRC, Meeting Nov. 27, 2012.
8. Scientific Advisory Board Invitee (declined attendance due to family health issues), NanoLund, Lund University Sweden, Oct 19-21, 2015

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9. Scientific Advisory Board Mediterranean Excellence in Computing and Ontology, Point of Contact: Prof. Veljko Milutinovic, April 2017 – present.

National Advisory Board Service

1. Advisory Board Meeting, NCRR Resource for Macromolecular Modelling and Bioinformatics, May 16, 2005, Chicago IL, PI.: Prof. Klaus Schulten, U Illinois Urbana-Champaign.
2. Advisory Board Meeting, NSF NMI project, "nanoHUB Deployment", West Lafayette, IN 47907, PI: Sebastien Goasguen, Oct 2004-2007.
3. Non-voting Ex-Officio AdCom member of the IEEE EDS Compact Modeling Committee.
4. CUAC - Cyberinfrastructure and User Advisory Committee of the NSF Teragrid, June 2006 - present, PI.: Charlie Catlett, Formal meetings at TG 06 conference in Indianapolis, June 2006, TG 07 conference in Madison, June 2007.
5. Teragrid governance planning board, June 2007 – April 2008
6. NSF Future of TeraGrid working Group, October 2007 – April 2008.
7. Oak Ridge Leadership Facility (OLCF) User council, Advise OLCF on operational and user aspects, meets throughout the year in conference calls, Aug. 2009-present,
8. KIM Governance Committee, “KIM – Knowledgebase of Interatomic Models”, Workshop, San Diego, Feb. 26-27, 2011

Industrial Committee Service

- SRC Multi-Scale Modeling Working Group, Feb. 2004 – Fall 08.
- ITRD – ERM (Emerging Research Materials) working group, July 2004 – Fall 08.
- ITRS (International Technology Roadmap For Semiconductors) - PIDS (Process Integration, Devices & Structures) working group, July 2011 – present, Transition the roadmap device modeling from non-physical lumped device models to physics-based well defined transport models. Direct impact of NEMO on global roadmap.

Local Committee Service

- JPL Supercomputing Steering Committee, Sept. 2003-Dec 2003.
- Purdue Computing Research Institute (CRI) Steering Committee, Jan 2004-Aug 2006.
- Purdue Engineering Computing Network (ECN) Director Search Committee, Dec. 2003-Feb. 2004.
- Purdue Engineering Teaching Awards Committee, Jan. 2005-Jan 2007.
- Intel Alumni Meeting co-organizer, spring 2004.
- Birck Nanotechnology Center Internal Advisory Committee (spring 2007 – 2012)
- ECE Wang Hall Building Planning Committee member (2008-09) (Original plan for discovery park)
- Co-Chair Predictive Science Cluster Hire with Prof. Alejandro Strachan (2014-2015)
- Advisory Board Member: GLASS-Net let by Prof. Thomas Hertel, Purdue (2021-present)

Journal Reviewer / Referee

- Physical Review B
- Applied Physics Letters, Journal of Applied Physics
- physica status solidi b
- Superlattices and Microstructures

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- IEEE Transactions on Electron Devices, IEEE Transactions on Nanotechnology
- Journal for Computational Electronics
- Nature Nanotechnology

SERVICE - FOREIGN EXCHANGE PROGRAM

- Organizer of Bochum-Purdue student exchange program. Jan 2004-present. This Program exists since 1979, originally under the leadership of Prof. Fritz Friedlaender (Purdue) and Eckard Kneller (Bochum). It is now lead from Bochum by Prof. Ulrich Kunze.
 - AY04/05 students (3/3): Tillmann Falk, Jannik Emde, Ralf Georg Hetmanczyk
 - AY05/06 students (4/7): Monica Siepmann, Markus Kasper, Hayg Dabag, Winfried Schüngel
 - AY06/07 students (3/10): Lars Wolleschensky, Martin Schiffner, Martin Oettmeier
 - AY07/08 students (3/13): Gesine Hinterwälder, Lukas Lohaus, Oliver Mischke
 - AY08/09 students (3/16): Michael Szelong, Matthias (Yui-Hong) Tan, Martin Beckmann
 - AY09/10 students (3+1/19) : Matthias (Yui-Hong) Tan, Patrick Wesskamp, Jan Trieschmann, Cornel Reuber
 - AY10/11 students (3+1/22): Matthias (Yui-Hong) Tan, Melanie Schmidt, Hendrik Vogt, Richard Ronig
 - AY11/12 students (3/25): Vadim Barkov, Markus Bienholz, Christian Tendency
 - AY12/13 students (3/28): Johnny Chor, Fabian Just, Dennis Michaelis
 - AY13/14 students (3/31): Lukas Bernhard, Thomas Busch, Frederik Schmidt
 - AY14/15 students (3/34): Thilo Balke, Steffen Becker, Dominik Preikschat
 - AY15/16 students (3/37): Tim Wingender, Jacek Rzeniewicz, Jan Kaiser

MENTOR / ADVISOR**Current advisor to 10 undergraduate students, 4 graduate students, 1 post-doc****Current Post-doc advisor to 1 individual**

- Jinying Jessica Wang (Aug. 2018 – present)

Current (year 2022 and AY 22/23) Ph.D. student advisor to 4 individuals

1. Xinchun Guo – defended successfully, thesis to be submitted Dec. 2022 (Aug. 2015 – Dec. 2022)
2. Han-Wei Hsiao (left research group – Kubis) (Aug. 2019 – Aug. 2022)
3. Hong-Yang Lin (Aug. 2021 – present)
4. Dain Kang (Aug. 2022 – present)

Current Master Student advisor to 0 individuals

- 1.

Current (year 2022 and AY 22/23) Undergraduate Research Student advisor to 12 individuals

1. Darin Tsai (VIP program) (Aug 2021 – Aug. 2022)
2. Alan Zhang (VIP program) (Aug 2021 – May 2022)
3. Aloysius Rebeiro (VIP program) (Aug 2021 – May 2022)
4. Maximilian Drach (VIP program) (Aug 2021 – present)
5. Dheeraj Kumar (VIP program, summer) (Jan 2022 – present)
6. Zachary Hunter (summer) (May 2022 – present)
7. Maximilian Drach (VIP program, summer) (Aug. 2021 – present)
8. Aneesh Chakravarthula (VIP fall, continued independent) (Aug. 2022 – present)
9. Jonathan Kao (VIP fall) (Aug. 2022 - Dec. 2022)
10. Samy Rajaraman (VIP Fall) (Aug. 2022 - Dec. 2022)
11. Kihunn Anderson (VIP Spring) (Jan. 2023 – present)
12. Lakshay Goel (VIP Spring) (Jan. 2023 – present)
13. Roosh Parikh (Jan. 2023 – present)

PAST MENTORSHIPS**Graduated 43 Ph.D. students**

- 1) Anisur Rahman, Co-advisor with Mark Lundstrom (Dec 2003-Aug 2005)
Exploring New Channel Materials for Nanoscale CMOS Devices: A Simulation Approach
- 2) Ahmed Ali Yanik (Physics), Co-advisor with S Datta and R Reifengerger (Dec 2003-Aug. 2007)
Spin Dependent Electron Transport in Nanostructures
- 3) Neophytos Neophytou, Co-Advisor with Mark Lundstrom (Aug. 2005 – Aug. 2008)
Quantum and Atomistic Effects in Nanoelectronic Transport Devices
- 4) Rajib Rahman, Co-advisor with Lloyd Hollenberg (Dec 2005-March 2009)
Stark Tuning of the Electronic Properties of Impurities for Quantum Computing Applications
- 5) Neerav Kharche, Co-advisor Timothy Boykin (Jan 2005-Jan 2010)
Atomistic Modeling of Electronic Structure and Transport in Disordered Nanostructures
- 6) Muhammad Usman, (Aug. 2005 – Aug. 2010)
Multi-million Atom Electronic Structure Calculations for Quantum Dots
- 7) Samarth Agarwal (Physics), Co-advisor with Ron Reifengerger (June 2004 – Dec. 2010)
Design Guidelines for High Efficiency Photovoltaics and Low Power Transistors using Quantum Transport
- 8) Amritanshu Palaria, Co-advisor with Alejandro Strachan (Aug. 2005 – Dec. 2010)
Multi-Scale Predictive Modeling of Nano-Material and Realistic Devices
- 9) Hoon Ryu, (July 2006 – Aug. 2011)
Electronic Structure and Quantum Transport in Controlled Impurity Systems (Aug. 2008 – Aug. 2011)

- 10) Abhijeet Paul (Aug. 2006 – Oct. 2011)
Computational modeling and simulation study of
electronic and thermal properties of semiconductor nanostructures
- 11) Sunhee Lee (Aug. 2006 – Nov. 2011)
Development of a Massively Parallel Nanoelectronic Modeling Tool
and its Application to Quantum Computing Devices
- 12) Ganesh Hegde (May 2010 – Nov. 2013)
Modeling the atomic and electronic structure of Meta-Metal,
Metal-Semiconductor and III-V/Oxide interfaces
- 13) Sung Geun Kim (Aug. 2007 – Nov. 2013)
Electron Scattering in Quasi-one Dimensional Nanoscale Transistors
- 14) Saumitra Mehrotra (Aug. 2007 – Jan 2014)
Physics and Simulation Study of Nanoscale Electronic Devices
- 15) Parijat Sengupta (Aug. 2008 – Jan 2014)
Theory of Topological Insulators and its Applications
- 16) Sung Hyon Park (Jan. 2010 – Jul 2014)
Advanced III-V / Si Nano-scale Transistors and Contacts: Modeling and Analysis
- 17) Mehdi Salmani Jelodar (Jan. 2009 – Dec. 2014)
Scaling Issues and Solutions in Ultra Scaled MOSFETs using Predictive Modeling
- 18) Yui-Hong Matthias Tan (Dec. 2010 – Sept. 2015)
Development of Hybrid Atomistic / Empirical Modeling Methods
for Donor-Based Quantum Computing
- 19) Yu He (Aug. 2010 – Nov. 2015)
Advanced Boundary Condition Method in Quantum Transport and its Application in Nanodevices
- 20) Zhengping Jiang (May 2011 – Nov. 2015)
Multi-Scale Simulations for High Efficiency Low Power Nanoelectronics Devices
- 21) Yaohua Tan (Aug. 2008 – Nov. 2015)
Mapping from *ab-initio* to Tight-Binding and its Applications.
- 22) Hesameddin Ilatikhameneh (Aug. 2011 – July 2016)
Steep Sub-threshold Swing Transistors
- 23) Kai Miao (Aug. 2010 – Feb. 2017)
“Quantum Thermal Transport in Semiconductor Nanostructure with Diffusion”
- 24) Fan Chen (physics) (Oct. 2012 – Feb. 2017)
“Low Power Transistors and Quantum Physics Based On Low Dimensional Materials”
- 25) Yu Wang (July 2015 – March 2017)
“Design and Optimization of Donor-Based Spin Qubits in Silicon”
- 26) Archana Tankasala (Aug. 2012 – July 2017)
“Engineering Multi-Electron Interactions for Quantum Logic in Silicon”
- 27) Junzhe Geng (Aug. 2012 – July 2017)
“Multi-Scale Quantum Transport Modeling of Light Emitting Diodes”
- 28) Yu-Ling Hsueh (Aug. 2011 – Oct. 2017)
“Electron Spin Relaxation of Donors in Silicon Nanoelectronic Devices
- 29) Pengyu Long (May 2015 – Nov. 2017)
“Engineering steep transistors towards ultra low supply voltage
- 30) Tarek Ameen (Aug. 2013 – Feb. 2018)
“Experimentally Validated Quantum Transport Models for Tunneling Devices based on novel
Materials”
- 31) Daniel Mejia (May 2011 – May 2018)
“Visual Analytics to Support Atomistic Simulations Design”
- 32) Daniel Valencia (Aug. 2012 – June 2018)
“Modeling Electronic Transport in Metal Interconnects”
- 33) Rifat Ferdous (Jan 2013 – July 2018)
“Spin-Orbit Interaction and Electron Spin Qubits in Silicon Quantum Dots”
- 34) Harshad Sahasrabudhe (physics) (June 2013 – July 2018)
“Low Temperature Simulations Framework for Quantum Dots and Point Contacts”

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- 35) Prasad Sarangapani (Aug. 2013 - Sept. 2018)
“Quantitative Prediction of Non-Local Material and Transport Properties Through Quantum Scattering Models”
- 36) James Charles (July 2016 - Sept 2018)
“Modeling Non-Locality in Quantum Systems”
- 37) Gustavo A. Valencia-Zapata (Jan. 2015 - Aug. 2019)
“Probabilistic Diagnostic Model For Handling Classifier Degredation in Machine Learning”
- 38) Chin-Yi Chen (Aug. 2014 - Oct. 2019)
“The promising candidate for low power computation: tunneling FETs”
- 39) Xinchun Guo (Aug. 2015 - Oct. 2019)
“General Resource Management for Computationally Demanding Scientific Software”
- 40) Kuang-Chung Wang (Aug. 2014 - Oct. 2019)
“Method Development in the NEGF Framework for Nano-Device Simulation: Ab-Initio Tight-Binding and Multi-Particle Interaction with Büttiker Probe”
- 41) Yuanchen Chu (Jan 2014 - Nov. 2019)
“Predictive Electro and Thermal Quantum Transport in Nanoscale Devices”
- 42) Daniel Lemus (Aug. 2012 - April 2020)
“Low-rank Approximations in Quantum Transport Simulations”
- 43) Timothy Wolfe (Jan. 2018 – Aug. 2021)
„Electronic and Optical Properties of First-Row Transition Metals in 4H-SiC For Photoconductive Switching”

Graduated 16 Master students

- 1) Rajib Rahman (non-thesis MS, continued on PhD.) (Aug. 2004-Dec. 2005)
- 2) Kaushik Balamukundan, (first Job at Intel Corp.) (Aug. 2006 – Aug. 2008)
Carrier Transport in Ultra-Scaled Devices
- 3) Alissa Nedossekina, Feb. 2009, “Evaluating the Effectiveness of a Virtual Economy System Within an Advanced Scientific Cyberinfrastructure”
- 4) Sung Hyon Park (continued for PhD) (Aug. 2007 – Dec. 2009)
Hyperfine Mapping of Donor Wave Function Deformations in Silicon Phosphorous Based Quantum Devices
- 5) Ganesh Hegde (continued for PhD) (Aug. 2007 – May 2010)
Generation and Optimization of Tight Binding Parameters Using Genetic Algorithms and Their Validation Using NEMO-3D
- 6) Xufeng Wang, co-advised with M. Lundstrom (continued for PhD Lundstrom)(Aug. 2008 – May 2010)
nanoMOS 4.0: A tool to explore ultimate Si transistors and beyond.
- 7) Yui-Hong Matthias Tan, Exchange Ruhr-University Bochum, (cont. for PhD) (Aug. 2009 – Dec. 2010)
Atomistic Modeling of an experimental GaAs/InGaAs Quantum Dot Molecule using NEMO-3D
- 8) Zhengping Jiang (continued for PhD) (Aug. 2008 – May 2011)
Quantum Transport in RTD and Atomistic Modeling of Nanostructures
- 9) Woo-Suhl Cho (transferred to other Purdue research group) (Aug. 2008 – Aug. 2011)
Investigation of Homo-junction InGaAs Band-to-Band Tunneling Diodes
- 10) Arun Goud Akkala (transferred to K. Roy) (June 2010 – Dec. 2011)
NEGF Simulation of Electron Transport in Resonant Tunneling and Resonant Interband Tunneling Diodes
- 11) Junzhe Geng (continued on PhD) (June 2010 – Aug. 2012)
Atomistic Modeling of Graphene Nanostructures and Single Electron Quantum Dots
- 12) Pengyu Long (continued on PhD) (Aug. 2012 – May 2015)
Design and Simulation of Two-dimensional Superlattice Steep Transistors
- 13) Yu Wang (continued on PhD) (Aug. 2012 – July 2015)
Manipulating and Characterizing Spin Qubits based on Donors in Silicon with Electromagnetic Fields

- | | |
|---|--------------------------|
| 14) James Charles (continued on PhD) | (May 2013 – July 2016) |
| Efficient Inelastic Scattering in Atomistic Tight Binding | |
| 15) Evan Wilson (terminal M.S. non-thesis) | (Aug. 2012 – May 2018) |
| 16) Samik Mukherjee (terminal M.S. non-thesis) | (June. 2012 – Dec. 2018) |

Past Advisor to 41 Undergrads, 6 Research Faculty, 16 Post-Docs, 1 Research Scientist

Past Research Faculty Mentor to 6 individuals

- | | |
|------------------------------|-------------------------|
| 1) Prof. Mathieu Luisier | (Feb. 2008 –Aug. 2011) |
| 2) Prof. Hong-Hyon Park | (July 2011 – Nov. 2011) |
| 3) Prof. Jean Michel Sellier | (Nov. 2011 – Oct. 2012) |
| 4) Prof. Tillmann Kubis | (July 2011 – Nov. 2016) |
| 5) Prof. Michael Povolotskyi | (Sept. 2009 – May 2017) |
| 6) Prof. Rajib Rahman | (Oct. 2012 – May 2017) |

Past Post-doc advisor to 16 individuals

- | | |
|---------------------------------------|--------------------------|
| 1) Dr. Olga Lazarenkova (at NASA/JPL) | (Feb 2002-Jan 2004) |
| 2) Dr. Marek Korkusinski | (July 2004-June 2005) |
| 3) Dr. Marta Prada | (Jan 2006 – Sept. 2006) |
| 4) Dr. Clemens Heitzinger | (Aug. 2005 - Dec. 2006) |
| 5) Dr. Shaikh Ahmed | (Feb. 2005-Aug. 2007) |
| 6) Dr. Ben Haley | (Nov. 2006 – Jan. 2010) |
| 7) Dr. Jean Michel Sellier | (Nov. 2008 – May 2010) |
| 8) Dr. Hong-Hyon Park | (July 2009 – July 2011) |
| 9) Dr. Tillmann Kubis | (Feb. 2010 – July 2011) |
| 10) Dr. Sebastian Steiger | (Jan. 2010 – Aug 2011) |
| 11) Dr. Denis Areshkin | (June 2010 – Oct 2011) |
| 12) Dr. James Fonseca | (July 2011 – Aug. 2012) |
| 13) Dr. Arvind Ajoy | (Sept. 2012 – June 2013) |
| 14) Dr. Bozidar Novakovic | (Aug. 2012 – June 2017) |
| 15) Dr. Jun Huang | (Nov. 2013 – Aug. 2017) |
| 16) Dr. Namita Narendra | (Aug. 2018 – May. 2021) |

Past Research Scientist Supervisor to 1 individual

- | | |
|----------------------|------------------------|
| 1) Dr. James Fonseca | (Aug. 2012 – May 2017) |
|----------------------|------------------------|

Past Undergraduate Research Student advisor to 60 individuals

- | | |
|-------------------------|---|
| 1) Aaron Christensen | June - Aug 04 |
| 2) Adrian Rios | June - Aug 04 |
| 3) Patrick Macnamara | June - Aug 04 |
| 4) Laurie St. Ange | June - Aug 04 |
| 5) Muriel Fort | June - Aug 04 |
| 6) Sameer Hamdan | June - Aug 04 |
| 7) Akira Matsudaira | (June 2005-Jan 2006) |
| 8) Katie Ikuku Kitamura | (June 2005-Dec 2005) |
| 9) Matteo Mannino | (May 2005-May 2006), (Jan 2007 – June 2007) |
| 10) Anish Dhanekula | (June 2006 – Jan 2007) |
| 11) Xufeng Wang | (June 2006 – Aug. 2008) |
| 12) Sriraman Damodaran | (Sept 2006 – Dec. 2007) |
| 13) Amanda Weitzel | (Sept 2006 – May 2007) |
| 14) Thomas Andrews | May 08-Aug 08 |
| 15) Drew Schuster | May 08-Aug 08 |
| 16) Gloria Budiman | May 08-Aug 08, May 09-Aug. 09 |
| 17) Mario Salomon | May 08-Aug 08 |

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18) Naman Chopra	(Nov. 2008 – Aug. 09)
19) Gloria Budiman	May 09-Aug 09
20) Matthias Tan	(Aug. 2008 – May 09)
21) Junzhe Geng	May 09-Aug 09
22) Victoria Savikhin	May 09-Aug 09
23) Abhinav Sinha <abhinavsinha@iitb.ac.in>,	May-Aug. 2010
24) Matthew Buresh <mjburesh@asu.edu>,	May-Aug. 2010
25) Lars Bjaalie <bjaalie1@illinois.edu>,	May-Aug. 2010
26) Siqi Wang <wang340@purdue.edu>,	May-Aug. 2010
27) Muhammad Zulkifli <mzulkifl@purdue.edu>,	May-Aug. 2010
28) Krystal Hoganson <khoganson@miners.utep.edu>	May-Aug. 2010
29) Win Than Aung	Dec. 2008 – May 2011
30) Siqi Wang,	May 2010 – Dec. 2011
31) Adit Ghosh	Aug. 2013 – Dec. 2013
32) José David Bermeo López (Colombia Exchange Student)	(Aug. 2013 – July 2014)
33) Santiago Alonso Pérez Rubiano (Colombia Exchange Student)	(Aug. 2013 – July 2014)
34) Woodrow (Woody) Gilbertson (Purdue)	(May 2014 – Dec 2014)
35) Liang Yuan (Richard) Dai ld@njit.edu	(May 2015 – Aug. 2015)
36) Jungbo Wu wu622@purdue.edu	(May 2016-Aug. 2016)
37) Matt Bliss blissm@purdue.edu	(May 2016-Aug. 2016)
38) Unmesha Kale ukale@purdue.edu	(May 2016-Aug. 2016)
39) Kyeonghoon Son (VIP program)	(Jan. 2020 – Dec. 2020)
40) Cassie Lin You	(May 2021 – Sept. 2021)
41) Shreya Rastogi (VIP program)	(Aug 2021 – Dec. 2021)
42) Ben Shatkowski (VIP program)	(Aug 2021 – May 2022)
43) Catherine Mayer (VIP program)	(Aug. 2021 – Dec. 2021)
44) Dingyan Shang (VIP program and independent)	(Jan 2021-May 2022)
45) Suyash Mishra (independent)	(Aug. 2021-May 2022)
46) Poonyapat Sinpanyalert (VIP program)	(Aug 2021 – May 2022)
47) Aswin Ramaswamy (VIP program, summer)	(Aug. 2021 – May 2022)
48) Alan Zhang (VIP and summer program)	(Aug. 2021 – Aug. 2022)
49) Darin Tsai (VIP and summer program)	(Aug. 2021 – Aug. 2022)
50) Aloysius Ribeiro (VIP and summer program)	(Aug. 2021 – May 2022)
51) Maximilian Drach (VIP program, summer)	(Aug. 2021 – present)
52) Dheeraj Kumar (VIP program, summer, continued)	(Jan 2022 – present)
53) Zachary Hunter (summer, continued)	(May 2022 - present)
54) Aneesh Chakravarthula (VIP fall, continued independent)	(Aug. 2022 – present)
55) Jonathan Kao (VIP fall)	(Aug. 2022 – Dec. 2022)
56) Samy Rajaraman (VIP Fall)	(Aug. 2022 – Dec. 2022)
57) Kihunn Anderson (VIP Spring)	(Jan. 2023 – present)
58) Lakshay Goel (VIP Spring)	(Jan. 2023 – present)
59) Roosh Parikh	(Jan. 2023 – present)

Past Ph.D. student advisor to 9 individuals (did not complete their PhD in my group)

1) Srikant Srinivasan, Co-advisor with Leonid Rokhinson	(Aug. 2005 – Dec. 2006)
2) Abu Naser Zainuddin, (transitioned to S. Datta)	(Aug. 2006 – Aug. 2007)
3) Robert Andrawis, transitioned to Kaushik Roy	(Aug. 2014 – Jan. 2016)
4) Evan Wilson (finished with non-thesis MS)	(Aug. 2012 – May 2017)
5) Frederico Severgnini (transitioned to other group)	(June 2016 – May 2017)
6) Enrique Jesus Aldana Sigoña (transitioned to another group)	(Aug. 2015 – Dec. 2017)
7) Samik Mukerjee (finished with non-thesis MS)	(June 2012 – Dec. 2018)
8) Shree Hari Sureshbabu (transitioned to another group)	(Aug. 2018 – May 2019)
9) Han-Wei Hsiao (transitioned to Kubis group)	(Aug. 2019 – Aug. 2022)

Past Master Student advisor to 9 individuals (did not complete their Master's degree in my group)

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- | | |
|--|-------------------------|
| 1) Jing Li, transitioned to K. Roy | (Aug 2004 – Aug. 2005). |
| 2) Selvakumaran Vadivelmurugan | Aug 2006 – Jan. 2007). |
| 3) Hemanth Hedge, | (Aug. 2006 – May 2007) |
| 4) Rezwan Chowdhury, transitioned to CE | (Aug. 2006 – May 2007) |
| 5) Seungmin Kim, (transitioned to J. Appenzeller to complete PhD) | (Aug. 2007 – Aug. 2008) |
| 6) Ahmed Reza (did not defend a master's thesis), transitioned to K. Roy | (Aug. 2012 – May 2014) |
| 7) Sicong Chen, abandoned graduate program | (Aug. 2013 – May 2014) |
| 8) Kyle Aiken (failed master's thesis), transitioned to Physics | (June 2013 – May 2014) |
| 9) Saima Sharmin (did not defend master's thesis), transitioned K. Roy | (Aug. 2012 – Aug. 2015) |

Master Student Committee Member

- Wei Qiao (August 2004-Dec. 2005), advised by Prof. David Ebert
- Prabhakar Srinivastava (Jan 2004 – Dec. 2006), advised by Prof. Supriyo Datta
- Zhen Huang (Aug 2006 – Aug. 2008), non-thesis
- Kurtis Cantley (Aug 2005 – Aug 2007), advised by Prof. Mark Lundstrom

Ph.D. Student Committee Member

- Bhaskaran Muralidharan (Aug. 2004 – May 08), advised by Prof. Supriyo Datta
- Wei Qiao (Dec. 2005 – Aug. 2006), advised by Prof. David Ebert
- Kirk Bevan (Dec 2004 – July 2008), advised by Prof. Supriyo Datta
- Ninad Pimparkar (Aug. 2004 – June 2008), advised by Prof. Ashraf Alam
- Behash Behinaein (Aug 2004 – May 2010), advised by Prof. Supriyo Datta
- Stephen Cauley (Aug 2005 – Aug. 2009), advised by Prof. Cheng-Kok Koh and Balakrishnan
- Krishnaswamy Uday Chettiar (Aug. 2005 – Aug 08), advised by Prof. Vladimir Shaleev
- Roksana Mojarad Golizadeh (Aug 2005 – May 09), advised by Prof. Supriyo Datta
- Tehseen Zahra Kazmi (Aug 2005 – Jan. 2011), advised by Prof. Supriyo Datta
- Adina Deborah Scott (Aug 2005 – Dec. 08), advised by Prof. David Janes
- Nathan Lawrence Anderson (Aug. 2008 – May 2012), advised by Prof. Alejandro Strachan
- Eduardo A. Garcia (May 2008 – ?), advised by Prof. David Janes
- Xingjie Ni (Dec. 2007 – May 2012), advised by Prof. Vladimir Shalaev
- Yumi Park (Aug. 2006 – Dec. 2011), advised by Prof. Alejandro Strachan
- Srikant Skinivasan (Aug. 2006 – May 2012), advised by Prof. Supriyo Datta
- Bangda Zhou, (Aug. 2010 – Aug. 2015), advised by Dan Jiao
- Samiran Ganguly (Jan 2011 – May 2016), advised by Prof. Supriyo Datta
- Brian Sutton (Aug. 2012 – ~Aug 2017_, advised by Prof. Supriyo Datta
- David Guzman (Aug. 2013 – ~Aug. 2016), advised by Prof. Alejandro Strachan (MSE)
- Zexi Lu (Aug. 2012 – May 2018), advised by Prof. Xiulin Ruan (ME)
- Abhijith Prakash, (Aug. 2012 – Jan 2018), advised by Prof. Joerg Appenzeller
- Kelsey Rodgers, (Aug. 2011 – May 2016), advised by Prof. Krishna Madhavan (ENE)
- JingJing Shi, (Aug. 2012 – Aug. 2018), advised by Timothy Fisher (ME)
- Zuyuan Wang, (Aug. 2012 – Aug. 2018), advised by Xiulin Ruan (ME)

PRE-PURDUE SCIENTIFIC MENTOR / ADVISOR

- Post-Doc advisor for the National Research Council.to Dr. Olga Lazarenkova at JPL. 01/2003-01/2005.
- Post-Doc mentor / collaborator to Dr. Paul Sotirelis, Texas Instruments, 09/96-01/98.
- Mentor to several summer students in a governmental or industrial laboratory environment:
 - Daniela Francovicchio, Texas Instruments, UT Dallas, 08/95-12/95, NEMO benchmarking.
 - Mukund Swaminathan, Texas Instruments, 06/97-01/98, NEMO software development.
 - William McMahon, Texas Instruments, 05/97-08/97, NEMO database development.
 - Kalen Jordan, JPL, academic part time, 05/01-08/01, Java interface development.
 - Hook Hua, academic part time, 04/02-02/03, Java/XML interface development.
 - Lei Pan, academic part time, 08/03-12/03, parallel application development.

TECHNICAL GROUP SUPERVISOR (APPLIED CLUSTER COMPUTING TECHNOLOGY GROUP):

Position held from April 2002 – December 2003

- Supervision of 11 computer science, electrical engineering and physics professionals (6 Ph.D., 3 master, 2 bachelor) and one National Research Council post-doc. Responsibilities include:
 - Technical quality of the work produced in the group.
 - Mentoring of the professional careers of the group members (promotions, salary management).
 - Direct interface between two axes of management at JPL: 1) line management (people) and 2) project management (tasks, money). Matching of technical expertise with project requirements.
 - Enforcement of JPL policies.
 - Equipment purchase responsibilities of up to \$150,000.
- Direct technical involvement in a diverse set of tasks:
 - Nanoelectronic modeling for quantum computing gates.
 - Nanoelectronic modeling development of numerically tractable open boundary conditions.
 - Spintronic modeling.
 - Evolvable computing (optimization and synthesis using genetic algorithms).
 - Java and portlet-based graphical user interface development.
 - Cluster computing technologies applied to science applications such as optical as well as synthetic aperture radar (SAR) image processing.
 - Adaptive, unstructured mesh refinement.
 - COTS-based on-board image processing.
 - XML-based non relational database design for project descriptions and evaluations.

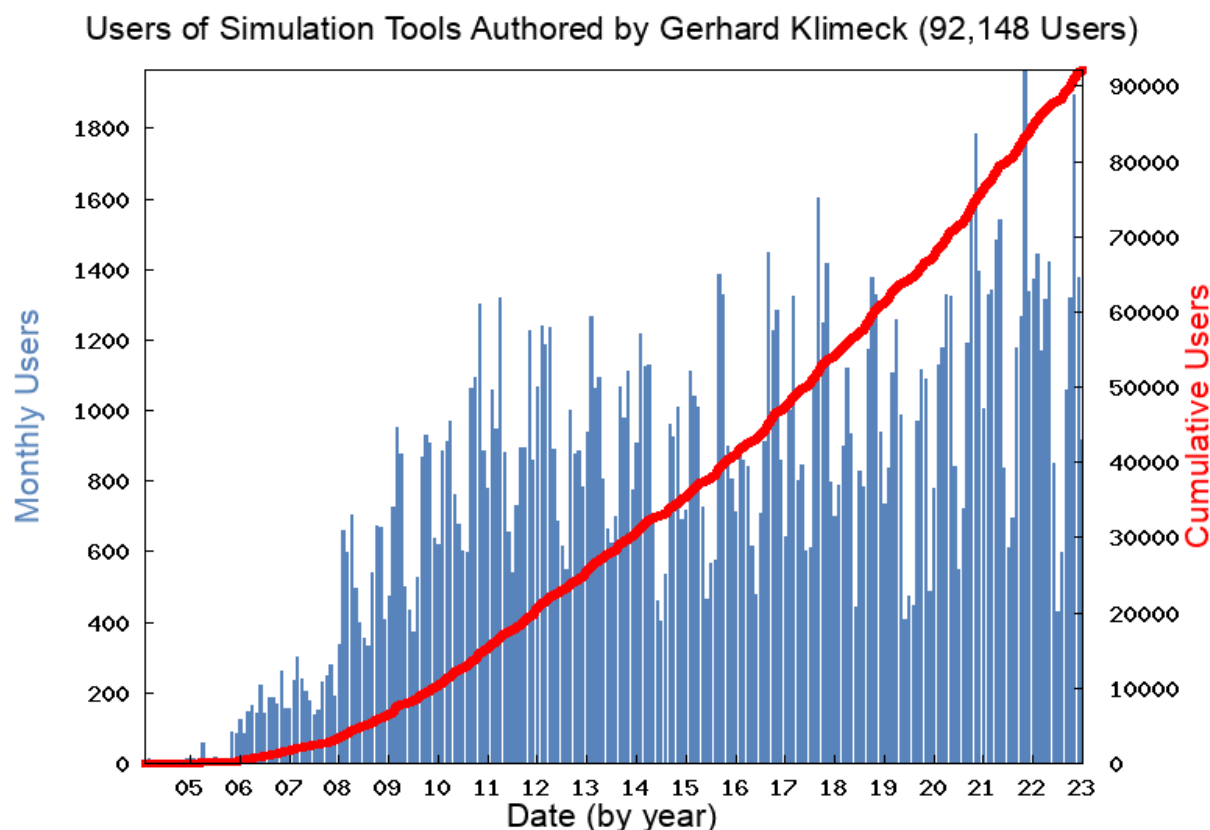
PUBLICATIONS**PUBLICATION AND CITATION SUMMARY**

Publication Type	total	Publication Type	total
- Peer reviewed Journals:	305	- Patents:	6
- Peer reviewed proceedings:	239	- Scientific Apps, Tools, Data:	42
- Invited Conference papers:	284	- Technical Reports:	36+
- Contributed conference papers:	520	- Technical Program Reviews:	98+
- Invited Seminars:	191	- Technical Briefings:	111+

Year	Journals	Proceedings	Inv. Conf	Conferences	Tech Rep.	Inv. Sem.	Reviews	Briefings
1990	1/1	0/0	0/0	2/2	0/0	0/0	0/0	0/0
1991	1/2	0/0	0/0	0/2	1/1	0/0	0/0	0/0
1992	1/3	0/0	0/0	3/5	0/1	0/0	0/0	0/0
1993	2/5	0/0	1/1	3/8	1/2	1/1	0/0	0/0
1994	3/8	0/0	3/4	8/16	1/3	2/3	2/2	0/0
1995	2/10	5/5	2/6	6/22	1/4	0/3	8/10	0/0
1996	2/12	3/8	3/9	4/26	0/4	5/8	7/17	0/0
1997	5/17	8/16	4/13	9/35	1/5	3/11	4/21	0/0
1998	7/24	1/17	5/18	5/40	4/9	4/15	0/21	0/0
1999	3/27	5/22	1/19	9/49	2/11	1/16	1/22	0/0
2000	2/29	5/27	2/21	8/57	0/11	3/19	2/24	0/0
2001	6/35	5/32	3/24	12/69	0/11	1/20	1/25	0/0
2002	6/41	2/34	6/30	22/91	9/20	10/30	3/28	0/0
2003	5/46	8/42	9/39	15/106	0/20	4/34	1/29	0/0
2004	9/55	14/56	11/50	20/126	1/21	11/45	7/36	14/14
2005	11/66	12/68	18/68	20/146	3/24	10/55	6/42	9/23
2006	7/73	13/81	18/86	36/182	2/26	13/68	9/51	3/26
2007	17/90	10/91	19/105	29/211	3/29	11/79	4/55	11/37
2008	21/111	21/112	14/119	31/242	3/32	11/90	8/63	6/43
2009	14/125	17/129	8/127	34/276	1/33	10/100	8/71	6/49
2010	16/141	15/144	20/147	35/311	1/34	7/107	6/77	0/49
2011	29/170	18/162	24/171	36/347	1/35	13/120	6/83	20/69
2012	13/183	6/168	24/195	40/387	0/35	15/135	7/90	3/72
2013	21/204	10/178	14/209	18/405	0/35	8/143	3/93	13/85
2014	16/220	10/188	15/224	17/422	0/35	6/149	4/97	1/86
2015	25/245	17/205	8/232	31/453	0/35	10/159	1/98	1/87
2016	24/269	8/213	9/241	25/478	1/36	9/168	x/98	x/87
2017	10/279	5/218	7/248	19/497	x/36	0/168	x/98	x/87
2018	16/295	7/225	6/254	7/504	x/36	6/174	x/98	x/87
2019	8/303	2/227	7/261	6/510	x/36	4/178	x/98	x/87
2020	1/304	0/227	4/265	0/510	x/36	1/179	x/98	x/87
2021	1/305	4/233	8/273	2/513		3/182		3/90
2022	4 subm	6/239	10/283	7/520		9/191		19/109
2023			1/284					2/111

Secondary Citations and h-index from Web of Science (WoS), Scopus (Sc), Google Scholar (GS)

Date	WoS Citations	Scopus Citations	GS Citations	WoS h-index	SC h-index	GS h-index	Years past PhD
2/2002	291						8
2/2003	425						9
4/19/2004	565						10
2/16/2005	672						11
2/15/2006	805						12
2/13/2007	954						13
8/24/2008	1342		1710				14
2/7/2009	1627		1916	22			15
1/27/2010			2516	26			16
1/8/2011	2525		3182	28		27	17
1/27/2012	3191		4956	31		35	18
1/14/2013	3978		6133	34		39	19
1/10/2014	4558		7402	35		44	20
1/14/2015	5349		8672	39		47	21
01/14/2016	6230		10058	41		50	22
02/11/2017	6730	8085	12250	45	45	55	23
01/17/2018	6810	9327	14301	48	50	58	24
09/02/2018	9077	10337	15309	49	51	60	24
01/09/2019	9485	10617	15817	51	51	61	25
01/23/2020	10701	11849	17768	53	55	65	26
1/18/2021	11,739	12,808	19,345	56	56	68	27
1/16/2022	12,520	13,891	20,855	57	58	70	28
1/16/2023	13,599	14,944	22,555	59	60	72	29

ELECTRONIC TOOL AND DATA PUBLICATIONS (42 TOTAL) > 92,148 USERS

- [T42] Daniel Mejia, Gerhard Klimeck (2019), "Periodic Potential Lab - Kronig Penney Model - New Interactive Version," <https://nanohub.org/resources/kronigpenneylab>. (DOI: 10.21981/TT2Y-A185). First publication 23 Aug 2019 doi:10.21981/96WV-5M37
- [T41] Prasad Sarangapani, James Fonseca, Daniel F Mejia, James Charles, Woody Gilbertson, Tarek Ahmed Ameen, Hesameddin Ilatikhameneh, Andrew Roché, Lars Bjaalie, Sebastian Steiger, David Ebert, Matteo Mannino, Hong-Hyun Park, Tillmann Christoph Kubis, Michael Povolotskyi, Michael McLennan, Gerhard Klimeck (2021), "Quantum Dot Lab," <https://nanohub.org/resources/qdot>. (DOI: 10.21981/QMEB-HW44). First publication 11 Nov 2005 doi:10.4231/D3MG7FV4Q
- [T40] Mark R. Pinto, Kent Smith, Muhammad Alam, Steven Clark, Xufeng Wang, Gerhard Klimeck, Dragica Vasileska (2014), "Padre," <https://nanohub.org/resources/padre>. (DOI: 10.4231/D30C4SK7Z). 29 Mar 2005 doi:10.4231/D30V89G94
- [T39] Dragica Vasileska, Shaikh S. Ahmed, Gokula Kannan, Matteo Mannino, Gerhard Klimeck, Mark Lundstrom, Akira Matsudaira, Junzhe Geng (2015), "Schred," <https://nanohub.org/resources/schred>. (DOI: 10.4231/D34T6F441). 02 Nov 2005 doi:10.4231/D3XS5JG64
- [T37] Shaikh S. Ahmed, Saumitra Raj Mehrotra, SungGeun Kim, Matteo Mannino, Gerhard Klimeck, Dragica Vasileska, Xufeng Wang, Himadri Pal, Gloria Wahyu Budiman (2017), "MOSFet," <https://nanohub.org/resources/mosfet>. (DOI: 10.4231/D34T6F54G). First publication 07 Oct 2005 doi:10.4231/D3Z60C178
- [T36] Akira Matsudaira, Saumitra Raj Mehrotra, Shaikh S. Ahmed, Gerhard Klimeck, Dragica Vasileska (2014), "MOSCap," <https://nanohub.org/resources/moscap>. (DOI: 10.4231/D3736M30D). First publication 02 Nov 2005
- [T36] Samik Mukherjee, Kai Miao, Abhijeet Paul, Neophytos Neophytou, Raseong Kim, Junzhe Geng, Michael Povolotskyi, Tillmann Christoph Kubis, Arvind Ajoy, Bozidar Novakovic, James Fonseca, Hesameddin Ilatikhameneh, Sebastian Steiger, Michael McLennan, Mark Lundstrom, Gerhard Klimeck (2015), "Band Structure Lab," <https://nanohub.org/resources/bandstrlab>. (DOI: 10.4231/D3Z02Z95M). First publication 18 May 2006 doi:10.4231/D3P843V6Z
- [T35] Hong-Hyun Park, Lang Zeng, Matthew Buresh, Siqi Wang, Gerhard Klimeck, Saumitra Raj Mehrotra, Clemens Heitzinger, Benjamin P Haley (2021), "Nanowire," <https://nanohub.org/resources/nanowire>. (DOI: 10.21981/QVXN-1H95). First publication 07 Dec 2005 doi:10.4231/D3NK36466

- [T34] M. E. Klausmeier-Brown, C. M. Maziar, Paul Dodd, M. A. Stettler, Xufeng Wang, Gerhard Klimeck (2019), "demons," <https://nanohub.org/resources/demons>. (DOI: 10.21981/3K4Y-JK38). First publication 17 Jul 2006 doi:10.4231/D3FB4WK6D
- [T33] Gyungseon Seol, Youngki Yoon, James K Fodor, Jing Guo, Akira Matsudaira, Diego Kienle, Gengchiao Liang, Gerhard Klimeck, Mark Lundstrom, Ahmed Ibrahim Saeed (2019), "CNTbands," <https://nanohub.org/resources/cntbands-ext>. (DOI: 10.21981/QT2F-0B32). First publication 30 May 2006 doi:10.4231/D3H98ZC6B
- [T32] M. P. Anantram, Shaikh S. Ahmed, alexei svizhenko, Derrick Kearney, Gerhard Klimeck (2019), "NanoFET," <https://nanohub.org/resources/nanofet>. (DOI: 10.21981/KNFS-1475). First publication 10 Mar 2006 doi:10.4231/D3H12V68S
- [T31] Neophytos Neophytou, Shaikh S. Ahmed, POLIZZI ERIC, Gerhard Klimeck, Mark Lundstrom (2019), "CNTFET Lab," <https://nanohub.org/resources/cntfet>. (DOI: 10.21981/WBMS-PX40). First publication 10 Mar 2006 doi:10.4231/D3VM42W9F
- [T30] Yuanchen Chu, Daniel F Mejia, Fan Chen, James Fonseca, Michael Povolotskyi, Gerhard Klimeck (2020), "Crystal Viewer Tool," https://nanohub.org/resources/crystal_viewer. (DOI: 10.21981/K3EK-R382). First publication 11 Jan 2008 doi:10.4231/D3PV6B640
- [T29] Saumitra Raj Mehrotra, Abhijeet Paul, Gerhard Klimeck (2014), "Carrier Statistics Lab," <https://nanohub.org/resources/fermi>. (DOI: 10.4231/D3K931706). First publication 22 Jan 2008 doi:10.4231/D3610VR4G
- [T28] Abhijeet Paul, Junzhe Geng, Gerhard Klimeck (2014), "Periodic Potential Lab," https://nanohub.org/resources/kronig_penney. (DOI: 10.4231/D3VT1GQ74). First publication 28 Jan 2008 doi:10.4231/D33N20D36
- [T27] Saumitra Raj Mehrotra, Abhijeet Paul, Gerhard Klimeck, Gloria Wahyu Budiman (2021), "Drift-Diffusion Lab," <https://nanohub.org/resources/semi>. (DOI: 10.21981/G0QV-VD57). First publication 04 Feb 2008 doi:10.4231/D3251FJ88
- [T26] Saumitra Raj Mehrotra, Abhijeet Paul, Gerhard Klimeck, Dragica Vasileska, Gloria Wahyu Budiman (2014), "BJT Lab," <https://nanohub.org/resources/bjt>. (DOI: 10.4231/D3BR8MH1H). First publication doi:10.4231/D3ZG6G65T
- [T25] Xufeng Wang, Sriraman Damodaran, Gerhard Klimeck, Clemens Heitzinger, POLIZZI ERIC (2014), "Prophet Nanowire," <https://nanohub.org/resources/nanowireclassic>. (DOI: 10.4231/D37D2Q81Z). First publication 26 Jun 2007
- [T24] Xufeng Wang, Bhaskaran Muralidharan, Gerhard Klimeck (2014), "Coulomb Blockade Simulation," <https://nanohub.org/resources/coulombsim>. (DOI: 10.4231/D3C24QP1W). First publication 06 Jul 2006
- [T23] SungGeun Kim, Gerhard Klimeck, Sriraman Damodaran, Benjamin P Haley (2014), "MuGFET," <https://nanohub.org/resources/NANOFINFET>. (DOI: 10.4231/D3HM52K86). First publication 01 May 2008 doi:10.4231/D35Q4RK62
- [T22] Amritanshu Palaria, Xufeng Wang, Benjamin P Haley, Matteo Mannino, Gerhard Klimeck (2021), "ABINIT," <https://nanohub.org/resources/abinit>. (DOI: 10.21981/CZMZ-XB31). First publication 09 May 2003
- [T21] Xufeng Wang, Samarth Agarwal, Gerhard Klimeck, Dragica Vasileska, Mathieu Luisier, Jean Michel D Sellier (2016), "Piece-Wise Constant Potential Barriers Tool," <https://nanohub.org/resources/pcpbt>. (DOI: 10.4231/D3WS8HN1C). First publication 08 Aug 2008 doi:10.4231/D36W9682D
- [T20] Xufeng Wang, Daniel Mejia, Dragica Vasileska, Gerhard Klimeck (2021), "ABACUS - Assembly of Basic Applications for Coordinated Understanding of Semiconductors," <https://nanohub.org/resources/abacus>. (DOI: 10.21981/YYFZ-7868). First publication 08 Aug 2008 doi:10.4231/D3348GF9F
- [T19] Pranay Kumar Reddy Baikadi, Michael Povolotskyi, Viswanathan Naveen Kumar Nolasname, Dragica Vasileska, Xufeng Wang, Gerhard Klimeck (2020), "Bound States Calculation Lab," <https://nanohub.org/resources/bsclab>. (DOI: 10.21981/6CJZ-SW77). First publication 21 Aug 2008 doi:10.4231/D3WH2DD7V
- [T18] Dragica Vasileska, Mark Lundstrom, Stephen M. Goodnick, Gerhard Klimeck (2014), "Bulk Monte Carlo Lab," <https://nanohub.org/resources/bulkmc>. (DOI: 10.4231/D3GT5FG5Q). First publication 21 Aug 2008 doi:10.4231/D3H70804F
- [T17] Gerhard Klimeck, Xufeng Wang, Dragica Vasileska (2019), "AQME - Advancing Quantum Mechanics for Engineers," <https://nanohub.org/resources/aqme>. (DOI: 10.21981/4PKZ-Q312). First publication 21 Aug 2008 doi:10.4231/D37S7HR99
- [T16] Dragica Vasileska, Gerhard Klimeck, Xufeng Wang, Stephen M. Goodnick (2015), "ACUTE," <https://nanohub.org/resources/acute>. (DOI: 10.4231/D3MK6590Z). First publication 25 Aug 2008 doi:10.4231/D3M03XW8J
- [T15] Arun Goud Akkala, Sebastian Steiger, Jean Michel D Sellier, Sunhee Lee, Michael Povolotskyi, Tillmann Christoph Kubis, Hong-Hyun Park, Samarth Agarwal, Gerhard Klimeck, James Fonseca, Archana Tankasala, Kuang-Chung Wang, Chin-Yi Chen (2015), "1D Heterostructure Tool,"

- <https://nanohub.org/resources/1dhetero>. (DOI: 10.4231/D3QR4NR6C). First publication 04 Sep 2008 doi:10.4231/D39K45S4M
- [T14] Hong-Hyun Park, Zhengping Jiang, Arun Goud Akkala, Sebastian Steiger, Michael Povolotskyi, Tillmann Christoph Kubis, Jean Michel D Sellier, Yaohua Tan, SungGeun Kim, Mathieu Luisier, Samarth Agarwal, Michael McLennan, Gerhard Klimeck, Junzhe Geng (2018), "Resonant Tunneling Diode Simulation with NEGF," <https://nanohub.org/resources/rtdnegf>. (DOI: 10.4231/D3125QC2M). First publication 05 Sep 2008 doi:10.4231/D35T3FZ9C
- [T13] Gerhard Klimeck, Dragica Vasileska (2016), "a TCAD Lab," <https://nanohub.org/resources/atcadlab>. (DOI: 10.4231/D3QR4NR7V). First publication 31 Oct 2008 doi:10.4231/D3PG1HN3Q
- [T12] Gerhard Klimeck, Dragica Vasileska (2019), "Assembly for Nanotechnology Survey Courses," <https://nanohub.org/resources/antsy>. (DOI: 10.21981/C3F8-2G69). First publication 06 Nov 2008 doi:10.4231/D39882M6H
- [T11] Dragica Vasileska, Gerhard Klimeck, Saumitra Raj Mehrotra (2014), "MESFET Lab," <https://nanohub.org/resources/mesfet>. (DOI: 10.4231/D3VM42Z2Z). First publication 25 Nov 2008 doi:10.4231/D30R9M36T
- [T10] SungGeun Kim, Mathieu Luisier, Benjamin P Haley, Abhijeet Paul, Saumitra Raj Mehrotra, Gerhard Klimeck, Hesameddin Ilatikhameneh (2021), "OMEN Nanowire," <https://nanohub.org/resources/omenwire>. (DOI: 10.21981/SX3C-YN45). First publication 15 Dec 2008 doi:10.4231/D3MK6577F
- [T9] Neerav Kharche, Mathieu Luisier, George A. Howlett, Gerhard Klimeck, Mehdi Salmani Jelodar (2016), "OMEN_FET," <https://nanohub.org/resources/omenhfet>. (DOI: 10.4231/D3BR8MH4Z) First publication 08 Sep 2009 doi:10.4231/D3GQ6R200
- [T8] Prasad Sarangapani, Arun Goud Akkala, Sebastian Steiger, Hong-Hyun Park, Yosef Borga, Tillmann Christoph Kubis, Michael Povolotskyi, Gerhard Klimeck (2014), "Brillouin Zone Viewer," <https://nanohub.org/resources/brillouin>. (DOI: 10.4231/D3DB7VQ35). First publication 15 Apr 2011 doi:10.4231/D36W9686B
- [T7] Jorge Mario Monsalve, German Felipe Giraldo, Alba Graciela Avila, Gerhard Klimeck (2014), "MEMS Piezoelectric Vibrational Energy Harvesting Lab," <https://nanohub.org/resources/piezoharvest>. (DOI: 10.4231/D3P26Q44Q). First publication 30 Jul 2014 doi:10.4231/D3P26Q44Q
- [T6] Hesameddin Ilatikhameneh, Tarek Ahmed Ameen, Fan Chen, Ramon Salazar, Gerhard Klimeck, Joerg Appenzeller, Rajib Rahman (2016), "Tunnel FET Compact Model," <https://nanohub.org/resources/tunnelfet>. (DOI: 10.4231/D36D5PC3P). First publication 24 Aug 2016 doi:10.4231/D36D5PC3P
- [T5] Khaled Aboumerhi (2017), "Quantum Dot Lab via Jupyter," <https://nanohub.org/resources/qdotjupyter>. (DOI: 10.4231/D38G8FK6C). First publication 11 Sep 2017 doi:10.4231/D38G8FK6C
- [T4] Daniel A. Valencia-Hoyos, Zhengping Jiang, Gustavo A Valencia, Kuang-Chung Wang, Gerhard Klimeck, Michael Povolotskyi (2017), "Specific Resistivity for Copper Interconnects," <https://nanohub.org/resources/resist>. (DOI: 10.4231/D3FF3M25J). First publication 20 Nov 2017 doi:10.4231/D3FF3M25J
- [T3] Daniel F Mejia, Gerhard Klimeck, Yuanchen Chu (2022), "Crystal Viewer Lab (New Interactive Front End)," <https://nanohub.org/resources/crystalviewer>. (DOI: 10.21981/3RCG-8S98). First publication 16 Aug 2019 doi:10.21981/25YY-W591
- [T2] Prasad Sarangapani, James Fonseca, Daniel F Mejia, James Charles, Woody Gilbertson, Tarek Ahmed Ameen, Hesameddin Ilatikhameneh, Andrew Roché, Lars Bjaalie, Sebastian Steiger, David Ebert, Matteo Mannino, Hong-Hyun Park, Tillmann Christoph Kubis, Michael Povolotskyi, Michael McLennan, Gerhard Klimeck (2021), "Quantum Dot Lab," <https://nanohub.org/resources/qdot> . (DOI: 10.21981/QMEB-HW44). First publication 11 Nov 2005. doi:10.4231/D3MG7FV4Q...
- [T1] Dragica Vasileska, Matteo Mannino, Michael McLennan, Xufeng Wang, Gerhard Klimeck, Saumitra Raj Mehrotra, Benjamin P Haley (2014), "PN Junction Lab," <https://nanohub.org/resources/pntoy> (DOI: 10.4231/D3GH9B95N). First publication Sept 12, 2005 (doi:10.4231/D3KK94B76)

PATENTS – 6 GRANTED

- [Pat1] US Patent 6,490,193: "Forming and storing data in a memory cell", Paul van der Wagt and Gerhard Klimeck, work performed at Texas Instruments and Raytheon TI Systems.
- [Pat2] US Patent 6,667,490: "Method and System for Generating a Memory Cell", Paul van der Wagt and Gerhard Klimeck, work performed at Texas Instruments and Raytheon TI Systems.
- [Pat3] U.S. Patent 2012/0043607, "Tunneling Field-Effect Transistor with Low Leakage Current", Mathieu Luisier, Samarth Agarwal, Gerhard Klimeck (2012)
- [Pat4] U.S. patent No. 9,858,365, "Physical modeling of electronic devices/systems", Ganesh Hegde, Yaohua Tan, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck (2017)

- [Pat5] U.S. patent 10680088, “Tunnel Effect Transistor Having Anisotropic Effective Mass Channel”, Hesameddin Ilatikhameneh, Tarek Ameen, Bozidar Novakovic, Rajib Rahman, Gerhard Klimeck, 2020/6/9,
U.S. patent application serial No. 15/479,247, “Tunnel Effect Transistor Having Anisotropic Effective Mass Channel”, Hesameddin Ilatikhameneh, Tarek Ameen, Bozidar Novakovic, Rajib Rahman, Gerhard Klimeck, Provisional Patent Filed 2017, final submission 2018, Patent update 2019
- [Pat6] U.S. patent US11093667B2, “Method and system for realistic and efficient simulation of light emitting diodes having multi-quantum-wells”, Gerhard Klimeck, Tillmann Kubis, Junzhe Geng. (2022)
U.S. patent application serial serial no. 62/509,318, “Method and System for realistic and efficient simulation of light emitting diodes having multi-quantum-wells”, Gerhard Klimeck, Tillmann Kubis, Junzhe Geng , provisional patent filed 2017,final submission 2018.

PATENT APPLICATIONS / DISCLOSURES

- U.S. patent Application Serial No.61/429,953, “Method for the Discovering Behavioral Similarities in Sequential/Temporal Event Streams”, Michael G. Zentner, Gerhard Klimeck, George B. Adams III., Nathan Denny.

BOOK (1) AND BOOK CHAPTERS (10)**BOOK (1)**

- [Book1] Computational Electronics: From Semi-Classical to Quantum Transport Modeling, D. Vasileska, S. M. Goodnick and G. Klimeck, 2010 Taylor and Francis.

BOOK CHAPTERS (10 TOTAL)

- [B10] Gerhard Klimeck, Timothy B. Boykin, "Tight-Binding Models, Their Applications to Device Modeling, and Deployment to a Global Community", In: Rudan, M., Brunetti, R., Reggiani, S. (eds) Springer Handbook of Semiconductor Devices . Springer Handbooks. Springer, Cham. https://doi.org/10.1007/978-3-030-79827-7_45 (2022)
- [B9] Gerhard Klimeck, et al., "Triennial Review of the National Nanotechnology Initiative" in "A report of National Academies of Sciences, Engineering, and Medicine", THE NATIONAL ACADEMIES PRESS, Washington, DC, ISBN:978-0-309-44794-2,
- [B8] Jun Huang, Lining Zhang, Pengyu Long, Michael Povolotskyi, Gerhard Klimeck, "Quantum Transport Simulation of III-V TFETs with Reduced-Order k-p Method" in "Tunneling Field Effect Transistor Technology", Chapter: 6, Springer International Publishing , ISBN:978-3-319-31651-2 (print) 978-3-319-31653-6 (online),
- [B7] Michael Zentner, Lynn Zentner, Dwight McKay, Swaroop Samek, Nathan Denny, Sabine Brunswicker, Gerhard Klimeck, "In the Flow: Evolving from Utility Based Social Medium to Community Peer" in "Transparency in Social Media, Tools, Methods and Algorithms for Mediating Online Interactions", Chapter: Part III, Springer International Publishing , ISBN:978-3-319-18551-4 (Print) 978-3-319-18552-1 (Online),
- [B6] Alan Seabaugh, Zhengping Jiang, Gerhard Klimeck, "Tunnel transistors" in "CMOS and Beyond: Logic Switches for Terascale Integrated Circuits", Chapter: 6, Cambridge University Press, ISBN:9781107043183, April 2015,
- [B5] Rajib Rahman, Lloyd Hollenberg, Gerhard Klimeck, "Theory and Simulations of Controlled Electronic States Bound to a Single Dopant in Silicon" in "Single Atom Nanoelectronics", Chapter: 3, Pan Stanford Publishing, ISBN:9789814316316, April 30, 2013,
- [B4] Giuseppe Tettamanzi, Abhijeet Paul, Sunhee Lee, Gerhard Klimeck, Sven Rogge, "New Tools for the direct characterisation of FinFets" in "CMOS Nanoelectronics: Innovative Devices, Architectures, and Applications", Chapter: 2, Nadine Collaert, Pan Stanford Publishing, ISBN:9789814364027, January 31, 2012,
- [B3] Gabriel Lansbergen, Rajib Rahman, Giuseppe Tettamanzi, Jan Verduijn, Lloyd Hollenberg, Gerhard Klimeck, Sven Rogge, "Dopant Metrology in Advanced FinFets" in "CMOS Nanoelectronics: Innovative Devices, Architectures, and Applications", Chapter: 1, Nadine Collaert , Pan Stanford Publishing, ISBN:9789814364027, January 31, 2012,
- [B2] Michael McLennan, George Adams III., Gerhard Klimeck, "HUBzero™ Platform for Scientific Collaboration" in "Distributed and Cloud Computing, From Parallel Processing to the Internet of Things", Chapter: 5.3.2, Morgan Kaufmann, ISBN:9780123858801, October 17, 2011,
- [B1] Shaikh Ahmed, Neerav Kharche, Rajib Rahman, Muhammad Usman, Sunhee Lee, Hoon Ryu, Hansang Bae, Steven Clark, Benjamin Haley, Maxim Naumov, Faisal Saied, Marek Korkusinski, Rick Kennel, Michael McLennan, Timothy Boykin, Gerhard Klimeck, "Multimillion Atom Simulations with Nemo3D" in "Encyclopedia of Complexity and Systems Science", Chapter: 13, Robert A Meyers, Springer, ISBN:9780387304403, Jan 1, 2009,

RECENTLY SUBMITTED JOURNAL PUBLICATIONS IN ARXIV (5)

- [xxx] Veljko Milutinovic, Erfan Sadeqi Azer, Kristy Yoshimoto, Gerhard Klimeck, Miljan Djordjevic, Milos Kotlar, Miroslav Bojovic, Bozidar Miladinovic, Nenad Korolija, Stevan Stankovic, Nenad Filipović, Zoran Babovic, Miroslav Kosanic, Akira Tsuda, Mateo Valero, Massimo De Santo, Erich Neuhold, Jelena Skoručak, Laura Dipietro, Ivan Ratkovic, "The Ultimate DataFlow for Ultimate SuperComputers-on-a-Chip, for Scientific Computing, Geo Physics, Complex Mathematics, and Information Processing", [arXiv:2009.10593](https://arxiv.org/abs/2009.10593)
- [xxx] Zoran Babovic¹, Branislav Bajat², Vladan Djokic², Filip Djordjevic², Drazen Draskovic², Nenad Filipovic^{1,11}, Stephan French⁸, Borko Furht¹³, Marija Ilic⁹, Ayhan Irfanoglu⁴, Gerhard Klimeck⁴, Nenad Korolija², Milos Kotlar², Milos Kovacevic², Vladan Kuzmanovic², Marko Marinkovic², Miodrag Mateljevic¹², Avi Mendelson⁷, Fedor Mesinger¹², Gradimir Milovanovic¹², Veljko Milutinovic^{5,14,15}, Nenad Mitic², Aleksandar Neskovic², Natasa Neskovic², Bosko Nikolic², Konstantin Novoselov⁶, Arun Prakash⁴, Ivan Ratkovic³, Diego Rios⁸, Dan Shechtman⁷, Zoran Stojadinovic², Andrey Ustyuzhanin¹⁰, Stan Zak⁴, "TEACHING COMPUTING FOR COMPLEX PROBLEMS IN CIVIL ENGINEERING AND GEO SCIENCES USING BIG DATA AND MACHINE LEARNING: SYNERGIZING FOUR DIFFERENT COMPUTING PARADIGMS AND FOUR DIFFERENT MANAGEMENT DOMAINS", submitted
- [xxx] Zoran Babovic¹, Branislav Bajat², Vladan Djokic², Filip Djordjevic², Drazen Draskovic², Nenad Filipovic^{1,11}, Borko Furht¹⁵, Nikola Gacic³, Igor Ikodinovic¹³, Marija Ilic⁹, Ayhan Irfanoglu⁴, Branislav Jelenkovic^{2,12}, Gerhard Klimeck⁴, Nenad Korolija², Milos Kotlar², Milos Kovacevic², Vladan Kuzmanovic², Marko Marinkovic², Slobodan Markovic^{5,12}, Avi Mendelson¹⁰, Veljko Milutinovic^{8,14}, Aleksandar Neskovic², Natasa Neskovic², Nenad Mitic², Bosko Nikolic², Konstantin Novoselov⁶, Arun Prakash⁴, Ivan Ratkovic³, Zoran Stojadinovic², Andrey Ustyuzhanin⁷, Stan Zak⁴, "RESEARCH IN COMPUTING-INTENSIVE SIMULATIONS FOR NATURE-ORIENTED CIVIL-ENGINEERING AND RELATED SCIENTIFIC FIELDS, USING MACHINE LEARNING AND BIG DATA: AN OVERVIEW OF OPEN PROBLEMS", submitted
- [xxx] Gesing, Sandra; Stirn, Claire ; Klimeck, Gerhard; Zentner, Lynn; Wang, Su; Villegas Martinez, Braulio; Moya-Cessa, Héctor Manuel ; Diaz Eaton, Carrie ; Donovan, Sam; Song, Carol; Zhao, Lan; Kim, I Luk ; Strachan, Alejandro; Zentner, Michael ; Kalyanam, Rajesh, "Hubzero: Community Engagement in Numbers for Four Science Gateways Supporting Open Science", submitted to CISE – Computers in Science and Engineering
- [xxx] nanoHUB: towards pervasive and FAIR simulations and data", submitted

JOURNAL PUBLICATIONS IN ARXIV (5) – UNCLEAR STATUS

- [xxx] Chin-Yi Chen, Hsin-Ying Tseng, Hesameddin Ilatikhameneh, Tarek A Ameen, Gerhard Klimeck, Mark J Rodwell, Michael Povolotskyi, Doping profile engineered triple heterojunction TFETs with 12 nm body thickness, arXiv preprint arXiv:2010.12964
- [xxx] Jun Huang, Yu Wang, Pengyu Long, Yaohua Tan, Michael Povolotskyi, Gerhard Klimeck, "High-Performance Complementary III-V Tunnel FETs with Strain Engineering", arXiv:1605.00955
- [xxx] Robert Andrawis, Jose Bermeo, James Charles, Jianbin Fang, Jim Fonseca, Yu He, Gerhard Klimeck, Zhengping Jiang, Tillmann Kubis, Daniel Mejia, Daniel Lemus, Michael Povolotskyi, Santiago Rubiano, Prasad Sarangapani, Lang Zeng, "NEMO5: Achieving High-end Internode Communication for Performance Projection Beyond Moore's Law", arXiv:1510.04686
- [xxx] Rajib Rahman, Jan Verduijn, Yu Wang, Chunming Yin, Gabriele Boo, Gerhard Klimeck, Sven Rogge, "Bulk and sub-surface donor bound excitons in silicon under electric fields", arXiv:1510.00065
- [xxx] Gustavo A. Valencia-Zapata, Carolina Gonzalez-Canas, Michael G. Zentner, Okan Ersoy, Gerhard Klimeck, "Probabilistic Diagnostic Tests for Degradation Problems in Supervised Learning", arXiv:2004.02988

JOURNAL PUBLICATIONS (305 TOTAL)**Work Performed at Purdue (249 Total)**

- [305] Chin-Yi Chen, Hsin-Ying Tseng, Hesameddin Ilatikhameneh, Tarek Ameen, Gerhard Klimeck, Mark Rodwell, Michael Povolotskyi, "Doping Profile Engineered Triple Heterojunction TFETs With 12-nm Body Thickness" IEEE Transactions on Electron Devices, June 2021, Vol. 68, No. 6, Pages 3104-3111 (2021); [doi: 10.1109/TED.2021.3075190](https://doi.org/10.1109/TED.2021.3075190)
- [304] Chin-Yi Chen, Hesam Ilatikhameneh, Huang, J.Z., Klimeck, G., Povolotskyi, M., Impact of Body Thickness and Scattering on III-V Triple Heterojunction TFET Modeled with Atomistic Mode-Space Approximation, IEEE Transactions on Electron Devices, 67(8),9132705, pp. 3478-3485
- [303] Tingting Shen, Daniel Valencia, Qingxiao Wang, KuangChung Wang, Michael Povolotskyi, Moon Kim, Gerhard Klimeck, Zhihong Chen, Joerg Appenzeller, "MoS2 for Enhanced Electrical Performance of Ultrathin Copper Films", ACS Applied Materials and Interfaces 11(31), pp. 28345-2835; doi:10.1021/acsami.9b03381

- [302] Wan Hwang, Pei Zhao, SungGeun Kim, Rusen Yan, Gerhard Klimeck, Alan Seabaugh, Susan Fullerton-Shirey, Huili Xing, Debdeep Jena, "Room-Temperature Graphene-Nanoribbon Tunneling Field-Effect Transistors", *npj 2D Mater Appl* 3, 43 (2019);doi:10.1038/s41699-019-0127-1
- [301] Chin-Sheng Pang, Chin-Yi Chen, Tarek Ameen, Shengjiao Zhang, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, Zhihong Chen, "WSe₂ Homo Junction Devices: Electrostatically Configurable as Diodes, MOSFETs, and Tunnel FETs for Reconfigurable Computing", *Small*, Vol. 15, Issue 14 (2019); doi:10.1002/sml.201902770
- [300] Yuanchen Chu, Jingjing Shi, Kai Miao, Yang Zhong, Prasad Sarangapani, Timothy Fisher, Gerhard Klimeck, Xiulin Ruan, Tillmann Kubis, "Thermal boundary resistance predictions with non-equilibrium Green's function and molecular dynamics simulations", *Applied Physics Letters*, Vol. 115, Issue 23 (2019)
- [299] Prasad Sarangapani, Yuanchen Chu, James Charles, Gerhard Klimeck, Tillmann Kubis, "Band-tail Formation and Band-gap Narrowing Driven by Polar Optical Phonons and Charged Impurities in Atomically Resolved III-V Semiconductors and Nanodevices", *Physical Review Applied* 12, 044045, October 2019
- [298] Jana Meyer, Jan Scharnetzky, Matthias Berl, Werner Wegscheider, Maik Hauser, Werner Dietsche, Kuang-chun Wang, Gerhard Klimeck, Lars Tiemann, Robert Blick, "Microwave-induced capacitance resonances and anomalous magneto resistance in double quantum wells", *Journal of Applied Physics*, Vol. 125, Issue 23, June 2019
- [297] Yuanchen Chu, Shang-Chun Lu, Nadim Chowdhury, Michael Povolotskyi, Gerhard Klimeck, Mohamed Mohamed, Tomas Palacios, "Superior Performance of 5-nm Gate Length GaN Nanowire nFET for Digital Logic Applications", *IEEE Electron Device Letters*, Volume: 40, Issue: 6, Pages: 874 - 877, June 2019
- [296] Timothy Boykin, Prasad Sarangapani, Gerhard Klimeck, "Non-orthogonal tight-binding models: Problems and possible remedies for realistic nano-scale devices", *Journal of Applied Physics*, Vol. 125, Issue 14, April 2019
- [295] Daniel Mejia, Tillmann Kubis, Gerhard Klimeck, "NemoViz: A visual interactive system for atomistic simulations design", *Visualization in Engineering*, November 2018, Volume 6, Number 6
- [294] Peng Wu, Tarek Ameen, Huairuo Zhang, Leonid Bendersky, Hesameddin Ilatikhameneh, Gerhard Klimeck, Rajib Rahman, Albert Davydov, Joerg Appenzeller, "Complementary Black Phosphorus Tunneling Field-Effect Transistors", *ACS Nano*, Publication Date (Web): December 18, 2018
- [293] Tarek Ameen, Hesameddin Ilatikhameneh, Patrick Fay, Alan Seabaugh, Rajib Rahman, Gerhard Klimeck, "Alloy Engineered Nitride Tunneling Field Effect Transistor: A solution for the challenge of heterojunction TFETs", *IEEE Transactions on Electron Devices*, 2018 (Early Access)
- [292] Prasad Sarangapani, Cory Weber, Jiwon Chang, Stephen Cea, Michael Povolotskyi, Gerhard Klimeck, Tillmann Kubis, "Atomistic tight-binding study of contact resistivity in Si/SiGe PMOS Schottky contacts", *IEEE Transactions on Electron Devices*, 2018 (Early Access), Pages 1-1
- [291] Fan Chen, Hesameddin Ilatikhameneh, Yaohua Tan, Gerhard Klimeck, Rajib Rahman, "Switching Mechanism and the Scalability of vertical-TFETs", , 2018, Vol. 65, No. 7, Pages 3065-3068
- [290] Hesameddin Ilatikhameneh, Tarek Ameen, Fan Chen, Harshad Sahasrabudhe, Gerhard Klimeck, Rajib Rahman, "Dramatic Impact of Dimensionality on the Electrostatics of P-N Junctions and Its Sensing and Switching Applications", *IEEE Transactions on Nanotechnology*, 2018, Vol. 17, No. 2, Pages 293-298
- [289] Yuanchen Chu, Prasad Sarangapani, James Charles, Gerhard Klimeck, Tillmann Kubis, "Explicit screening full band quantum transport model for semiconductor nanodevices", *Journal of Applied Physics* 123, 244501 (2018)
- [288] Tarek Ameen, Hesameddin Ilatikhameneh, Archana Tankasala, Yuling Hsueh, James Charles, Jim Fonseca, Michael Povolotskyi, Jun Kim, Sanjay Krishna, Monica Allen, Jeffery Allen, Rajib Rahman, Gerhard Klimeck, "Theoretical study of strain-dependent optical absorption in doped Stranski-Krastanov grown InAs/InGaAs/GaAs/AlGaAs quantum dots", *Beilstein Journal of Nanotechnology*, 2018, 9, 1075–1084
- [287] Rifat Ferdous, Kok , Menno Veldhorst, Jason Hwang, C.H. Yang, Gerhard Klimeck, Andrea Morello, Andrew Dzurak, Rajib Rahman, "Interface induced spin-orbit interaction in silicon quantum dots and prospects for scalability", *Physical Review B* 97, 241401 (2018)
- [286] Chin-Yi Chen, Tarek Ameen, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, Joerg Appenzeller, "Channel Thickness Optimization for Ultrathin and 2-D Chemically Doped TFETs", *IEEE Transactions on Electron Devices*, 2018, Vol. 65, No. 10, Pages 4614-4621
- [285] Daniel Valencia, Evan Wilson, Zhengping Jiang, Gustavo Valencia-Zapata, KuangChung Wang, Gerhard Klimeck, Michael Povolotskyi, "Grain-Boundary Resistance in Copper Interconnects: From an Atomistic Model to a Neural Network", *Physical Review Applied* 9 (4), 044005
- [284] Harshad Sahasrabudhe, Bozidar Novakovic, James Nakamura, Saeed Fallahi, Michael Povolotskyi, Gerhard Klimeck, Rajib Rahman, Michael Manfra, "Optimization of edge state velocity in the integer quantum Hall regime", *Physical Review B* 97, 085302 (2018)
- [283] Hesameddin Ilatikhameneh, Tarek Ameen, Chin-Yi Chen, Gerhard Klimeck, Rajib Rahman, "Sensitivity Challenge of Steep Transistors", *IEEE TRANSACTIONS ON ELECTRON DEVICES*, VOL. 65, NO. 4, APRIL 2018

- [282] Archana Tankasala, Joe Salfi, Juanita Bocquel, Benoit Voisin, Muhammad Usman, Gerhard Klimeck, Michelle Simmons, Lloyd Hollenberg, Sven Rogge, Rajib Rahman, "Two-electron states of a group V donor in silicon from atomistic full configuration interaction", *Phys. Rev. B* 97, 195301 – Published 2 May 2018
- [281] Jun Huang, Hesameddin Ilatikhameneh, Michael Povolotskyi, Gerhard Klimeck, "Robust Mode Space Approach for Atomistic Modeling of Realistically Large Nanowire Transistors", *Journal of Applied Physics* 123, 044303 (2018)
- [280] Pengyu Long, Jun Huang, Michael Povolotskyi, Prasad Sarangapani, Gustavo Valencia-Zapata, Tillmann Kubis, Mark Rodwell, Gerhard Klimeck, "Atomistic Modeling trap-assisted tunneling in hole tunnel FETs", *Journal of Applied Physics* 123 (2018)
- [279] Yu Wang, Chin-Yi Chen, Gerhard Klimeck, Michelle Simmons, Rajib Rahman, "All-electrical control of donor-bound electron spin qubits in silicon", *Nature Nanotechnol.* 2017 Oct
- [278] KuangChung Wang, Teodor Stanev, Daniel Valencia, James Charles, Alex Henning, Vinod Sangwan, Aritra Lahiri, Daniel Mejia, Prasad Sarangapani, Michael Povolotskyi, A. Afzal, Jesse Maassen, Gerhard Klimeck, Mark Hersam, Lincoln Lauhon, Nathaniel Stern, Tillmann Kubis, "Control of interlayer delocalization in 2H transition metal dichalcogenides", *Journal of Applied Physics* 122, 224302 (2017)
- [277] Junzhe Geng, Prasad Sarangapani, KuangChung Wang, Erik Nelson, Ben Browne, Carl Wordelman, James Charles, Yuanchen Chu, Tillmann Kubis, Gerhard Klimeck, "Quantitative Multi-Scale, Multi-Physics Quantum Transport Modeling of GaN-Based Light Emitting Diodes", *Phys. Status Solidi A* 2017, 1700662, 27 December 2017
- [276] Fan Chen, Hesameddin Ilatikhameneh, Yaohua Tan, Daniel Valencia, Gerhard Klimeck, Rajib Rahman, "Transport in vertically stacked hetero-structures from 2D materials", *IOP Journal of Physics: Conf. Series* 864 (2017) 012053
- [275] Fan Chen, Hesameddin Ilatikhameneh, Tarek Ameen, Gerhard Klimeck, Rajib Rahman, "Thickness Engineered Tunnel Field-Effect Transistors based on Phosphorene", *IEEE Electron Device Letters*, Volume: 38, Issue: 1, Jan. 2017, Pages: 130 - 133
- [274] Tarek Ameen, Hesameddin Ilatikhameneh, Jun Huang, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, "Combination of Equilibrium and Nonequilibrium Carrier Statistics Into an Atomistic Quantum Transport Model for Tunneling Heterojunctions", *IEEE Transactions on Electron Devices*, Vol: 64, Issue: 6, Page(s): 2512 - 2518, June 2017
- [273] Gustavo Valencia-Zapata, Daniel Mejia, Gerhard Klimeck, Michael Zentner, Okan Ersoy, "Statistical Approach for Increasing the Accuracy in Supervised Learning Algorithms", *The IPSI BGD Transactions on Internet Research. Special Issue: Machine Learning and Signal/Image Processing*, 2017.
- [272] Guilherme Tosi, Fahd Mohiyaddin, Tenberg, Rajib Rahman, Gerhard Klimeck, Andrea Morello, "Silicon quantum processor with robust long-distance qubit couplings", *Nature Communications* 8, Article number: 450 (2017)
- [271] Parijat Sengupta, Yaohua Tan, Gerhard Klimeck, Junxia Shi, "Low-temperature thermal transport and thermopower of monolayer transition metal dichalcogenide semiconductors", *JOURNAL OF PHYSICS-CONDENSED MATTER*, Vol: 29, Issue: 40, Article Number: 405701, OCT 11, 2017
- [270] Jun Huang, Michael Povolotskyi, Hesameddin Ilatikhameneh, Tarek Ameen, Rajib Rahman, Mark Rodwell, Pengyu Long, Gerhard Klimeck, "A Multiscale Modeling of Triple-Heterojunction Tunneling FETs", *IEEE Transactions on Electron Devices*, Volume: 64, Issue: 6, Pages: 2728 - 2735, June 2017
- [269] Sorin Matei, Michael Zentner, Lynn Zentner, Gerhard Klimeck, "Creating impact in the digital space: digital practice dependency in communities of digital scientific innovations", *Scientometrics*, January 2017, Volume 110, Issue 1, pp 417–442
- [268] Timothy Boykin, Gerhard Klimeck, "Insights from simple models for surface states in nanostructures", *European Journal of Physics*, Volume 38, 025501
- [267] Pengyu Long, Jun Huang, Zhengping Jiang, Gerhard Klimeck, Mark Rodwell, Michael Povolotskyi, "Performance degradation of superlattice MOSFETs due to scattering in the contacts", *Journal of Applied Physics*, Vol 120, 224501, December 2016
- [266] James Charles, Prasad Sarangapani, Roksana Golizadeh-Mojarad, Robert Andrawis, Daniel Lemus, Xinchun Guo, Daniel Mejia, Jim Fonseca, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Incoherent transport in NEMO5: realistic and efficient scattering on phonons", *Journal of Computational Electronics*, pp 1–7, 2016
- [265] Jun Huang, Pengyu Long, Michael Povolotskyi, Gerhard Klimeck, Mark Rodwell, "Scalable GaSb/InAs tunnel FETs with non-uniform body thickness", *IEEE Transactions on Electron Devices*, Volume: 64, Issue: 1, Pages: 96 - 101, Jan. 2017
- [264] Jun Huang, Pengyu Long, Michael Povolotskyi, Gerhard Klimeck, Mark Rodwell, "P-Type Tunnel FETs With Triple Heterojunctions", *IEEE Journal of the Electron Devices Society*, Volume: 4, Issue: 6, Page(s): 410 - 415, Nov. 2016

- [263] Yu Wang, Chin-Yi Chen, Gerhard Klimeck, Michelle Simmons, Rajib Rahman, "Characterizing Si:P quantum dot qubits with spin resonance techniques", *Scientific Reports* 6, Article number: 31830 (2016)
- [262] Kai Miao, S. Sadasivam, James Charles, Gerhard Klimeck, Timothy Fisher, Tillmann Kubis, "Büttiker probes for dissipative phonon quantum transport in semiconductor ", *APPLIED PHYSICS LETTERS* 108, 113107 (2016)
- [261] Tillmann Kubis, Yu He, Robert Andrawis, Gerhard Klimeck, "General Retarded Contact Self-energies in and beyond the Non-equilibrium Green's Function Method", *Journal of Physics: Conference Series* Volume 696, conference 1, 012019 (2016)
- [260] Yu He, Yaohua Tan, Zhengping Jiang, Michael Povolotskyi, Gerhard Klimeck, Tillmann Kubis, "Surface Passivation in Empirical Tight Binding", *IEEE TRANSACTIONS ON ELECTRON DEVICES* VOL. 63, Issue: 3, Page(s): 954 - 958, February (2016)
- [259] Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "Transferable tight-binding model for strained group IV and III-V materials and heterostructures", *PHYSICAL REVIEW B* 94, 045311 (2016), published 21 July 2016
- [258] Hesameddin Ilatikhameneh, Tarek Ameen, Bozidar Novakovic, Yaohua Tan, Gerhard Klimeck, Rajib Rahman, "Saving Moore's Law Down To 1nm Channels With Anisotropic Effective Mass", *Scientific Reports* 6, Article number: 31501
- [257] Mehdi Salmani-Jelodar, Hesameddin Ilatikhameneh, SungGeun Kim, Kwok Ng, Prasad Sarangapani, Gerhard Klimeck, "Optimum High-k Oxide for the Best Performance of Ultra-scaled Double-Gate MOSFETs", *IEEE Transactions on Nanotechnology* (2016)
- [256] Tarek Ameen, Hesameddin Ilatikhameneh, Gerhard Klimeck, Rajib Rahman, "Few-layer Phosphorene: An Ideal 2D Material For Tunnel Transistors", *Scientific Reports* 6, Article number: 28515 (2016)
- [255] Hesameddin Ilatikhameneh, Gerhard Klimeck, Joerg Appenzeller, Rajib Rahman, "Design Rules for High Performance Tunnel Transistors from 2D Materials", *IEEE Journal of Electron Device Society (J-EDS)*, Volume: 4, Issue: 5, Page(s): 260 - 265, Sept. 2016
- [254] Hesameddin Ilatikhameneh, Tarek Ameen, Gerhard Klimeck, Rajib Rahman, "Universal Behavior of Atomistic Strain in Self-Assembled Quantum Dots", *IEEE JOURNAL OF QUANTUM ELECTRONICS*, vol. 52, no. 7, July 2016
- [253] Hesameddin Ilatikhameneh, Ramon Salazar, Gerhard Klimeck, Rajib Rahman, Joerg Appenzeller, "From Fowler-Nordheim to Non-Equilibrium Green's Function Modeling of Tunneling", *IEEE Transactions on Electron Devices*, Volume:63 , Issue: 7, July 2016
- [252] Fahd Mohiyaddin, Rachpon Kalra, Arne Laucht, Rajib Rahman, Gerhard Klimeck, Andrea Morello, "Transport of Spin Qubits with Donor Chains under Realistic Experimental Conditions", *PHYSICAL REVIEW B* 94, 045314 (2016), published 25 July 2016
- [251] Fan Chen, Hesameddin Ilatikhameneh, Gerhard Klimeck, zhihong chen, Rajib Rahman, "Configurable Electrostatically Doped High Performance Bilayer Graphene Tunnel FET", *IEEE Journal of the Electron Devices Society*, Volume:4 ,Issue: 3, Page(s): 124 - 128, May 2016
- [250] Muhammad Usman, Juanita Bocquel, Joe Salfi, Benoit Voisin, Archana Tankasala, Rajib Rahman, Michelle Simmons, Sven Rogge, Lloyd Hollenberg, "Spatial Metrology of Dopants in Silicon with Exact Lattice Site Precision", *Nature Nanotechnology* 11, 763–768 (2016)
- [249] Pengyu Long, Jun Huang, Michael Povolotskyi, Gerhard Klimeck, "High-Current Tunneling FETs With (1\bar{1}0) Orientation and a Channel Heterojunction", *IEEE Electron Device Letters*, Volume:37 , Issue: 3, Page(s): 345 - 348, March 2016
- [248] Timothy Boykin, Arvind Ajoy, Hesameddin Ilatikhameneh, Michael Povolotskyi, Gerhard Klimeck, "Unfolding and effective bandstructure calculations as discrete real-and reciprocal-space operations", *Physica B: Condensed Matter*, Volume 491, 15 June 2016, Pages 22–30
- [247] Omid Nohadani, Jocelyn Dunn, Gerhard Klimeck, "Categorizing Users of Cloud Services", *Service Science*, Volume 8 Issue 1, March 2016, In Progress, pp. 59-70
- [246] Yu Wang, Archana Tankasala, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, Rajib Rahman, "Highly tunable exchange in donor qubits in silicon", *npj Quantum Information* 2, 16008 (2016)
- [245] Joe Salfi, J. Mol, Rajib Rahman, Gerhard Klimeck, Michelle Simmons, Lloyd Hollenberg, Sven Rogge, "Quantum simulation of the Hubbard model with dopant atoms in silicon", *Nature Communications* 7, 11342, 20 April 2016
- [244] Pengyu Long, Evan Wilson, Jun Huang, Gerhard Klimeck, Mark Rodwell, Michael Povolotskyi, "Design and Simulation of GaSb/InAs 2D Transmission-Enhanced Tunneling FETs", *IEEE ELECTRON DEVICE LETTERS*, VOL: 37, Issue: 1, Pages: 107 - 110, JANUARY 2016
- [243] Zhengping Jiang, Yeqing Lu, Yaohua Tan, Yu H, Michael Povolotskyi, Tillmann Kubis, Alan Seabaugh, Patrick Fay, Gerhard Klimeck, "Quantum Transport in AlGaSb/InAs TFETs With Gate Field In-Line With Tunneling Direction", *IEEE TRANSACTIONS ON ELECTRON DEVICES*, VOL. 62, Issue: 8, Page(s): 2445 - 2449, AUGUST 2015

- [242] Tarek Ameen, Hesameddin Ilatikhameneh, Yuling Hsueh, James Charles, Jim Fonseca, Michael Povolotskyi, Jun Kim, Sanjay Krishna, Monica Allen, Jeffery Allen, Brett Wenner, Rajib Rahman, Gerhard Klimeck, "Theoretical study of strain-dependent optical absorption in Stranski-Krastanov grown InAs/InGaAs/GaAs/AlGaAs quantum dots", arXiv:1502.07726
- [241] Long-Qing Chen, Li-Dong Chen, Sergei Kalinin, Gerhard Klimeck, Sanat Kumar, Jörg Neugebauer, Ichiro Terasaki, "Design and discovery of materials guided by theory and computation", npj Computational Materials 1, Article number: 15007 (2015)
- [240] Hesameddin Ilatikhameneh, Gerhard Klimeck, Rajib Rahman, "Can Homo Junction Tunnel FETs Scale Below 10nm?", IEEE ELECTRON DEVICE LETTERS, vol. 37, Issue: 1, Page(s): 115-118, January, 2016
- [239] Tao Chu, Hesameddin Ilatikhameneh, Gerhard Klimeck, Rajib Rahman, zhihong chen, "Electrically Tunable Bandgaps in Bilayer MoS₂", Nano Lett., 2015, 15 (12), pp 8000–8007
- [238] Ramon Salazar, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, Joerg Appenzeller, "A predictive analytic model for high-performance tunneling field-effect transistors approaching non-equilibrium Green's function simulations", Journal of Applied Physics, 118, 164305 (2015)
- [237] Hesameddin Ilatikhameneh, Tarek Ameen, Gerhard Klimeck, Joerg Appenzeller, Rajib Rahman, "Dielectric Engineered Tunnel Field-Effect Transistor", IEEE ELECTRON DEVICE LETTERS, vol. 36, Issue: 10, Page(s): 1097-1100, October, 2015
- [236] Fan Chen, Luis Jauregui, Yaohua Tan, Michael Manfra, Yong Chen, Gerhard Klimeck, Tillmann Kubis, "In-surface confinement of topological insulator nanowire surface states", Appl. Phys. Lett., vol. 107, no. 12, pp. 121605, Sep. 2015
- [235] Parijat Sengupta, Hoon Ryu, Sunhee Lee, Yaohua Tan, Gerhard Klimeck, "Numerical guidelines for setting up a k.p simulator with applications to quantum dot heterostructures and topological insulators", Journal of Computational Electronics, 02 Aug 2015
- [234] Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "Tight-binding analysis of Si and GaAs ultrathin bodies with subatomic wave-function resolution", Phys. Rev. B 92, 085301 – Published 4 August 2015
- [233] Parijat Sengupta, Gerhard Klimeck, Enrico Bellotti, "The evaluation of non-topological components in Berry phase and momentum relaxation time in a gapped 3D topological insulator", J. Phys.: Condens. Matter 27 (2015) 335505
- [232] Muhammad Usman, C. Hill, Rajib Rahman, Gerhard Klimeck, Michelle Simmons, Sven Rogge, Lloyd Hollenberg, "Strain and electric field control of hyperfine interactions for donor spin qubits in silicon", PHYSICAL REVIEW B 91, 245209 (2015), Published 25 June 2015
- [231] Muhammad Usman, Rajib Rahman, Joe Salfi, Juanita Bocquel, Benoit Voisin, Sven Rogge, Gerhard Klimeck, Lloyd Hollenberg, "Donor hyperfine Stark shift and the role of central-cell corrections in tight-binding theory", Journal of Physics: Condensed Matter, 27 (2015) 154207 (7pp)
- [230] Hesameddin Ilatikhameneh, Gerhard Klimeck, Joerg Appenzeller, Rajib Rahman, "Scaling Theory of Electrically Doped 2D Transistors", IEEE Electron Device Letters, vol. 36, Issue: 7, Page(s): 726-728, July 2015
- [229] J. Mol, Joe Salfi, Rajib Rahman, Yuling Hsueh, Jill Miwa, Gerhard Klimeck, Michelle Simmons, Sven Rogge, "Interface-induced heavy-hole/light-hole splitting of acceptors in silicon", Appl. Phys. Lett. 106, 203110 (2015)
- [228] Ravi Vedula, Saumitra Mehrotra, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, Alejandro Strachan, "Optimal Ge/SiGe nanofin geometries for hole mobility enhancement: Technology limit from atomic simulations", J. Appl. Phys. 117, 174312 (2015)
- [227] Wenjun Li, Saima Sharmin, Hesameddin Ilatikhameneh, Rajib Rahman, Yeqing Lu, Jingshan Wang, Xiaodong Yan, Alan Seabaugh, Gerhard Klimeck, Debdeep Jena, Patrick Fay, "Polarization-Engineered III-Nitride Heterojunction Tunnel Field-Effect Transistors", IEEE Journal of Exploratory Solid-State Computational Devices and Circuits, Volume:1, Pages: 28 - 34, Dec. 2015
- [226] Hesameddin Ilatikhameneh, Bozidar Novakovic, Yaohua Tan, Gerhard Klimeck, Rajib Rahman, Joerg Appenzeller, "Tunnel field effect transistors in two dimensional transition metal dichalcogenides", IEEE Journal on Exploratory Solid-State Computational Devices and Circuits, vol. 1, Page(s):12-18, 14 April 2015
- [225] Arne Laucht, Juha Muhonen, Fahd Mohiyaddin, Rachpon Kalra, Juan Dehollain, Solomon Freer, Fay Hudson, Menno Veldhorst, Rajib Rahman, Gerhard Klimeck, Kohei Itoh, David Jamieson, Jeffrey McCallum, Andrew Dzurak, Andrea Morello, "Electrically controlling single-spin qubits in a continuous microwave field", Science Advances 10 Apr 2015: Vol. 1 no. 3 e1500022
- [224] Zhengping Jiang, Behtash Behin-Aein, Zoran Krivokapic, Michael Povolotskyi, Gerhard Klimeck, "Tunneling and Short Channel Effects in Ultrascaled InGaAs Double Gate MOSFETs", IEEE Transactions on Electron Devices, Volume:62, Issue: 2, Page(s): 525 - 531, Feb. 2015
- [223] Parijat Sengupta, Gerhard Klimeck, "The influence of proximity induced ferromagnetism, superconductivity and Fermi-velocity on evolution of Berry phase in Bi₂Se₃ topological insulator", Semicond. Sci. Technol. Volume:30, 045004

- [222] Mehdi Salmani-Jelodar, Saumitra Mehrotra, Hesameddin Ilatikhameneh, Gerhard Klimeck, "Design Guidelines for Sub-12 nm Nanowire MOSFETs", IEEE Transactions on Nanotechnology, vol. 14, Issue: 2, Page(s): 210 - 213, March 2015
- [221] Parijat Sengupta, Tillmann Kubis, Yaohua Tan, Gerhard Klimeck, "Proximity induced ferromagnetism, superconductivity, and finite-size effects on the surface states of topological insulator nanostructures", J. Appl. Phys. 117, 044304 (2015)
- [220] Bent Weber, Yui-Hong Tan, Gerhard Klimeck, Michelle Simmons, "Limits to Metallic Conduction in Atomic-Scale Quasi-One-Dimensional Silicon Wires", Phys. Rev. Lett. 113, 246802 – Published 10 December 2014
- [219] Pengyu Long, Michael Povolotskyi, Bozidar Novakovic, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, "Design and Simulation of Two-dimensional Superlattice Steep Transistors", IEEE ELECTRON DEVICE LETTERS., vol. 35, Issue: 12, Page(s): 1212 - 1214, Dec. 2014
- [218] Marcelo Kuroda, Zhengping Jiang, Michael Povolotskyi, Gerhard Klimeck, Dennis Newns, Glenn Martyna, "Anisotropic strain in SmSe and SmTe: Implications for electronic transport", Phys. Rev. B 90, 245124, Published 15 December 2014
- [217] Yu He, Yu Wang, Gerhard Klimeck, Tillmann Kubis, "Non-equilibrium Green's functions method: Non-trivial and disordered leads", Appl. Phys. Lett. 105, 213502 (2014)
- [216] Jarryd Pla, Fahd Mohiyaddin, Kuan Tan, Juan Dehollain, Rajib Rahman, Gerhard Klimeck, David Jamieson, Andrew Dzurak, Andrea Morello, "Coherent Control of a Single Silicon-29 Nuclear Spin Qubit", Phys. Rev. Lett. 113, 246801, Published 9 December 2014
- [215] Hoon Ryu, Sunhee Lee, Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, Lloyd Hollenberg, Michelle Simmons, Gerhard Klimeck, "A Tight-Binding Study of Single-Atom Transistors", Small, Volume 11, Issue 3 January 21, 2015 Pages 374–381
- [214] Yuling Hsueh, Holger Buch, Yaohua Tan, Yu Wang, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, Rajib Rahman, "Spin-lattice relaxation times of single donors and donor clusters in silicon", Phys. Rev. Lett. 113, 246406, Published 11 December 2014
- [213] Mehdi Salmani-Jelodar, S. Kim, K. , Gerhard Klimeck, "Transistor roadmap projection using predictive full-band atomistic modeling", Appl. Phys. Lett. 105, 083508 , published online 28 August 2014
- [212] Timothy Boykin, A. Ajoy, Hesameddin Ilatikhameneh, Michael Povolotskyi, Gerhard Klimeck, "Brillouin zone unfolding method for effective phonon spectra", Physical Review B 90, 205214 (2014)
- [211] Lynn Zentner, Michael Zentner, Victoria Farnsworth, Michael McLennan, Krishna Madhavan, Gerhard Klimeck, "nanoHUB.org: Experiences and Challenges in Software Sustainability for a Large Scientific Community", Published on 9 July 2014, Journal of Open Research Software, Volume: 2, Issue: 1: e19, pp. 1-5
- [210] SungGeun Kim, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Computational study of heterojunction graphene nanoribbon tunneling transistors with p-d orbital tight-binding method", Appl. Phys. Lett. 104, 243113 (2014)
- [209] Ali Razavieh, Parsian Mohseni, Kyoocho Jung, Saumitra Mehrotra, Saptarshi Das, Sergey Suslov, Xiuling Li, Gerhard Klimeck, David Janes, Joerg Appenzeller, "Effect of Diameter Variation on Electrical Characteristics of Schottky Barrier Indium Arsenide Nanowire Field Effect Transistors", ACS Nano, Publication Date (Web): 21 May 2014
- [208] Bent Weber, Yui-Hong Tan, Suddhasatta Mahapatra, Thomas Watson, Hoon Ryu, Rajib Rahman, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, "Spin blockade and exchange in Coulomb-confined silicon double quantum dots", Nature Nanotechnology 9, 430–435 (2014), Published online 13 April 2014
- [207] Ganesh Hegde, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "An environment-dependent semi-empirical tight binding model suitable for electron transport in bulk metals, metal alloys, metallic interfaces, and metallic nanostructures. I. Model and validation", JOURNAL OF APPLIED PHYSICS 115, 123703 (2014), published online 25 March 2014
- [206] Joe Salfi, J. Mol, Rajib Rahman, Gerhard Klimeck, Michelle Simmons, Lloyd Hollenberg, Sven Rogge, "Spatially resolving valley quantum interference of a donor in silicon", Nature Materials 13, 605–610 (2014), Published online 06 April 2014
- [205] Ganesh Hegde, Michael Povolotskyi, Tillmann Kubis, James Charles, Gerhard Klimeck, "An Environment-dependent Semi-Empirical Tight Binding Model Suitable for Electron Transport in Bulk Metals, Metal Alloys, Metallic Interfaces and Metallic Nanostructures II - Effect of Confinement and Homogeneous Strain on Cu Conductance", J. Appl. Phys. 115, 123703 (2014)
- [204] Bijesh Rajamohanam, Dheeraj Mohata, Yan Zhu, Mantu Hudait, Zhengping Jiang, Matthew Hollander, Gerhard Klimeck, Suman Datta, "Design, fabrication, and analysis of p-channel arsenide/antimonide hetero-junction tunnel transistors", Published online 23 January 2014, J. Appl. Phys. 115, 044502 (2014)
- [203] Anya Samek, Gerhard Klimeck, "A Field Experiment on Using Messaging and Virtual Rewards to Increase User Participation on NanoHUB.org", (May 13, 2013). Available at SSRN: <https://ssrn.com/abstract=2344049> or <http://dx.doi.org/10.2139/ssrn.2344049>

- [202] Krishna Madhavan, Lynn Zentner, Victoria Farnsworth, Swaroop Shivarajapura, Michael Zentner, Nathan Denny, Gerhard Klimeck, "nanoHUB.org: cloud-based services for nanoscale modeling, simulation, and education", *Nanotechnology Reviews*. Volume 2, Issue 1, Pages 107–117, ISSN (Online) 2191-9097, ISSN (Print) 2191-9089, January 2013
- [201] Dragica Vasileska, Gerhard Klimeck, Alejandra Magana, S. Goodnick, "Tool-Based Curricula and Visual Learning", *ELECTRONICS*, VOL. 17, NO. 2, DECEMBER 2013
- [200] Krishna Madhavan, Michael Zentner, Gerhard Klimeck, "Learning and research in the cloud", Published online 07 November 2013, *Nature Nanotechnology* 8, 786–789 (2013)
- [199] Jim Fonseca, Tillmann Kubis, Michael Povolotskyi, Bozidar Novakovic, A. Ajoy, Ganesh Hegde, Hesameddin Ilatikhameneh, Zhengping Jiang, Parijat Sengupta, Yaohua Tan, Gerhard Klimeck, "Efficient and realistic device modeling from atomic detail to the nanoscale", *Journal of Computational Electronics* December 2013, Volume 12, Issue 4, pp 592-600
- [198] Xueping Jiang, Neerav Kharche, Paul Kohl, Timothy Boykin, Gerhard Klimeck, Mathieu Luisier, Pulickel Ajayan, Saroj K.Nayak, "Giant Quasiparticle Bandgap Modulation in Graphene Nanoribbons Supported on Weakly Interacting Surfaces", *Appl. Phys. Lett.* 103, 133107 (2013)
- [197] Hoon Ryu, Sunhee Lee, Bent Weber, Suddhasatta Mahapatra, Lloyd Hollenberg, Michelle Simmons, Gerhard Klimeck, "Atomistic modeling of metallic nanowires in silicon", *Nanoscale*, 2013,5, 8666-8674, Received 10 Apr 2013, Accepted 02 Jul 2013, First published online 11 Jul 2013
- [196] C.H. Yang, A. Rossi, R. Ruskov, N.S. Lai, Fahd Mohiyaddin, S. Lee, C. Tahan, Gerhard Klimeck, Andrea Morello, Andrew Dzurak, "Spin-valley lifetimes in a silicon quantum dot with tunable valley splitting.", Received 11 January, Accepted 27 May, Published 27 June 2013 in *Nature Communications* 4, Article number: 2069
- [195] Christoph Deutsch, Hermann Detz, Tobias Zederbauer, Andrews, Pavel Klang, Tillmann Kubis, Gerhard Klimeck, Manfred Schuster, Werner Schrenk, Strasser, Karl Unterrainer, "Probing scattering mechanisms with symmetric quantum cascade lasers", Accepted February 14, Published: March 14, 2013 in *Optics Express*, Vol. 21, Issue 6, pp. 7209-7215
- [194] Parijat Sengupta, Tillmann Kubis, Yaohua Tan, Michael Povolotskyi, Gerhard Klimeck, "Design principles for HgTe based topological insulator devices", Published online 22 July, *J. Appl. Phys.* 114, 043702 (2013)
- [193] Mathieu Luisier, Timothy Boykin, Z. Ye, A. Martini, Gerhard Klimeck, Neerav Kharche, Xueping Jiang, Saroj K.Nayak, "Investigation of ripple-limited low-field mobility in large-scale graphene nanoribbons", *Appl. Phys. Lett.* Volume 102, Issue 25 (2013), Published online 26 June 2013
- [192] Hoon Ryu, Dukyun Nam, Bu-Young Ahn, JongSuk Lee, Kumwon Cho, Sunhee Lee, Gerhard Klimeck, Mincheol Shin, "Optical TCAD on the Net: A tight-binding study of inter-band light transitions in self-assembled InAs/GaAs quantum dot photodetectors", *Mathematical and Computer Modelling* Volume 58, Issues 1–2, July 2013, Pages 288–299, Financial IT & Security and 2010 International Symposium on Computational Electronics
- [191] Saumitra Mehrotra, Pengyu Long, Michael Povolotskyi, Gerhard Klimeck, "Atomistic simulation of phonon and alloy limited hole mobility in Si1-xGex nanowires", *Phys. Status Solidi RRL* 7, No. 10, 903–906 (2013)
- [190] Zhengping Jiang, Marcelo Kuroda, Yaohua Tan, Dennis Newns, Michael Povolotskyi, Timothy Boykin, Tillmann Kubis, Gerhard Klimeck, Glenn Martyna, "Electron transport in nano-scaled piezoelectronic devices", *Appl. Phys. Lett.* 102, 193501 (2013)
- [189] Saumitra Mehrotra, SungGeun Kim, Tillmann Kubis, Michael Povolotskyi, Mark Lundstrom, Gerhard Klimeck, "Engineering Nanowire n-MOSFETs at Lg < 8nm", *IEEE TRANSACTIONS ON ELECTRON DEVICES*, VOL. 60, Issue: 7, Page(s): 2171 - 2177, July 2013
- [188] Saumitra Mehrotra, Michael Povolotskyi, Doron Elias, Tillmann Kubis, Jeremy Law, Mark Rodwell, Gerhard Klimeck, "Simulation Study of Thin-Body Ballistic n-MOSFET Involving Transport in Mixed Γ -L valleys", *IEEE Electron Device Letters*, vol.34, Issue: 9, Page(s): 1196 - 1198, Sept. 2013
- [187] Fahd Mohiyaddin, Rajib Rahman, Rachpon Kalra, Gerhard Klimeck, Lloyd Hollenberg, Jarryd Pla, Andrew Dzurak, Andrea Morello, "Non-invasive spatial metrology of single-atom devices", *Nano Lett.*, Published April 9, 2013, 13 (5), pp 1903–1909
- [186] Ali Razavih, Saumitra Mehrotra, Navab Singh, Gerhard Klimeck, David Janes, Joerg Appenzeller, "Utilizing the Unique Properties of Nanowire MOSFETs for RF Applications", *Nano Lett.*, March 6, 2013 (Communication)
- [185] Floris Zwanenburg, Andrew Dzurak, Andrea Morello, Michelle Simmons, Lloyd Hollenberg, Gerhard Klimeck, Sven Rogge, Susan Coppersmith, Mark Eriksson, "Silicon Quantum Electronics", Published 10 July 2013 in *Reviews of Modern Physics*, Volume 85, Issue 3, 961–1019
- [184] Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Yu He, Zhengping Jiang, Gerhard Klimeck, Timothy Boykin, "Empirical tight binding parameters for GaAs and MgO with explicit basis through DFT mapping", *Journal of Computational Electronics*, January 2013

- [183] Ramon Salazar, Saumitra Mehrotra, Gerhard Klimeck, Navab Singh, Joerg Appenzeller, "Observation of 1D Behavior in Si Nanowires: Towards High-Performance TFETs", *Nano Lett.*, 2012, 12 (11), pp 5571–5575
- [182] Yamanishi Masamichi, Edamura Tadataka, Fujita Kazuue, Tillmann Kubis, Gerhard Klimeck, "Indirectly pumped 3.7 THz InGaAs/InAlAs quantum-cascade lasers grown by metal-organic vapor-phase epitaxy", accepted in *Optics Express*, 2012, Published August 27, 2012, Vol. 20, Issue 18, pp. 20647-20658 (2012)
- [181] Somaia Sylvia, Hong-Hyun Park, M. Khayer, Khairul Alam, Gerhard Klimeck, Roger Lake, "Material Selection for Minimizing Direct Tunneling in Nanowire Transistors", *IEEE TRANSACTIONS ON ELECTRON DEVICES*, VOL. 59, Issue: 8, Page(s): 2064 - 2069, Aug. 2012
- [180] Seung Park, Yang Liu, Neerav Kharche, Mehdi Salmani-Jelodar, Gerhard Klimeck, Mark Lundstrom, Mathieu Luisier, "Performance Comparisons of III-V and strained-Si in Planar FETs and Non-planar FinFETs at Ultra-short Gate Length (12nm)", *IEEE Transactions on Electron Devices*, vol. 59, Issue: 8, Page(s): 2107 - 2114, Aug. 2012
- [179] Hoon Ryu, Hong-Hyun Park, Mincheol Shin, Dragica Vasileska, Gerhard Klimeck, "Feasibility, Accuracy, and Performance of Contact Block Reduction method for multi-band simulations of ballistic quantum transport", *Journal of Applied Physics* 111, 063705 (2012), Published 21 March 2012
- [178] Stephen Cauley, Venkataramanan Balakrishnan, Gerhard Klimeck, Cheng-Kok Koh, "A two-dimensional domain decomposition technique for the simulation of quantum-scale devices", *Journal of Computational Physics* Volume 231, Issue 4, 20 February 2012, Pages 1293–1313
- [177] Muhammad Usman, Vittorianna Tasco, Maria Todaro, Milena Giorgi, Eoin O'Reilly, Gerhard Klimeck, Adriana Passaseo, "The polarization response in InAs quantum dots: theoretical correlation between composition and electronic properties", *IOP Nanotechnology*, Volume 23, Number 16, Published 2 April 2012
- [176] Zhengping Jiang, Neerav Kharche, Timothy Boykin, Gerhard Klimeck, "Effects of Interface Disorder on Valley Splitting in SiGe/Si/SiGe Quantum Wells", *Applied Physics Letters* Vol100 issue10, Mar 6, 2012
- [175] Qi Wang, Tao Liu, Tillmann Kubis, Gerhard Klimeck, "Design of three-well indirect pumping terahertz quantum cascade lasers for high optical gain based on nonequilibrium Green's function analysis", *Appl. Phys. Lett.* 100, 122110 (2012)
- [174] Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, Hoon Ryu, Sunhee Lee, Oliver Warschkow, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, "A single-atom transistor", *Nature Nanotechnology* 7, 242–246 (2012)
- [173] Woo-Suhl Cho, Mathieu Luisier, Dheeraj Mohata, Suman Datta, David Pawlik, Sean Rommel, Gerhard Klimeck, "Full Band Modeling of Homo-junction InGaAs Band-to-Band Tunneling Diodes including Band Gap Narrowing", *Applied Physics Letters* 100, 063504, Published 7 February 2012
- [172] Bent Weber, Suddhasatta Mahapatra, Hoon Ryu, Sunhee Lee, A. Fuhrer, T. Reusch, D. Thompson, W. C. T. Lee, Gerhard Klimeck, Lloyd Hollenberg, Michelle Simmons, "Ohm's Law Survives to the Atomic Scale", *Science* 335, 64 (2012)
- [171] Mehdi Salmani-Jelodar, Abhijeet Paul, Timothy Boykin, Gerhard Klimeck, "Calculation of Phonon Spectrum and Thermal Properties in Suspended $\text{InGa}_{1-x}\text{As}_x$ Nanowires", *Journal of Computational Electronics* March 2012, Volume 11, Issue 1, pp 22-28
- [170] Stephen Cauley, Mathieu Luisier, Venkataramanan Balakrishnan, Gerhard Klimeck, Cheng-Kok Koh, "Distributed non-equilibrium Green's function algorithms for the simulation of nanoelectronic devices with scattering", *Journal of Applied Physics*, V110, Issue: 4, 043713, Published: AUG 15 2011
- [169] SungGeun Kim, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Effects of Interface Roughness Scattering on Radio Frequency Performance of Silicon Nanowire Transistors", *Appl. Phys. Lett.* 99, 232107 (2011)
- [168] Abhijeet Paul, Shuaib Salamat, Changwook Jeong, Gerhard Klimeck, Mark Lundstrom, "An efficient algorithm to calculate intrinsic thermoelectric parameters based on Landauer approach", *Journal of Computational Electronics*, March 2012, Volume 11, Issue 1, pp 56-66
- [167] Sunhee Lee, Hoon Ryu, Huw Campbell, Lloyd Hollenberg, Michelle Simmons, Gerhard Klimeck, "Electronic structure of realistically extended, atomistically resolved disordered Si:P δ -doped layers", *Phys. Rev. B* 84, 205309 (2011) – Published November 14, 2011
- [166] R. Kotlyar, T. Linton, R. Rios, M. Giles, S. Cea, Kellin Kuhn, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Does the low hole transport mass in $\text{Si}_{1-x}\text{Ge}_x$ and $\text{Si}_{1-x}\text{Ge}_x$ nanowires lead to mobility enhancements at high field and stress: a self-consistent tight-binding study", *Journal of Applied Physics* Vol.111, Issue 12 published online 26 June 2012
- [165] Sebastian Steiger, Mehdi Salmani-Jelodar, Denis Areshkin, Abhijeet Paul, Tillmann Kubis, Michael Povolotskyi, Hong-Hyun Park, Gerhard Klimeck, "Enhanced valence force field model for the lattice properties of gallium arsenide", *Physical Review B*, Vol. 84, pg. 155204, Published 17 October 2011
- [164] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Influence of cross-section geometry and wire orientation on the phonon shifts in ultra-scaled Si nanowires", *J. Appl. Phys.* 110, 094308 (2011)

- [163] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Shape and orientation effects on the ballistic phonon thermal properties of ultra-scaled Si nanowires", *Journal of Applied Physics* 110, 114309 (2011), selected for the December 19, 2011 issue of *Virtual Journal of Nanoscale Science & Technology*, Published 6 December 2011
- [162] Sebastian Steiger, Michael Povolotskyi, Hong-Hyun Park, Tillmann Kubis, Gerhard Klimeck, "NEMO5: A Parallel Multiscale Nanoelectronics Modeling Tool", *IEEE Transactions on Nanotechnology*, Vol. 10, Issue: 6, Page(s): 1464 - 1474, Nov. 2011
- [161] Muhammad Usman, Tomoya Inoue, Yukihiro Harada, Gerhard Klimeck, Takashi Kita, "Experimental and atomistic theoretical study of degree of polarization from multilayer InAs/GaAs quantum dot stacks", *Physical Review B* 84, 115321, published September 23, 2011
- [160] Ganesh Hegde, Gerhard Klimeck, "Role of surface orientation on ALD Al₂O₃/GaAs interface structure and Fermi level pinning: a DFT study", *Applied Physics Letters* 99, 093508, Published 2 September 2011
- [159] Gabriel Lansbergen, Rajib Rahman, Jan Verduijn, Giuseppe Tettamanzi, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Lifetime enhanced transport in silicon due to spin and valley blockade", *Phys. Rev. Lett.* 107, 136602 – Published 19 September 2011
- [158] Rajib Rahman, Gabriel Lansbergen, Jan Verduijn, Giuseppe Tettamanzi, Seung Park, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Electric field reduced charging energies and two-electron bound excited states of single donors in silicon", *PHYSICAL REVIEW B* 84, 115428 (2011)
- [157] Abhijeet Paul, Gerhard Klimeck, "Strain effects on the phonon thermal properties of ultra-scaled Si nanowires", *APPLIED PHYSICS LETTERS* 99, 083115 (2011)
- [156] Abhijeet Paul, Giuseppe Tettamanzi, Sunhee Lee, Saumitra Mehrotra, Nadine Collaert, Sven Rogge, Gerhard Klimeck, "Interface trap density metrology from sub-threshold transport in highly scaled undoped Si n-FinFETs", *Journal of Applied Physics*. 110, 121301 (2011), 22 December 2011
- [155] Muhammad Usman, Yui-Hong Tan, Hoon Ryu, Shaikh Ahmed, Timothy Boykin, Gerhard Klimeck, Hubert Krenner, "Quantitative Excited State Spectroscopy of a Single InGaAs Quantum Dot Molecule through Multi-million Atom Electronic Structure Calculations", *Nanotechnology* 22 (2011) 315709 (14pp)
- [154] Neophytos Neophytou, Gerhard Klimeck, Hans Kosina, "Subband engineering for p-type silicon ultra-thin layers for increased carrier velocities: An atomistic analysis", *Journal of Applied Physics*, Vol 109, ppg: 053721 – 053726, Published 15 March 2011
- [153] Timothy Boykin, Mathieu Luisier, Gerhard Klimeck, Xueping Jiang, Neerav Kharche, Yu Zhou, Saroj K.Nayak, "Accurate Six-Band Nearest-Neighbor Tight-Binding Model for the π -Bands of Bulk Graphene and Graphene Nanoribbons", *J. Appl. Phys.* 109, 104304 (2011)
- [152] Giuseppe Tettamanzi, Abhijeet Paul, Sunhee Lee, Saumitra Mehrotra, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Sven Rogge, "Interface Trap Density Metrology of state-of-the-art undoped Si n-FinFETs", *Electron Device Letters*. 32,4 (2011)
- [151] Abhijeet Paul, Gerhard Klimeck, "Atomistic study of electronic structure of PbSe nanowires", *Applied Physics Letters* 98, 212105 (2011)
- [150] Rajib Rahman, Jan Verduijn, Gabriel Lansbergen, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Engineered valley-orbit splittings in quantum confined nanostructures in silicon", *Phys. Rev. B* 83, 195323
- [149] Neerav Kharche, Gerhard Klimeck, Dae-Hyun Kim, Jesús. Alamo, Mathieu Luisier, "Multiscale Metrology and Optimization of Ultra-Scaled InAs Quantum Well FETs", *IEEE Transactions on Electron Devices*, Volume:58, Issue: 7, Page(s): 1963 - 1971, July 2011
- [148] Saumitra Mehrotra, Abhijeet Paul, Gerhard Klimeck, "Atomistic Approach to Alloy Scattering in Si(1-x)Ge(x)", *Appl. Phys. Lett.* 98, 173503 (2011), Online Publication Date: 26 April 2011
- [147] Rajib Rahman, Seung Park, Gerhard Klimeck, Lloyd Hollenberg, "Stark tuning of the charge states of a two-donor molecule in silicon", *Nanotechnology* 22 225202
- [146] Muhammad Usman, Susannah Heck, Edmund Clarke, Peter Spencer, Hoon Ryu, Ray Murray, Gerhard Klimeck, "Experimental and Theoretical Study of Polarization-Dependent Optical Transitions in InAs Quantum Dots at Telecommunication-Wavelengths (1300-1500 nm)", *Journal of Applied Physics* 83 19 pages 104510, 26 May 2011
- [145] Abhijeet Paul, Gerhard Klimeck, "Tuning Lattice Thermal Conductance by Porosity Control in Ultrascaled Si and Ge Nanowires", *Applied Physics Letters* 98 8 pages 083106, published Feb. 22, 2011. arXiv:1012.1054, selected for the March 7, 2011 issue of *Virtual Journal of Nanoscale Science & Technology*
- [144] Shweta Deora, Abhijeet Paul, Bijesh R, Jeff Huang, Gerhard Klimeck, Gennadi Bersuker, Paul Krisch, Raj Jammy, "Intrinsic Reliability improvement in Biaxially Strained SiGe p-MOSFETs", *IEEE Electron Device Letters*, Vol. 32, Issue: 3, pages 255-257, March 2011
- [143] SungGeun Kim, Abhijeet Paul, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Full Three-Dimensional Quantum Transport Simulation of Atomistic Interface Roughness in Silicon Nanowire FETs", *IEEE Transactions on Electron Devices* (May 2011) Vol: 58 Issue:5, Page : 1371 - 1380

- [142] Martha Prada, Gerhard Klimeck, Robert Joynt, "Spin-orbit Splittings in Si/SiGe Quantum Wells: From Ideal Si Membranes to Realistic Heterostructures", *New Journal of Physics* 13 (2011) 013009
- [141] Tillmann Kubis, Saumitra Mehrotra, Gerhard Klimeck, "Design concepts of terahertz quantum cascade lasers: Proposal for terahertz laser efficiency improvements", *Appl. Phys. Lett.* 97, 261106 (2010)
- [140] Samarth Agarwal, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Adaptive quadrature for sharply spiked integrands", *Journal of Computation Electronics* vol 9 , No. 3-4, 252-255 (2010)
- [139] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Modified valence force field approach for phonon dispersion: from zinc-blende bulk to nanowires", *Journal of Computational Electronics* Volume 9, Numbers 3-4, 160-172, Abstract on arXiv:1009.6188
- [138] Rajib Rahman, Richard Muller, James Levy, Malcolm Carroll, Gerhard Klimeck, Andrew Greentree, Lloyd Hollenberg, "Coherent electron transport by adiabatic passage in an imperfect donor chain", *Phys. Rev. B.* (2010) Vol. 55, Issue 3
- [137] Hong-Hyun Park, Gerhard Klimeck, "Quantum approach to electronic noise calculations in the presence of electron-phonon interactions", *Phys. Rev.B*, Vol 81, 125328(2010)
- [136] Timothy Boykin, Mathieu Luisier, Gerhard Klimeck, "Current density and continuity in discretized models", *European Journal of Physics*, Vol 31, pg. 1077
- [135] Mincheol Shin, Sunhee Lee, Gerhard Klimeck, "Computational Study on the Performance of Si nanowire pMOSFETs based on the k.p method", *IEEE Transactions on Electron Devices*, Vol. 57, Issue: 9, Page(s): 2274 - 2283, Sept. 2010
- [134] Neophytos Neophytou, SungGeun Kim, Gerhard Klimeck, Hans Kosina, "On the bandstructure velocity and ballistic current of ultra-narrow silicon nanowire transistors as a function of cross section size, orientation, and bias", *J. Appl. Phys.*, Vol. 107, 113701 (2010)
- [133] Alejandro Strachan, Gerhard Klimeck, Mark Lundstrom, "Cyber-Enabled Simulations in Nanoscale Science and Engineering", *Computing in Science and Engineering*, Vol. 12, pg: 12-17 (2010)
- [132] Timothy Boykin, Mathieu Luisier, Mehdi Salmani-Jelodar, Gerhard Klimeck, "Strain-induced, off-diagonal, same-atom parameters in empirical tight-binding theory suitable for [110] uniaxial strain applied to a silicon parameterization", *Phys. Rev. B*, Vol 81, 125202 (2010)
- [131] Mathieu Luisier, Gerhard Klimeck, "Simulation of nanowire tunneling transistors: From the Wentzel-Kramers-Brillouin approximation to full-band phonon-assisted tunneling", *J. Appl. Phys.*, Vol. 107, 084507 (2010)
- [130] Samarth Agarwal, Gerhard Klimeck, Mathieu Luisier, "Leakage Reduction Design Concepts for Low Power Vertical Tunneling Field-Effect Transistors", *IEEE Electronic Device Letters*, Vol. 31, Issue: 6, Page(s):621 - 623, June 2010
- [129] Mathieu Luisier, Gerhard Klimeck, "Numerical Strategies towards Peta-Scale Simulations of Nanoelectronics Devices", *Parallel Computing (PARCO)*, Vol. 36, pg. 117-128 (2010)
- [128] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Performance Prediction of Ultra-scaled SiGe/Si Core/Shell Electron and Hole Nanowire MOSFETs", *IEEE Electron Device Letters*, Vol. 31, Issue: 4, Page(s): 278-280, April 2010
- [127] Gerhard Klimeck, Mathieu Luisier, "Atomistic Modeling of Realistically Extended Semiconductor Devices with NEMO/OMEN", *IEEE Computing in Science and Engineering (CISE)*, Vol.12, Issue: 2, Pages: 28-35, March-April 2010
- [126] Samarth Agarwal, Kyle Montgomery, Timothy Boykin, Gerhard Klimeck, Jerry Woodall, "Design Guidelines for True Green LEDs and High Efficiency Photovoltaics Using ZnSe/GaAs Digital Alloys", *Electrochemical and Solid-State Lett.*, Vol. 13, pp. H5-H7 (2010)
- [125] Muhammad Usman, Hoon Ryu, David Ebert, Gerhard Klimeck, "Moving towards nano-TCAD through multi-million atom quantum dot simulations matching experimental data", *IEEE Transactions on Nanotechnology*, Vol. 8, Issue: 3, Page(s): 330 - 344, May 2009
- [124] Giuseppe Tettamanzi, Abhijeet Paul, Gabriel Lansbergen, Jan Verduijn, Sunhee Lee, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Sven Rogge, "Thermionic Emission as a tool to study transport in undoped nFinFETs", *IEEE Electron Device Letters*, Vol. 31, Issue: 2, Page(s): 150 - 152, Feb. 2010
- [123] Mathieu Luisier, Gerhard Klimeck, "Atomistic Full-Band Simulations of Si Nanowire Transistors: Effects of Electron-Phonon Scattering", *Phys. Rev. B*, Vol. 80, 155430 (2009)
- [122] Rajib Rahman, Gabriel Lansbergen, Seung Park, Jan Verduijn, Gerhard Klimeck, Sven Rogge, Lloyd Hollenberg, "Orbital Stark effect and quantum confinement transition of donors in silicon", *Phys. Rev. B*, Vol. 80, 098936 (2009) arXiv 0904.4281
- [121] Rajib Rahman, Seung Park, Timothy Boykin, Gerhard Klimeck, Sven Rogge, Lloyd Hollenberg, "Gate induced g-factor control and dimensional transition for donors in multi-valley semiconductors", *Physical Review B*, Vol. 80 134935 (2009)
- [120] Seung Park, Rajib Rahman, Gerhard Klimeck, Lloyd Hollenberg, "Mapping donor electron wave function deformations at sub-Bohr orbit resolution", *Phys. Rev. Lett.*, Vol. 103, 106802 (2009)

- [119] Benjamin Haley, Gerhard Klimeck, Mathieu Luisier, Dragica Vasileska, Abhijeet Paul, Swaroop Shivarajapura, Diane Beaudoin, "Computational nanoelectronics research and education at nanoHUB.org", *Journal of Computational Electronics*, Vol. 8, pp. 124–131 (2009)
- [118] Rajib Rahman, Seung Park, Andrew Greentree, Richard Muller, Gerhard Klimeck, Lloyd Hollenberg, "Atomistic simulations of adiabatic coherent electron transport in triple donor systems", *Phys. Rev. B*, Vol. 80, 035302 (2009)
- [117] Mathieu Luisier, Gerhard Klimeck, "Performance analysis of statistical samples of graphene nanoribbon tunneling transistors with line edge roughness", *Applied Physics Lett.*, Vol. 94, 223505 (2009)
- [116] Hui Zhao, Raseong Kim, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, Fa-Jun Ma, Subhash Rustagi, Ganesh Samudra, Navab Singh, Guo-Qiang Lo, Dim-Lee Kwong, "Characterization and Modeling of Subfemtofarad Nanowire Capacitance Using the CBCM Technique", *IEEE Electron Device Letters*, Vol. 30, Issue: 5, Page(s): 526-528, May 2009
- [115] Mathieu Luisier, Gerhard Klimeck, "Atomistic, Full-Band Design Study of InAs Band-to-Band Tunneling Field-Effect Transistors", *IEEE Electron Device Letters*, Vol. 30, Issue: 6, Page(s): 602-604, June 2009
- [114] Gerhard Klimeck, Neophytos Neophytou, "Design Space for Low Sensitivity to Size Variations in [110] PMOS Nanowire Devices: The Implications of Anisotropy in the Quantization Mass", *Nano Lett.*, Vol. 9, pp. 623–630, Published January 13, 2009
- [113] Neerav Kharche, Seongmin Kim, Timothy Boykin, Gerhard Klimeck, "Valley Degeneracies in (111) Silicon Quantum Wells", *Applied Physics Lett.*, Vol. 94, 042101 (2009)
- [112] Timothy Boykin, Neerav Kharche, Gerhard Klimeck, "Non-primitive rectangular cells for tight-binding electronic structure calculations", *Physica E*, Vol. 41, pp. 490-494 (2009)
- [111] Amritanshu Palaria, Gerhard Klimeck, Alejandro Strachan, "Structures and energetics of Silicon nanotubes from molecular dynamics and density functional theory", *Phys. Rev. B*, Vol. 78, 205315 (2008)
- [110] Mark Lundstrom, Gerhard Klimeck, George Adams III., Michael McLennan, "HUB is where the heart is", *IEEE Nanotechnology Magazine*, Vol. 2, Issue: 1, Page(s): 28-31, March 2008
- [109] Neophytos Neophytou, Abhijeet Paul, Gerhard Klimeck, "Bandstructure Effects in Silicon Nanowire Hole Transport", *IEEE Transactions on Nanotechnology*, Vol. 7, Issue: 6, Page(s): 710-719, Nov. 2008, - Special issue on nanowires
- [108] Nancy Wilkins-Diehr, Dennis Gannon, Gerhard Klimeck, Scott Oster, Sudhakar Pamidighantam, "TeraGrid Science Gateways and Their Impact on Science", *IEEE Computer*, Vol. 41, Issue: 11, Page(s): 32-41, June 2008
- [107] Raseong Kim, Neophytos Neophytou, Abhijeet Paul, Gerhard Klimeck, Mark Lundstrom, "Dimensionality in metal-oxide-semiconductor field-effect transistors: A comparison of one-dimensional and two-dimensional ballistic transistors", *J. Vac. Sci. Technol. B*, Vol. 26, pp. 1628-1631 (2008)
- [106] Srikant Srinivasan, Gerhard Klimeck, Leonid Rokhinson, "Valley splitting in Si quantum dots embedded in SiGe", *Applied Physics Letters*, Vol. 93, pg. 112102 (2008)
- [105] Marek Korkusinski, Pawel Hawrylak, M. Zielinski, W. Sheng, Gerhard Klimeck, "Building semiconductor nanostructures atom by atom", *Microelectronics Journal* Vol. 39 pg. 318-326 (2008)
- [104] Shaikh Ahmed, Neerav Kharche, Rajib Rahman, Muhammad Usman, Sunhee Lee, Hoon Ryu, Hansang Bae, Steven Clark, Benjamin Haley, Maxim Naumov, Faisal Saied, Marek Korkusinski, Rick Kennel, Michael McLennan, Timothy Boykin, Gerhard Klimeck, "Multimillion Atom Simulations with NEMO 3-D", *Springer Encyclopedia for Complexity*, pp 5745-5783, 2008, Published 2009
- [103] Song Li, Shaikh Ahmed, Gerhard Klimeck, Eric Darve, "Computing entries of the inverse of a sparse matrix using the FIND algorithm", *Journal of Computational Physics*, Vol 227, pp. 9408-9427 (2008)
- [102] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, J. Caro, Nadine Collaert, Serge Biesemans, Jerry Woodall, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Gate induced quantum confinement transition of a single dopant atom in a Si FinFET", *Nature Physics*, Vol. 4, pg. 656 (2008)
- [101] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Bandstructure Effects in Silicon Nanowire Electron Transport", *IEEE Transaction on Electron Devices*, Vol. 55, Issue: 6, Page(s): 1286 - 1297, June 2008, pg. 1286 - 1297
- [100] Yang Liu, Neophytos Neophytou, Gerhard Klimeck, Mark Lundstrom, "Band-Structure Effects on the Performance of III-V Ultrathin-body SOI MOSFETs", *IEEE Transaction on Electron Devices*, Vol. 55, Issue 5, Page(s): 1116 - 22, May 2008
- [99] Gianluca Fiori, Giuseppe Iannaccone, Gerhard Klimeck, "Corrections to: A Three-Dimensional Simulation Study of the Performance of Carbon Nanotube Field-Effect Transistors With Doped Reservoirs and Realistic Geometry", *IEEE Transaction on Electron Devices*, Vol. 55, Issue: 4, Page(s): 1094 - 1095, April 2008
- [98] Gerhard Klimeck, Michael McLennan, Sean Brophy, George Adams III., Mark Lundstrom, "nanoHUB.org: Advancing Education and Research in Nanotechnology", *IEEE Computers in Engineering and Science (CISE)*, Vol. 10, Issue: 5, Page(s): 17 - 23, Sept.-Oct. 2008

- [97] Timothy Boykin, Mathieu Luisier, Gerhard Klimeck, "Multiband transmission calculations for nanowires using an optimized renormalization method", *Phys Rev B*, Vol. 77, 165318 (2008)
- [96] Maxim Naumov, Sunhee Lee, Benjamin Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Steven Clark, Gerhard Klimeck, "Eigenvalue Solvers for Atomistic Simulations of Electronic Structures with NEMO-3D", *Journal of Computational Electronics*, 2008, Vol. 7, pg. 297-300 (2008)
- [95] Roksana Golizadeh-Mojarad, A.N.M. Zainuddin, Shaikh Ahmed, Gerhard Klimeck, Supriyo Datta, "Atomistic Non-equilibrium Green's Function Simulations of Graphene Nano-Ribbons in the Quantum Hall Regime", *Journal of Computational Electronics*, 2007, Vol. 7, pg. 407-410 (2008)
- [94] Neerav Kharche, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Electronic Structure and Transmission Characteristics of SiGe Nanowires", *Journal of Computational Electronics*, 2007, Vol. 7, pg. 350-354 (2008)
- [93] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Simulation of nanowire transistors: Atomistic vs. Effective Mass Models", *Journal of Computational Electronics*, 2007, Vol. 7, pg. 363-366 (2008)
- [92] Bhaskaran Muralidharan, Hoon Ryu, Zhen Huang, Gerhard Klimeck, "NEMO-3D based Atomistic Simulation of a Double Quantum Dot Structure for Spin-Blockaded Transport", *Journal of Computational Electronics*, Vol 7, pg. 403-406 (2008)
- [91] Yang Liu, Neophytos Neophytou, Tony Low, Gerhard Klimeck, Mark Lundstrom, "A Tight-binding Study of the Ballistic Injection Velocity for Ultrathin-body SOI MOSFETs", *IEEE Transaction on Electron Devices*, Vol. 55, Issue: 3, Page(s): 866 - 871, March 2008
- [90] Timothy Boykin, Neerav Kharche, Gerhard Klimeck, "Valley Splitting in Finite Barrier Quantum Wells", *Phys. Rev. B*, Vol. 77, 245320 (2007)
- [89] Rajib Rahman, Cameron. Wellard, Forrest Bradbury, Martha Prada, Gerhard Klimeck, Lloyd Hollenberg, "High precision quantum control of single donor spins in Si", *Physical Review Letters*, Vol 99, pg 036403 (2007)
- [88] Timothy Boykin, Neerav Kharche, Gerhard Klimeck, "Brillouin-zone unfolding of perfect supercells having nonequivalent primitive cells illustrated with a Si / Ge tight-binding parameterization", *Phys. Rev. B* Vol 76, 035310 (2007)
- [87] Ahmet Yanik, Gerhard Klimeck, Supriyo Datta, "Quantum Transport with Spin Dephasing: A Nonequilibrium Green's function Approach", *Phys. Rev.* Vol. 76, 045213 (2007)
- [86] Gerhard Klimeck, Shaikh Ahmed, Neerav Kharche, Marek Korkusinski, Muhammad Usman, Martha Prada, Timothy Boykin, "Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D: Part II - Applications", *IEEE Transactions on Electron Devices*, Vol. 54, Issue 9, Page(s):2090 - 2099, Sept. 2007, (INVITED) Special Issue on Nanoelectronic Device Modeling
- [85] Gerhard Klimeck, Shaikh Ahmed, Hansang Bae, Neerav Kharche, Rajib Rahman, Steven Clark, Benjamin Haley, Sunhee Lee, Maxim Naumov, Hoon Ryu, Faisal Saied, Martha Prada, Marek Korkusinski, Timothy Boykin, "Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D: Part I - Models and Benchmarks", *IEEE Transactions on Electron Devices*, Vol. 54, Issue 9, Page(s):2079 - 2089, Sept. 2007, (INVITED) Special Issue on Nanoelectronic Device Modeling
- [84] Timothy Boykin, Neerav Kharche, Gerhard Klimeck, "Evolution Time and Energy Uncertainty", *Eur. J. Phys.* 28 (2007) 673-678 (2007)
- [83] Neophytos Neophytou, Shaikh Ahmed, Gerhard Klimeck, "Influence of Vacancies on Metallic Nanotube Transport Properties", *Applied Physics Letters*, Vol 90, 182119 (2007)
- [82] Gianluca Fiori, Giuseppe Iannaccone, Gerhard Klimeck, "Coupled mode space approach for the simulation of realistic Carbon Nanotube Field Effect Transistors", *IEEE Transaction on Nanotechnology*, Vol. 6, Issue: 4, Page(s): 475 - 480, July 2007
- [81] Gengchiao Liang, Jie Xiang, Neerav Kharche, Gerhard Klimeck, Charles Lieber, Mark Lundstrom, "Performance Analysis of a Ge/Si Core/Shell Nanowire Field Effect Transistor", *Nano letters*, Vol. 7, 642-646 (2007)
- [80] Shaikh Ahmed, Gerhard Klimeck, Derrick Kearney, Michael McLennan, M. Anantram, "Quantum Simulations of Dual Gate MOSFET Devices: Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org", *Journal of High Speed Electronics and Systems*, Vol. 17, No 3, pp. 485-494 (2007)
- [79] Neerav Kharche, Martha Prada, Timothy Boykin, Gerhard Klimeck, "Valley-splitting in strained Silicon quantum wells modeled with 2 miscuts, step disorder, and alloy disorder", *Applied Phys. Lett.* Vol. 90, 092109 (2007)
- [78] Clemens Heitzinger, Gerhard Klimeck, "Computational aspects of the three-dimensional feature-scale simulation of silicon-nanowire field-effect sensors for DNA detection", *Journal of Computational Electronics*, Vol. 6, pg. 387-390, (2007)
- [77] Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, Gerhard Klimeck, "Transport Calculation of Semiconductor Nanowires Coupled to Quantum Well Reservoirs", *Journal of Computational Electronics*, Vol. 6, pg. 199-202, 2007

- [76] Vladimir Mitin, Nizami Vagidov, Mathieu Luisier, Gerhard Klimeck, "Energy Dispersion Relations for Holes in Silicon Quantum Wells and Quantum Wires", *Journal of Computational Electronics* Vol. 6, pg. 227-230, 2007
- [75] Timothy Boykin, Neerav Kharche, Gerhard Klimeck, Marek Korkusinski, "Approximate bandstructures of semiconductor alloys from tight-binding supercell calculations", *J. Phys.: Condens. Matter* 19 (2007) 036203 (14pp)
- [74] Timothy Boykin, Mathieu Luisier, Andreas Schenk, Neerav Kharche, Gerhard Klimeck, "The electronic Structure and Transmission Characteristics of AlGaAs Nanowires", *IEEE Transactions on Nanotechnology*, Vol. 6, Issue: 1, Page(s): 43 - 47, Jan. 2007
- [73] Neophytos Neophytou, Shaikh Ahmed, Gerhard Klimeck, "Non-Equilibrium Green's Function (NEGF) Simulation of Metallic Carbon Nanotubes including Vacancy Defects", *Journal of Computational Electronics*, Vol. 6, pg. 317-320, 2006
- [72] Wei Qiao, Michael McLennan, Rick Kennel, David Ebert, Gerhard Klimeck, "Hub-based Simulation and Graphics Hardware Accelerated Visualization for Nanotechnology Applications", *IEEE Transactions on Visualization and Computer Graphics*, Vol. 12, Issue: 5, Page(s): 1061-1068, Sept.-Oct. 2006
- [71] Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, Gerhard Klimeck, "Atomistic Simulation of Nanowires in the sp³d⁵s* Tight-Binding Formalism: from Boundary Conditions to Strain Calculations", *Phys. Rev. B* 74, 205323 (2006)
- [70] Gianluca Fiori, Giuseppe Iannaccone, Gerhard Klimeck, "A Three-dimensional simulation study of the performance of Carbon Nanotube Field Effect Transistors with doped reservoirs and realistic geometry", *IEEE Transactions on Electron Devices*, vol. 53, Issue: 8, Page(s): 1782 - 1788, Aug. 2006
- [69] Marek Korkusinski, Gerhard Klimeck, "Atomistic simulations of long-range strain and spatial asymmetry molecular states of seven quantum dots", *Journal of Physics: Conference Series* Vol. 38, pg 75-78 (2006)
- [68] Timothy Boykin, Neerav Kharche, Gerhard Klimeck, "Allowed wavevectors under the application of incommensurate periodic boundary conditions", *European Journal of Physics*, vol 27, p 5 (2006)
- [67] V. Drachev, H.-K. Yuan, A. Sarychev, A. Kildishev, Gerhard Klimeck, V. Shalaev, "Experimental verification of an optical negative-index material", *Laser Phys. Lett.* Vol. 3, 49-55 (2006)
- [66] A. Martins, Timothy Boykin, Gerhard Klimeck, Belita Koiller, "Conduction-band tight-binding description for silicon applied to P donors", *Phys. Rev. B* Vol. 72 pg. 193204 (2005)
- [65] Yong Joe, Arkady Satanin, Gerhard Klimeck, "Interactions of Fano resonances in the transmission for an Aharonov-Bohm ring with two embedded quantum dots in the presence of a magnetic field", *Physical Review B*, Vol. 72, pg. 115310 (2005)
- [64] Timothy Boykin, Gerhard Klimeck, "The discretized Schrödinger equation for the finite square well and its relationship to solid state physics", *European Journal of Physics*, Vol. 26 pp. 865-881(2005)
- [63] Jing Wang, Anisur Rahman, Avik Ghosh, Gerhard Klimeck, Mark Lundstrom, "On the Validity of the Parabolic Effective-Mass Approximation for the I-V Calculation of Silicon Nanowire Transistors", *IEEE Transactions on Electron Devices*, Volume:52, Issue: 7, Page(s): 1589-1595, July 2005
- [62] Yun Zheng, Christian Rivas, Roger Lake, Khairul Alam, Timothy Boykin, Gerhard Klimeck, "Electronic Properties of Silicon Nanowires", *IEEE Transactions on Electron Devices*, Vol. 52, Issue: 6, Page(s): 1097-1103, June 2005
- [61] Jeremy Green, Timothy Boykin, Corrie Farmer, Michel Garcia, Charles Ironside, Gerhard Klimeck, Roger Lake, Colin Stanley, "Quantum cascade laser gain medium modeling using a second-nearest-neighbor sp³s* tight-binding model", *Superlattices and Microstructures*, Vol. 37, pg. 410-424 (2005)
- [60] Timothy Boykin, Gerhard Klimeck, Paul Allmen, Seungwon Lee, Fabiano Oyafuso, "Valley-splitting in V-shaped quantum wells", *Journal of Applied Physics*, Vol. 97, pg. 113702 (2005)
- [59] Jing Wang, Anisur Rahman, Avik Ghosh, Gerhard Klimeck, Mark Lundstrom, "Performance Evaluation of Ballistic Silicon Nanowire Transistors with Atomic-basis Dispersion Relations", in *Applied Phys. Lett.* Vol. 86 (9): Art. No. 093113 (2005)
- [58] Timothy Boykin, Gerhard Klimeck, "Practical Application of Zone-Folding Concepts in Tight-Binding calculations", *Physical Review B*, V71, 115215 (2005)
- [57] Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, Nizami Vagidov, Timothy Boykin, "Atomistic Approach for NanoScale Devices at the Scaling Limit and Beyond - Valley Splitting in Si", *Japanese Journal of Applied Physics* Vol. 44, No. 4B, pp. 2187-2190 (2005)

Work Performed at JPL (32 Total)

- [56] Seungwon Lee, Paul Allmen, Fabiano Oyafuso, Gerhard Klimeck, K. Whaley, "Effect of electron-nuclear spin interactions on electron-spin qubits localized in self-assembled quantum dots", *Journal of Applied Physics*, Vol. 97, 043706 (2005)
- [55] Carl Gardner, Gerhard Klimeck, Christian Ringhofer, "Smooth Quantum Hydrodynamic Model vs. NEMO Simulation of a Resonant Tunneling Diode", *Journal of Computational Electronics*, Vol. 3, No. 2, 95-102, 2004

- [54] Timothy Boykin, Gerhard Klimeck, Mark Eriksson, Mark Friesen, Susan Coppersmith, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, "Valley splitting in low-density quantum-confined heterostructures studied using tight-binding models", *Phys. Rev. B*. Vol. 70, 165325 (2004)
- [53] Olga Lazarenkova, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, Gerhard Klimeck, "Effect of anharmonicity of the strain energy on band offsets in semiconductor nanostructures", *Appl. Phys. Lett.* 85, 4193 (2004)
- [52] Seungwon Lee, Olga Lazarenkova, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Effect of wetting layers on the strain and electronic structure of InAs self-assembled quantum dots", *Phys. Rev. B*. Vol. 70, pg. 125307 (2004)
- [51] Timothy Boykin, Gerhard Klimeck, "The discretized Schrodinger equation and simple models for semiconductor quantum wells", *Eur. J. Phys.*, Vol. 25 No 4, 503-514 (2004)
- [50] Olga Lazarenkova, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, Gerhard Klimeck, "An atomistic model for the simulation of acoustical phonons, strain distribution, and Grüneisen coefficients in zinc-blende semiconductors", *Superlattices and Microstructures*, Vol 34, pg. 553-556 (2004)
- [49] Seungwon Lee, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures", *Phys. Rev. B* 69, 045316 (2004)
- [48] Timothy Boykin, Gerhard Klimeck, Fabiano Oyafuso, "Valence band effective mass expressions in the sp³d⁵s* empirical tight-binding model applied to a new Si and Ge parameterization", *Phys. Rev. B*. 69, 115201, No 11 (2004)
- [47] Timothy Boykin, Gerhard Klimeck, Mark Eriksson, Mark Friesen, Susan Coppersmith, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, "Valley splitting in strained silicon quantum wells", *Applied Physics Letters*, Vol. 84, pg. 115-117, 2004
- [46] Gerhard Klimeck, "Quantum and semi-classical transport in RTDs in NEMO 1-D", *Journal of Computational Electronics*, Vol 2, pg. 177-182, 2003
- [45] Christian Rivas, Roger Lake, William Frensley, Gerhard Klimeck, Phillip Thompson, Karl Hobart, Sean Rommel, Paul Berge, "Full Band Modeling of the Excess Current in a Delta-Doped Silicon Tunnel Diode", *Journal of Appl. Phys.*, Vol 94, No. 8, pg 5005-5013 (2003)
- [44] Fabiano Oyafuso, Gerhard Klimeck, Paul Allmen, Timothy Boykin, R. Bowen, "Strain Effects in large-scale atomistic quantum dot simulations", *Phys. Stat. Sol. (b)*, Vol. 239, p 71-79 (2003)
- [43] Titus Sandu, Gerhard Klimeck, Wiley Kirk, "Off-Center Electron Transport in Resonant Tunneling Diodes due to Incoherent Scattering", *Phys. Rev. B*. Vol 68, pg 115320, (2003)
- [42] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, Paul Allmen, "Disorder Induced Broadening in Multimillion Atom Alloyed Quantum Dot Systems", *Phys. Stat. Sol. (c)*, vol 0004, pg 1149-1152 (2003)
- [41] Gerhard Klimeck, Fabiano Oyafuso, R. Bowen, Timothy Boykin, Thomas Cwik, Edith Huang, Edward Vinyard, "3-D Atomistic Nanoelectronic Modeling on High Performance Clusters: Multimillion Atom Simulations", *Superlattices and Microstructures*, Vol 31/2, pg 171-179, 2002
- [40] Gerhard Klimeck, "Parallelization of the Nanoelectronic Modeling Tool (NEMO 1-D) on a Beowulf Cluster", *Journal of Computational Electronics*, Vol 1, Issue 1-2, pp 75-79 (2002)
- [39] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", *Journal of Computational Electronics*, Vol 1. Issue 3, pp. 317-321 (2002)
- [38] Seungwon Lee, Jeungnim Kim, Lars Jönsson, John Wilkins, Garnett Bryant, Gerhard Klimeck, "Many-body levels of multiply charged and laser-excited InAs nanocrystals modeled by empirical tight binding", *Phys. Rev. B* 66, 235307 (2002)
- [37] Timothy Boykin, Gerhard Klimeck, R. Bowen, Fabiano Oyafuso, "Diagonal parameter shifts due to nearest-neighbor displacements in empirical tight-binding theory", *Phys. Rev. B* 66, 125207 (2002)
- [36] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, Paul Allmen, "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots (INVITED)", *Computer Modeling in Engineering and Science (CMES)* Volume 3, No. 5 pp 601-642 (2002)
- [35] Timothy Boykin, R. Bowen, Gerhard Klimeck, "Electromagnetic coupling and gauge invariance in the empirical tight-binding method", *Physical Review B*, Vol 63, pg. 245314 (2001)
- [34] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Strong wavevector dependence of hole transport in heterostructures", *Superlattices and Microstructures*, Vol 29, No. 3, pg. 187-216 (2001)
- [33] Seungwon Lee, Lars Jönsson, John Wilkins, Garnett Bryant, Gerhard Klimeck, "Electron-hole correlations in semiconductor quantum dots with tight-binding wave functions", *Phys. Rev. B* Vol. 63, 195318 (2001)
- [32] Gerhard Klimeck, "Indirect bandgap-like current flow in direct bandgap electron resonant tunneling diodes", *Physica Status Solidi (b)* Vol. 226, pg. 9-19 (2001)
- [31] Christian Rivas, Roger Lake, Gerhard Klimeck, William Frensley, Massimo Fischetti, Phillip Thompson, Sean Rommel, Paul Berge, "Full Band Simulation of Indirect Phonon-Assisted Tunneling in a Silicon Tunnel Diode with Delta-Doped Contacts", *Applied Physics Letters*, Vol. 78, pg 814, (2001)

- [30] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Off-zone-center (indirect bandgap like) hole transport in heterostructures", *Phys. Rev. B.*, Vol 63, pg. 195310 (2001)
- [29] Gerhard Klimeck, R. Bowen, Timothy Boykin, Thomas Cwik, "sp³s* Tight-Binding Parameters for Transport Simulations in Compound Semiconductors", *Superlattices and Microstructures* Vol. 27, pp. 519-524 (2000)
- [28] Gerhard Klimeck, R. Bowen, Timothy Boykin, Carlos Salazar-Lazaro, Thomas Cwik, Adrian Stoica, "Si tight-binding parameters from genetic algorithm fitting", *Superlattices and Microstructures*, Vol. 27, No. 2/3, Mar 2000, pp. 77-88.
- [27] Timothy Boykin, R. Bowen, Gerhard Klimeck, Kevin Lear, "Resonant-tunneling Diodes with Emitter Prewells", *Appl. Phys. Lett.*, Vol. 75, 1302 (1999)
- [26] Timothy Boykin, Lisa Gamble, Gerhard Klimeck, R. Bowen, "Valence-Band Warping in Tight-Binding Models", *Phys. Rev. B* Vol 59, 7301 (1999)
- [25] Timothy Boykin, Roger Lake, Gerhard Klimeck, Mukund Swaminathan, "Interface Effects in Tunneling Models with Identical Real and Complex Dispersions", *Phys. Rev. B* Vol 59, 7316 (1999)

Work Performed at UTD/TI (16 Total)

- [24] Gerhard Klimeck, Daniel Blanks, Roger Lake, R. Bowen, Chenjing Fernando, Manhua Leng, William Frensley, Dejan Jovanovic, Paul Sotirelis, "Writing Research Software in a Large Group for the NEMO Project", *VLSI Design*, Vol 8, p 79 (1998)
- [23] Sean Rommel, Thomas Dillon, M. Dashiell, H. Feng, J. Kolodzey, Paul Berge, Phillip Thompson, Karl Hobart, Roger Lake, Alan Seabaugh, Gerhard Klimeck, Daniel Blanks, "Room temperature operation of epitaxially grown Si/Si_{0.5}Ge_{0.5}/Si resonant interband tunneling diodes", *Applied Physics Letters*, Vol. 73, 2191 (1998)
- [22] Gerhard Klimeck, Roger Lake, Daniel Blanks, "Numerical Approximations to the Treatment of Interface Roughness Scattering in Resonant Tunneling Diodes", *Semicond. Sci. Technology*, Vol 13, pg. A165 (1998)
- [21] Roger Lake, Gerhard Klimeck, Daniel Blanks, "Interface Roughness and Polar Optical Phonon Scattering in InGaAs/AlAs/InAs RTDs", *Semicond. Sci. Technology*, Vol 13, pg. A163 (1998)
- [20] Gerhard Klimeck, Roger Lake, R. Bowen, Chenjing Fernando, William Frensley, "Resolution of Resonances in a General Purpose Quantum Device Simulator (NEMO)", *VLSI Design*, Vol. 6, p. 107 (1998)
- [19] Roger Lake, Gerhard Klimeck, R. Bowen, Dejan Jovanovic, Paul Sotirelis, William Frensley, "A Generalized Tunneling Formula for Quantum Device Modeling", *VLSI Design*, Vol. 6, pg 9 (1998)
- [18] Gerhard Klimeck, Roger Lake, Daniel Blanks, "Role of interface roughness scattering in self-consistent resonant tunneling diode simulation", *Phys. Rev. B*, Vol. 58, 7279 (1998)
- [17] Timothy Boykin, Gerhard Klimeck, R. Bowen, Roger Lake, "Effective Mass Reproducibility of the Nearest-Neighbor sp³s* Models: Analytic Results", *Phys. Rev. B* Vol 56, 4102 (1997)
- [16] Gerhard Klimeck, Roger Lake, Daniel Blanks, Chenjing Fernando, R. Bowen, Ted Moise, Y. Kao, "The Effects of Electron Screening Length and Emitter Quasi-Bound States on the Polar-Optical Phonon Scattering in Resonant Tunneling Diodes", *Physica Status Solidi (b)*, Vol 204, 408 (1997)
- [15] Roger Lake, Gerhard Klimeck, R. Bowen, Dejan Jovanovic, Daniel Blanks, Mukund Swaminathan, "Quantum Transport with Band-Structure and Schottky Contacts", *Physica Status Solidi (b)*, Vol 204, 354 (1997)
- [14] Roger Lake, Gerhard Klimeck, R. Bowen, Dejan Jovanovic, "Single and multiband modeling of quantum electron transport through layered semiconductor devices", *J. of Appl. Phys.* 81, 7845 (1997)
- [13] R. Bowen, Gerhard Klimeck, Roger Lake, William Frensley, Ted Moise, "Quantitative Simulation of A Resonant Tunneling Diode", *J. of Appl. Phys.* 81, 3207 (1997)
- [12] Roger Lake, Gerhard Klimeck, R. Bowen, Chenjing Fernando, Manhua Leng, Ted Moise, Y. Kao, "Interface Roughness, Polar Optical Phonon, And the Valley Current of a Resonant Tunneling Diode", *Superlattices and Microstructures*, Vol. 20, p.279 (1996)
- [11] Jim Tatum, Duncan MacFarlane, R. Bowen, Gerhard Klimeck, William Frensley, "Ultrafast Characteristics of InGaP/InGaAlP Laser Amplifiers", *IEEE Journal of Quantum Electronics*, Vol. 32, Issue: 4, Page(s): 664 - 669, Apr 1996
- [10] Gerhard Klimeck, Roger Lake, R. Bowen, William Frensley, Ted Moise, "Quantum Device Simulation with a Generalized Tunneling Formula", *Appl. Phys. Lett.*, Vol. 67, p.2539 (1995)
- [9] R. Bowen, William Frensley, Gerhard Klimeck, Roger Lake, "Transmission resonances and zeros in multi-band models", *Phys. Rev. B.*, Vol. 52, p.2754 (1995)

Work Performed in Graduate School (8 Total)

- [8] Gerhard Klimeck, Roger Lake, Supriyo Datta, Garnett Bryant, "Elastic and Inelastic Scattering in Quantum Dots in the Coulomb Blockade Regime", *Phys. Rev. B*, Vol. 50, 5484 (1994)
- [7] Guanlong Chen, Gerhard Klimeck, Supriyo Datta, G. Chen, William Goddard, "Resonant Tunneling through Quantum Dot arrays", *Phys. Rev. B*, Vol. 50, p.8035 (1994)
- [6] Gerhard Klimeck, Guanlong Chen, Supriyo Datta, "Conductance Spectroscopy in Coupled Quantum Dots", *Phys. Rev. B*, Vol. 50, p.2316 (1994)

- [5] Roger Lake, Gerhard Klimeck, M. Anantram, Supriyo Datta, "Rate Equations for the Phonon Peak in Resonant Tunneling Structures", Phys. Rev. B., Vol. 48, p.15132 (1993)
- [4] Roger Lake, Gerhard Klimeck, Supriyo Datta, "Rate Equations from the Keldysh Formalism Applied to the Phonon Peak in Resonant-Tunneling Diodes", Phys. Rev. B, Vol. 47, p.6427 (1993)
- [3] Yong Lee, Michael McLennan, Gerhard Klimeck, Roger Lake, Supriyo Datta, "Quantum Kinetic Analysis of Mesoscopic Systems: Linear Response", Superlattices and Microstructures, Vol. 11, p.137 (1992)
- [2] Gerhard Klimeck, Daniel Elliott, M. Hamilton, "Laser-Bandwidth-Induced Fluctuations in the Intensity Transmitted by a Fabry-Perot Interferometer", Phys. Rev. A, Vol. 44, p.3222 (1991)
- [1] Cheng Xie, Gerhard Klimeck, Daniel Elliott, "Generation and Intensity Correlation Measurements of the Real Gaussian Field", Phys. Rev. A Vol. 41, p.6376 (1990)

PEER REVIEWED CONFERENCE PROCEEDINGS (234 +5 TOTAL)

These peer-reviewed proceedings articles are full papers or extended abstracts made available to conference participants. Some of the articles are publicly available in conference archives such as IEEE IEDM, IEEE DRC, IEEE SISPAD, IEEE AP-S, and Inst. Phys. Conf. Ser.

Work Performed at Purdue (186 + 5 Total)

The conference participation is also shown in the list of contributed or invited conferences

- [P239] Gerhard Klimeck¹, Tanya Faltens¹, Daniel Mejia¹, Alejandro Strachan¹, Lynn Zentner¹, Michael Zentner², “nanoHUB.org: How to enable Rapid Curriculum Innovation through Translation of Research-Based Simulation Tools into Apps”, Workshop on Innovative Nanoscale Devices and Systems (WINDS) Conference, Kauai, HI, Dec. 12, 2022. Book of abstracts, ISBN 978-3-9504738-4-1, <https://www.winds-meeting.info/winds2022/book-of-abstracts>
- [P238] Gerhard Klimeck, Tillmann Kubis, Michael Povolotskyi, James E. Fonseca, Bozidar Novakovic, Rajib Rahman, Tarek Ameen, James Charles, Junzhe Geng, Kaspar Haume, Yu He, Ganesh Hegde, Yuling Hsueh, Hesam Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Lemus, Daniel Mejia, Kai Miao, Samik Mukherjee, Seung Hyun Park, Ahmed Reza, Mehdi Salmani, Parijat Sengupta, Saima Sharmin, Yaohua Tan, Archana Tankasala, Daniel Valencia, Evan Wilson, “NEMO5, a Multiscale, Multiphysics Nanoelectronics Modeling Tool used for Ultra-Scaled CMOS, 2D Transistor, Topological Materials, and Quantum Computing Devices”, Workshop on Innovative Nanoscale Devices and Systems (WINDS), Kauai, HI, Dec. 12, 2022. Book of abstracts, ISBN 978-3-9504738-4-1, <https://www.winds-meeting.info/winds2022/book-of-abstracts>
- [P237] G. Klimeck, T. Kubis, M. Povolotskyi, J. E. Fonseca, B. Novakovic, R. Rahman, T. Ameen, J. Charles, J. Geng, K. Haume, Yu He, G. Hegde, Y. Hsueh, H. Ilatikhameneh, Z. Jiang, S. G. Kim, D. Lemus, D. Mejia, K. Miao, Samik Mukherjee, S. H. Park, A. Reza, M. Salmani, P. Sengupta, S. Sharmin, Y. Tan, A. Tankasala, D. Valencia, E. Wilson, “
- [P236] Jay Alameda, Claire Stirm, Gregory Bauer, Timothy Boerner, Brett Bode, Maytal Dahan, William Gropp, Marlon Pierce, Cynthia Yewdall, Michael Zentner, Meghna Babbar-Sebens, Michael Barton, Daniele Bianchi, Michael Bell, Michel Boufadel, Michael Cianfrocco, Sean Cleveland, Cosan Daskiran, Kjersten Fagnan, Geoffrey Fox, Eleftherios Garyfallidis, Jerome Hajjar, Gerhard Klimeck, Mark Miller, Mark Perri, Victor Pinks II, Mohan Ramamurthy, Michel Regenwetter, Amy Roberts, Aldo Romero, Carol Song, Alejandro Strachan, Ellad Tadmor and Gregory Tucker, “The Delta Gateway: Exploring Community Use of GPU Resources through a Science Gateway”, Science Gateways Conference, San Diego, Oct. 18, 2022
- [P235] Gerhard Klimeck, Lynn Zentner, Alejandro Strachan, Michael Zentner, “Driving Sustainability of a Gateway with a Customer Relationship Management (CRM) System”, Science Gateways Conference, San Diego, Oct. 18, 2022
- [P234] Sandra Gesing, Claire Stirm, Gerhard Klimeck, Lynn Zentner, S. Wang, B.M. Martinez, Diaz, C. Donovan, L. Zhao, Carol Song, I.L. Kim, Alejandro Strachan, Michael Zentner, R. Kalyanam, "Open Science via HUBzero: Exploring Five Science Gateways Supporting and Growing their Open Science Communities", Proc. of HICSS-55 (55th Hawaii International Conference on System Sciences), Open Science Practices in Information Systems Research, January 2022
- [P233] Gerhard Klimeck, Alejandro Strachan, Tanya Faltens, Lynn Zentner, Michael Zentner, "Using nanoHUB.org in Research and Education – a Hands-on Tutorial", IEEE NMDC Conference, Dec. 12-15, 2021.
- [P232] Claire Stirm, Sandra Gesing, Lynn Zentner, Michael Zentner, Carly Dearborn, Gerhard Klimeck, "HUBzero's variations of sustainability: From simulation/modeling tools to communities" CEUR Workshop Proceedings, 2021, 2975
- [P231] Gerhard Klimeck, Gustavo Valencia-Zapata, Nathan Denny, Lynn Zentner, Michael Zentner, "NanoHUB user behavior: Moving from retrospective statistics to actionable behavior analysis" CEUR Workshop Proceedings, 2021, 2975
- [P230] Veliko Milutinović, Erfan Azer, Kristy Yoshimoto, Gerhard Klimeck, Miljan Djordjevic, Milos Kotlar, Miroslav Bojovic, Bozidar Miladinovic, Nenad Korolija, Stevan Stankovic, Nenad Filipović, Zoran Babovic, Miroslav Kosanic, Akira Tsuda, Mateo Valero, Massimo Santo, Erich Neuhold, Jelena Skorucak, Laura Dipietro, Ivan Ratkovic, "The Ultimate DataFlow for Ultimate SuperComputers-on-a-Chip, for Scientific Computing, Geo Physics, Complex Mathematics, and Information Processing" 10th Mediterranean Conference on Embedded Computing, MECO, 2021, 9459725, DOI 10.1109/MECO52532.2021.9459725
- [P229] Dewei Xu, KuangChung Chuang, Wayne Zhao, Keith Donegan, Seung-Yeop Kook, Rod Augur, Jeffery Chee, Gerhard Klimeck, "Resistivity Impact from Modulated Line-Edge-Roughness with Self-aligned Double Patterning", proceedings of 2020 IEEE International Interconnect Technology Conference (IITC), DOI: 10.1109/IITC47697.2020.9515619

- [P228] Gerhard Klimeck, Gustavo Valencia-Zapata, Nathan Denny, Lynn Zentner, Michael Zentner, "nanoHUB User Behavior: Moving From Retrospective Statistics to Actionable Behavior Analysis" 11th International Workshop on Science Gateways, Ljubljana, Slovenia, June 12-14, 2019
- [P227] Nathan Denny, Michael Zentner, Daniel Mejia, Gerhard Klimeck, "Instant On" Science Gateways: An Introduction to Caching Simulation Results and a Path Towards Data Exploration", Gateways 2019, Sept. 23–25, 2019, San Diego, California
- [P226] Gerhard Klimeck, Alejandro Strachan, Tanya Faltens, Brad Hallberg, Lynn Zentner, Michael Zentner, Martin Hunt, "Using nanoHUB.org in Research and Education—A Hands-on Tutorial", Proceedings of IWCN 2019 - International Workshop on Computational Nanotechnology, May 20-24, 2019 Evanston, IL, USA
- [P225] Nathan Denny, Gerhard Klimeck, Michael Zentner, "Visualizing User Interactions with Simulation Tool", Proceedings of the 13th Gateway Computing Environments Conference, September 25-27, 2018, Austin, TX
- [P224] Dwight McKay, Michael Zentner, Gerhard Klimeck, "Clustering Download Events to Identify Classrooms", Proceedings of the 13th Gateway Computing Environments Conference, September 25-27, 2018, Austin, TX
- [P223] Michael Zentner, Nathan Denny, Krishna Madhavan, Swaroop Samek, George Adams III., Gerhard Klimeck, "Using Automatic Detection and Characterization to Measure Educational Impact of nanoHUB", Proceedings of the 13th Gateway Computing Environments Conference, September 25-27, 2018, Austin, TX
- [P222] Shang-Chun Lu, Yuanchen Chu, Youngseok Kim, Mohamed Mohamed, Gerhard Klimeck, Thomas Palacios, Umberto Ravaioli, "Design Guidelines and Limitations of Multilayer Two-dimensional Vertical Tunneling FETs for Ultra-Low Power Logic Applications", Proceedings of the International Conference on Simulation of Semiconductor Processes and Devices, September 24-26, 2018, Austin, TX
- [P221] Yuanchen Chu, Prasad Sarangapani, James Charles, Gerhard Klimeck, Tillmann Kubis, "Electron-only explicit screening quantum transport model for semiconductor nanodevices", Proceedings of the International Conference on Simulation of Semiconductor Processes and Devices, September 24-26, 2018, Austin, TX
- [P220] Daniel Valencia, K. Wang, Y. Chu, Gerhard Klimeck, Michael Povolotskyi, "Surface and grain boundary effects on copper interconnects thin films modeling with an atomistic basis", Proceedings of the International Conference on Simulation of Semiconductor Processes and Devices, September 24-26, 2018, Austin, TX
- [P219] Gerhard Klimeck, Michael Zentner, Lynn Zentner, Tillmann Kubis, "NEMO5: Multi-Scale, Multi-Physics, Atomistic Modeling of Non-Equilibrium Processes in Nanometer-Scaled Compound Materials For Active Devices and Global Impact on nanoHUB.org", Collaborative Conference on Materials Research (CCMR) 2018, 25 - 29 June 2018, Incheon/Seoul, South Korea
- [P218] Prasad Sarangapani, Cory Weber, Jiwon Chang, Stephen Cea, Roksana Golizadeh-Mojarad, Michael Povolotskyi, Gerhard Klimeck, Tillmann Kubis, "Assessment of Si/SiGe PMOS Schottky contacts through atomistic tight binding simulations: Can we achieve the $10-9\Omega\cdot\text{cm}$? target?", Proceedings of the 2017 IEEE 17th International Conference on Nanotechnology (IEEE-NANO), Pages 83-84
- [P217] Jun Huang, Pengyu Long, Michael Povolotskyi, Gerhard Klimeck, Mark Rodwell, "Sb- and Al-free ultra-high-current tunnel FET designs", Proceedings of the 2017 Fifth Berkeley Symposium on Energy Efficient Electronic Systems & Steep Transistors Workshop (E3S), Pages 1-3
- [P216] Patrick Fay, W. Li, D. Digiovanni, L. Cao, Hesameddin Ilatikhameneh, Fan Chen, Tarek Ameen, Rajib Rahman, Gerhard Klimeck, C. Lund, S. Keller, S.M. Islam, A. Chaney, Y. Cho, Debdeep Jena, "III-N heterostructure devices for low-power logic", Proceedings of the Semiconductor Technology International Conference (CSTIC), 2017 China, Pages 1-3
- [P215] Pengyu Long, Michael Povolotskyi, Jun Huang, James Charles, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, "A high-current InP-channel triple heterojunction tunnel transistor design", Proceedings of the 75th Device Research Conference (DRC), University of Notre Dame (Indiana, USA) from June 25-28, 2017
- [P214] Junzhe Geng, Prasad Sarangapani, Carl Wordelman, Erik Nelson, Ben Browne, Tillmann Kubis, Gerhard Klimeck, "NEMO5: realistic and efficient NEGF simulations of GaN light-emitting diodes", Proc. SPIE 10098, Physics and Simulation of Optoelectronic Devices XXV, 1009813 (February 22, 2017)
- [P213] KuangChung Wang, Daniel Valencia, James Charles, Yu He, Michael Povolotskyi, Gerhard Klimeck, Jesse Maassen, Mark Lundstrom, Tillmann Kubis, "NEMO5: Predicting MoS₂ Heterojunctions", 2016 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)
- [P212] Daniel Valencia, Evan Wilson, Prasad Sarangapani, Gustavo Valencia-Zapata, Gerhard Klimeck, Michael Povolotskyi, Zhengping Jiang, "Grain boundary resistance in nanoscale copper interconnections", Simulation of Semiconductor Processes and Devices (SISPAD), 2016
- [P211] Patrick Fay, W. Li, L. Cao, K. Pourang, S.M. Islam, C. Lund, Saima Sharmin, Hesameddin Ilatikhameneh, Tarek Ameen, Jun Huang, Rajib Rahman, Debdeep Jena, S. Keller, Gerhard Klimeck, "Novel III-N heterostructure devices for low-power logic and more", Nanotechnology (IEEE-NANO), 2016 IEEE 16th International Conference on (pp. 767-769). IEEE
- [P210] Pengyu Long, Jun Huang, Michael Povolotskyi, Devin Verreck, James Charles, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, B. Calhoun, "A Tunnel FET Design for High-Current, 120 mV Operation", 2016 IEEE International Electron Devices Meeting, December 3-7, 2016, San Francisco, CA

- [P209] Jun Huang, Pengyu Long, Michael Povolotskyi, Mark Rodwell, Gerhard Klimeck, "Exploring Channel Doping Designs for High-Performance Tunneling FETs", Device Research Conference (DRC), June, 2016, Newark, Delaware, USA
- [P208] Pengyu Long, Michael Povolotskyi, Jun Huang, Hesameddin Ilatikhameneh, Tarek Ameen, Rajib Rahman, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, "Extremely high simulated ballistic currents in triple-heterojunction tunnel transistors", Device Research Conference (DRC), June, 2016, Newark, Delaware, USA
- [P207] Pengyu Long, Jun Huang, Michael Povolotskyi, Devin Verreck, Gerhard Klimeck, Mark Rodwell, "High-Current InP-Based Triple Heterojunction Tunnel Transistors", 28th International Conference on Indium Phosphide and Related Materials (IPRM), June, 2016, Toyama, Japan
- [P206] Fan Chen, Hesameddin Ilatikhameneh, Yaohua Tan, Daniel Valencia, Gerhard Klimeck, Rajib Rahman, "Transport in vertically stacked hetero-structures from 2D materials", 33rd International Conference on the Physics of Semiconductors, Beijing, China on July 31- August 5, 2016
- [P205] Hesameddin Ilatikhameneh, Gerhard Klimeck, Rajib Rahman, "2D tunnel transistors for ultra-low power applications: Promises and challenges", 2015 Fourth Berkeley Symposium on Energy Efficient Electronic Systems (E3S), 1-2 Oct. 2015, Berkeley, CA, Page(s): 1 - 3
- [P204] Krishna Madhavan, Daniel Mejia, Hanjun Xian, Lynn Zentner, Victoria Farnsworth, Swaroop Samek, Gerhard Klimeck, "Interactive Analytic Systems for Understanding the Scholarly Impact of Large-Scale E-science Cyberenvironments", 2015 IEEE 11th International Conference on e-Science (e-Science), Aug. 31 2015-Sept. 4 2015, Munich, Page(s): 288 - 291
- [P203] Hesameddin Ilatikhameneh, Rajib Rahman, Joerg Appenzeller, Gerhard Klimeck, "Electrically doped WTe₂ tunnel transistors", 2015 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), 9-11 Sept. 2015, Washington, DC, Page(s): 270 - 272
- [P202] Prasad Sarangapani, Daniel Mejia, James Charles, Woody Gilbertso, Hesameddin Ilatikhameneh, Tarek Ameen, Andrew Roche, Jim Fonseca, Gerhard Klimeck, "Quantum dot lab: an online platform for quantum dot simulations", International Workshop on Computational Electronics (IWCE), 2015, Page(s): 1 - 3
- [P201] Tanya Faltens, Alejandro Strachan, Gerhard Klimeck, "Nanohub as a Platform for Implementing ICME Simulations in Research and Education", Proceedings of the 3rd World Congress on Integrated Computational Materials Engineering (ICME 2015), 15 MAY 2015
- [P200] Jun Huang, KuangChung Wang, William Frensley, Gerhard Klimeck, "Finite difference schemes for k-p models: A comparative study", 18th International Workshop on Computational Electronics (IWCE), West Lafayette, Indiana, September 2-4, 2015, Page(s): 1 - 2
- [P199] Hesameddin Ilatikhameneh, Fan Chen, Rajib Rahman, Gerhard Klimeck, "Electrically Doped 2D material tunnel transistor", International Workshop on Computational Electronics (IWCE 2015) September 2, 2015 West Lafayette, Indiana USA, Pages: 1 - 3
- [P198] Fan Chen, Michael Manfra, Gerhard Klimeck, Tillmann Kubis, "NEMO5: Why must we treat topological insulator nanowires atomically?", IWCE, September 2, 2015 West Lafayette, Indiana USA
- [P197] Fan Chen, Hesameddin Ilatikhameneh, Gerhard Klimeck, Rajib Rahman, Tao Chu, zhihong chen, "Achieving a higher performance in bilayer graphene FET - strain engineering", the 20th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Washington DC, 9-11 Sep. 2015, Pages: 177 - 181
- [P196] Bozidar Novakovic, Gerhard Klimeck, "Atomistic quantum transport approach to time-resolved device simulations", in Proceedings of the 20th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Washington DC, 9-11 Sep. 2015, pp. 8-11
- [P195] Mehdi Salmani-Jelodar, Hesameddin Ilatikhameneh, Prasad Sarangapani, Saumitra Mehrotra, SungGeun Kim, Kwok Ng, Gerhard Klimeck, "Tunneling: The Major Issue in Ultra-scaled MOSFETs", IEEE Nano, Rome, Italy, July 26-30, 2015, Pages: 670 - 673
- [P194] Mark Rodwell, Cheng-Ying Huang, Arthur Gossard, Varistha Chobpattana, S. Stemmer, B. Thibeault, W. Mitchell, Pengyu Long, Evan Wilson, Saumitra Mehrotra, Michael Povolotskyi, Gerhard Klimeck, "Record-Performance Thermally-Limited Devices, Prospects for High-On-Current Steep Subthreshold Swing Devices", 2015 Conference on Indium Phosphide and Related Materials, June 8-July 2, Santa Barbara, CA
- [P193] Tarek Ameen, Hesameddin Ilatikhameneh, Daniel Valencia, Rajib Rahman, Gerhard Klimeck, "Engineering The Optical Transitions of Self-Assembled Quantum Dots", International Workshop on Computational Electronics (IWCE 2015) September 2, 2015 West Lafayette, Indiana USA, Pages: 1 - 4
- [P192] A. Afzalian, Jun Huang, Hesameddin Ilatikhameneh, James Charles, Daniel Lemus, Jose Bermeo, Santiago Rubiano, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, M. Passlack, Y.-C. Yeo, "Mode space tight binding model for ultra-fast simulations of III-V nanowire MOSFETs and heterojunction TFETs", International Workshop on Computational Electronics (IWCE 2015) September 2, 2015 West Lafayette, Indiana USA, Page(s): 1 - 3
- [P191] Cheng-Ying Huang, Sanghoon Lee, Evan Wilson, Pengyu Long, Michael Povolotskyi, Varistha Chobpattana, Susanne Stemmer, Arthur Gossard, Gerhard Klimeck, Mark Rodwell, "Comparison of Ultra-Thin

- InAs and InGaAs Quantum Wells and Ultra-Thin-Body Surface-Channel MOSFETs", 27th International Conference on Indium Phosphide and Related Materials, June 28-July 2, 2015 University of California Santa Barbara, CA, USA
- [P190] Mark Rodwell, Cheng-Ying Huang, J. Rode, P. Choudhary, Sanghoon Lee, Arthur Gossard, Pengyu Long, Evan Wilson, Saumitra Mehrotra, Michael Povolotskyi, Gerhard Klimeck, M. Urteaga, B. Brar, Varistha Chobpattana, S. Stemmer, "Transistors for VLSI, for Wireless: A View Forwards Through Fog", 73rd Device Research Conference (DRC), Ohio State University, June 21-24, 2015
- [P189] Mustafa Badaroglu, Kwok Ng, Mehdi Salmani-Jelodar, SungGeun Kim, Gerhard Klimeck, Chong-Ping Chang, Charles Cheung, Yuzo Fukuzaki, "More Moore landscape for system readiness-ITRS2. 0 requirements", 32nd IEEE International Conference on Computer Design (ICCD), pp. 147-152, Oct. 2014
- [P188] Tarek Ameen, Hesameddin Ilatikhameneh, James Charles, Yuling Hsueh, Sicong Chen, Jim Fonseca, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, "Optimization of the anharmonic strain model to capture realistic strain distributions in quantum dots", 14th IEEE International Conference on Nanotechnology, 18-21 Aug. 2014, Page(s): 921 - 924, Toronto, ON
- [P187] Mehdi Salmani-Jelodar, S. Kim, K. Ng, Gerhard Klimeck, "Performance degradation due to thicker physical layer of high k oxide in ultra-scaled MOSFETs and mitigation through electrostatics design", 2014 IEEE Silicon Nanoelectronics Workshop (SNW), 8-9 June 2014, Honolulu, HI, Page(s): 1 - 2
- [P186] Yui-Hong Tan, Hoon Ryu, Bent Weber, Sunhee Lee, Rajib Rahman, Lloyd Hollenberg, Michelle Simmons, Gerhard Klimeck, "Statistical Modeling of Ultra-Scaled Donor-Based Silicon Phosphorus Devices", 2014 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI USA June 8-9, 2014, Page(s): 1 - 2
- [P185] Fahd Mohiyaddin, Rajib Rahman, Rachpon Kalra, Sunhee Lee, Gerhard Klimeck, Lloyd Hollenberg, C.H. Yang, A. Rossi, Andrew Dzurak, Andrea Morello, "Designing a large scale quantum computer with atomistic simulations", 2014 IEEE Silicon Nanoelectronics Workshop (SNW), 8-9 June 2014, Honolulu, HI, Page(s): 1 - 2
- [P184] Hesameddin Ilatikhameneh, Bozidar Novakovic, Yaohua Tan, Mehdi Salmani-Jelodar, Tillmann Kubis, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, "Atomistic simulation of steep subthreshold slope Bi-layer MoS₂ transistors", 2014 IEEE Silicon Nanoelectronics Workshop (SNW), 8-9 June 2014, Honolulu, HI, Page(s): 1 - 2
- [P183] Bent Weber, Yui-Hong Tan, Suddhasatta Mahapatra, Thomas Watson, Hoon Ryu, Sunhee Lee, Rajib Rahman, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, "Silicon at the fundamental scaling limit-atomic-scale donor-based quantum electronics", IEEE Silicon Nanoelectronics Workshop (SNW), Page(s): 1 - 2, 8-9 June 2014
- [P182] Tanya Faltens, Peter Bermel, Amanda Buckles, K. Douglas, Alejandro Strachan, Lynn Zentner, Gerhard Klimeck, "nanoHUB.org: A Gateway to Undergraduate Simulation-Based Research in Materials Science and Related Fields", 2014 MRS Fall Meeting, Volume: 1762
- [P181] Yu He, Tillmann Kubis, Michael Povolotskyi, Jim Fonseca, Gerhard Klimeck, "Quantum Transport in NEMO5: Algorithm Improvements and High Performance Implementation", 2014 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Yokohama, Japan, September 9-11, 2014, Page(s): 361 - 364
- [P180] Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "Tight Binding analysis of Si/GaAs UTBs with subatomic resolution", 17th International Workshop on Computational Electronics (IWCE), Paris, France, 2014
- [P179] Prasad Sarangapani, Yaohua Tan, James Charles, Tarek Ameen, Junzhe Geng, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Atomistic Tight Binding Simulations with Real Space Basis Functions: Optical Properties of Quantum Wells and Dots", IWCE 2014, June 3-6, Paris, France
- [P178] Lynn Zentner, Michael Zentner, Victoria Farnsworth, Michael McLennan, Krishna Madhavan, Gerhard Klimeck, "nanoHUB.org: Experiences and Challenges in Software Sustainability for a Large Scientific Community", First Workshop on Sustainable Software for Science: Practice and Experiences (WSSSPE1), held in conjunction with SC12, 17 November 2013, Denver, CO.
- [P177] Hesameddin Ilatikhameneh, Saima Sharmin, Rajib Rahman, Gerhard Klimeck, "Atomistic Simulation of GaN/InN/GaN Tunnel FETs", Berkeley Symposium on Energy Efficient Electronic Systems, 2013
- [P176] Victoria Farnsworth, Mark Lundstrom, Supriyo Datta, Ron Reifengerger, Arvind Raman, Timothy Fisher, Alejandro Strachan, Michael McLennan, Swaroop Shivarajapura, Lynn Zentner, Krishna Madhavan, Gerhard Klimeck, "nanoHUB-U: A Science Gateway Ventures into Structured Online Education", 13th IEEE International Conference on Nanotechnology, August 5-8, 2013, Shangri-La Hotel, Beijing, China
- [P175] Parijat Sengupta, Tillmann Kubis, Yaohua Tan, Michael Povolotskyi, Gerhard Klimeck, "Thermal transport in topological insulator nanowires", Techon Sept 10-11, 2013. Austin

- [P174] Parijat Sengupta, Yaohua Tan, Tillmann Kubis, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, "Topological insulator states in a broken-gap GaN/InN/GaN system heterojunction", International Conference on Nitride Semiconductors. Aug 25 -30, 2013. Washington D.C
- [P173] Zhengping Jiang, Yu He, Guangle Zhou, Tillmann Kubis, Huili Xing, Gerhard Klimeck, "Atomistic Simulation on Gate-recessed InAs/GaSb TFETs and Performance Benchmark", Device Research Conference (DRC), Page(s): 145 - 146, June 2013, Notre Dame, IN, USA
- [P172] SungGeun Kim, Mehdi Salmani-Jelodar, Kwok Ng, Gerhard Klimeck, "Quantum Corrected Drift-Diffusion Simulation for Prediction of CMOS Scaling", Device Research Conference, 2013
- [P171] Seung Park, Neerav Kharche, D. Basu, Zhengping Jiang, Saroj K.Nayak, C. Weber, Ganesh Hegde, K. Haume, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Scaling Effect on Specific Contact Resistivity in Nanoscale Metal-Semiconductor Contacts", Device Research Conference (DRC), University of Notre Dame, IN, June 23-26, 2013, Page(s): 125 - 126, and International Workshop on Computational Electronics (IWCE), Nara, Japan, June 4-7, 2013
- [P170] Yu Wang, Yu He, Gerhard Klimeck, Tillmann Kubis, "Nonequilibrium Green's function method: Algorithm for regular and irregular leads", 16th International Workshop on Computational Electronics, Nara, Japan June 4-7, 2013
- [P169] Saumitra Mehrotra, Abhijeet Paul, Jin Cho, Michael Povolotskyi, Gerhard Klimeck, "Effect of Fin Tapering in Nanoscale Si FinFETs", 16th International Workshop on Computational Electronics, Nara, Japan June 4-7, 2013
- [P168] Jean Sellier, Jim Fonseca, Tillmann Kubis, Michael Povolotskyi, Yu He, Hesameddin Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Mejia, Parijat Sengupta, Yaohua Tan, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool", IEEE SISPAD 2012, pg: 388-391, International Conference on Simulation of Semiconductor Processes and Devices, Denver, CO, Sept. 2012
- [P167] Behtash Behin-Aein, Abhijeet Paul, Saumitra Mehrotra, Kerem Akarvardar, Ajey Jacob, Zoran Krivokapic, Gerhard Klimeck, "Atomistic Analysis of Electrical Performance of Highly Scaled Si1-xGex p-FinFETs", SISPAD 2012, International Conference on Simulation of Semiconductor Processes and Devices, Denver, CO, Sept. 2012
- [P166] Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, Hoon Ryu, Sunhee Lee, Oliver Warschkow, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, "Spectroscopy of a deterministic single-donor device in silicon", Proceedings of SPIE, V8400, Article Number: 840006, May 1, 2012
- [P165] Timothy Boykin, Mathieu Luisier, Neerav Kharche, Xueping Jiang, Saroj K.Nayak, A. Martins, Gerhard Klimeck, "Multiband tight-binding model for strained and bilayer graphene from DFT calculations ", Computational Electronics (IWCE), 2012 15th International Workshop on, 22-25 May 2012
- [P164] Jean Sellier, Jim Fonseca, Gerhard Klimeck, "Archimedes, the free Monte Carlo simulator: A GNU package for submicron semiconductor devices on nanoHUB ", IWCE 2012 proceeding, May 2012
- [P163] R. Pipes, Gerhard Klimeck, Mark Pipes, "The Composite Materials Manufacturing HUB – Crowd Sourcing as the Norm", The composite exhibition and convention (COMPOSITES 2012), Feb. 21-23, 2012 at Las Vegas, Nevada
- [P162] Mehdi Salmani-Jelodar, Yaohua Tan, Gerhard Klimeck, "Single Layer MoS2 Band Structure and Transport", International Semiconductor Device Research Symposium (ISDRS 2011), Dec 7-11, Univ of Maryland
- [P161] SungGeun Kim, Saumitra Mehrotra, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Effects of Interface Roughness Scattering on RF Performance of Nanowire Transistors", International Semiconductor Device Research Symposium (ISDRS 2011), Dec 7-11, Univ of Maryland
- [P160] Saumitra Mehrotra, Abhijeet Paul, Gerhard Klimeck, "Ballistic hole injection velocity analysis in Ge UTB pMOSFETs: Dependence on body thickness, orientation and strain", International Semiconductor Device Research Symposium (ISDRS 2011), Dec 7-11, Univ of Maryland
- [P159] Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Atomistic nanoelectronic device simulations with sustained performances up to 1.44 PFlop/s", Finalist in ACP/IEEE in Gordon Bell Prize Competition (5 finalists) Supercomputing Nov. 2011, IEEE Proceedings, E-ISBN: 978-1-4503-0771-0
- [P158] Parijat Sengupta, Yaohua Tan, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Tunability of the critical width of a 2D Topological Insulator", Presented at MRS Fall Meeting 2011, SYMPOSIUM L, Boston, MA
- [P157] Gerhard Klimeck, Lynn Zentner, Krishna Madhavan, Victoria Farnsworth, Mark Lundstrom, "Network for Computational Nanotechnology - A Strategic Plan for Global Knowledge Transfer in Research and Education", INVITED paper, IEEE proceedings of IEEE Nanotechnology Materials and Devices Conference (IEEE NMDC 2011), Oct. 18-21, 2011 at The Shilla Jeju, Korea
- [P156] Seung Park, Hong-Hyun Park, Mehdi Salmani-Jelodar, Sebastian Steiger, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Contact Modeling and Analysis of InAs HEMT Transistors", IEEE proceedings of IEEE Nanotechnology Materials and Devices Conference (IEEE NMDC 2011), Oct. 18-21, 2011 at The Shilla Jeju, Korea

- [P155] Lynn Zentner, Steven Clark, Preston Smith, Swaroop Shivarajapura, Victoria Farnsworth, Krishna Madhavan, Gerhard Klimeck, "Practical Considerations in Cloud Utilization for the Science Gateway nanoHUB.org", Utility and Cloud Computing (UCC), 2011 Fourth IEEE International Conference on, Publication Year: 2011 , Page(s): 287 - 292
- [P154] Abhijeet Paul, Kai Miao, Ganesh Hegde, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Enhancement of thermoelectric efficiency by uniaxial tensile stress in n-type GaAs nanowires", proceedings of IEEE nano conference, Portland, Aug, 2011.
- [P153] Gerhard Klimeck, George Adams III., Krishna Madhavan, Nathan Denny, Michael Zentner, Swaroop Shivarajapura, Lynn Zentner, Diane Beaudoin, "Social Networks of Researchers and Educators on nanoHUB.org", proceedings of the 11th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, CCGrid 2011, Newport Beach, CA, USA, May 23-26, 2011
- [P152] Mark Lundstrom, Changwook Jeong, Gerhard Klimeck, "Computational Study of the Electronic Performance of Cross-Plane Superlattice Peltier Devices", Proceedings of the MRS Spring Meeting, Published March 14 2011
- [P151] Lynn Zentner, Steven Clark, Krishna Madhavan, Swaroop Shivarajapura, Victoria Farnsworth, Gerhard Klimeck, "Automated Grid-Probe System to Improve End-To-End Grid Reliability for a Science Gateway", Proceedings of TeraGrid 2011 conference. July 18-21, 2011, Salt Lake City, ACM proceedings, ISBN: 978-1-4503-0888-5
- [P150] Abhijeet Paul, Saumitra Mehrotra, Gerhard Klimeck, Mark Rodwell, "Performance enhancement of GaAs UTB pFETs by strain, orientation and body thickness engineering", proceedings of the IEEE Device Research Conference (DRC), June 20-22 2011
- [P149] Sebastian Steiger, Michael Povolotskyi, Hong-Hyun Park, Tillmann Kubis, Ganesh Hegde, Benjamin Haley, Mark Rodwell, Gerhard Klimeck, "The Nanoelectronic Modeling Tool NEMO 5: Capabilities, Validation, and Application to Sb-Heterostructures", proceedings of the IEEE Device Research Conference (DRC), June 20-22 2011
- [P148] Kai Miao, Mathieu Luisier, Gerhard Klimeck, "Tuning lattice thermal conductance in ultra-scaled hollow SiNW: Role of porosity size, density and distribution", proceedings of the MRS Spring Meeting, 2011. San Francisco, April 25th - 29th
- [P147] Parijat Sengupta, Sebastian Steiger, Sunhee Lee, Hoon Ryu, Gerhard Klimeck, "Multiscale Modeling of a Quantum Dot Heterostructures", presented at MRS Spring Meeting 2011, YY10.2, San Francisco CA,
- [P146] Mehdi Salmani-Jelodar, Sebastian Steiger, Abhijeet Paul, Gerhard Klimeck, "Parameter Fitting for Lattice Properties of Gallium Arsenide using Parallel Genetic Algorithm", 2011 IEEE Congress on Evolutionary Computation, 5-8 June 2011
- [P145] Ali Razavieh, Navab Singh, Abhijeet Paul, Gerhard Klimeck, David Janes, Joerg Appenzeller, "A New Method to Achieve RF Linearity in SOI Nanowire MOSFETs", IEEE 2011 RFIC Symposium, ISBN: 978-1-4244-8293-1
- [P144] Neophytos Neophytou, Hans Kosina, Gerhard Klimeck, "A comprehensive atomistic analysis of bandstructure velocities in si nanowires", Computational Electronics (IWCE), 2010 14th International Workshop, Pisa, Italy, 26-29 Oct. 2010, Page(s): 1-4
- [P143] Ganesh Hegde, Gerhard Klimeck, Alejandro Strachan, "First Principles Study of the Energetics of Ideal GaAs Surfaces and Adsorption of Al and O as a Function of Surface Orientation", 41st IEEE Semiconductor Interface Specialists Conference, The Catamaran Hotel, San Diego, CA, December 2-4, 2010
- [P142] Mathieu Luisier, Gerhard Klimeck, "Phonon-limited mobility and injection velocity in n- and p-doped ultrascaled nanowire field-effect transistors with different crystal orientations", proceedings of IEDM 2010, 6-8 Dec. 2010
- [P141] Tillmann Kubis, Gerhard Klimeck, "Rough interfaces in THz quantum cascade lasers", International Workshop for Computational Electronics, Publication Year: 2010 , Page(s): 1 - 4, Pisa, Italy
- [P140] Zhengping Jiang, Neerav Kharche, Gerhard Klimeck, "Valley Degeneracy in (110) Si Quantum Wells - Strain and Misorientation Effects", Proceedings of the International Workshop for Computational Electronics, Pisa, Italy, October 2010
- [P139] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Atomistic modeling of the phonon dispersion and lattice properties of free-standing <100> Si nanowires", Proceedings of the International Workshop for Computational Electronics, Pisa, Italy, October 2010, Abstract on arXiv:1010.0367v1
- [P138] George Adams III., Krishna Madhavan, Michael Zentner, Nathan Denny, Swaroop Shivarajapura, Gerhard Klimeck, "User Flow Informatics to Personalize Learning in Engineering Cyber-environments - nanoHUB.org A Case Study", proceedings of the ASEE 9th Global Colloquium on Engineering Education in Singapore on October 18 -21,2010
- [P137] Krishna Madhavan, Diane Beaudoin, Swaroop Shivarajapura, George Adams III., Gerhard Klimeck, "nanoHUB.org serving over 120,000 users worldwide: it's first cyber-environment assessment", Nanotechnology (IEEE-NANO), 2010 10th IEEE Conference, Seoul Korea, Aug. 17-20, 2010, Page:90

- [P136] Sunhee Lee, Hoon Ryu, Gerhard Klimeck, Suddhasatta Mahapatra, Michelle Simmons, Lloyd Hollenberg, "Equilibrium Bandstructure of a Phosphorus δ -doped Layer in Silicon using a Tight-binding Approach", Proceedings of IEEE Nano 2010, Seoul Korea, Aug. 17-20, 2010
- [P135] Nabil Ashraf, Dragica Vasileska, Gerhard Klimeck, "Modeling Fluctuations in the Threshold Voltage and ON-Current and Threshold Voltage Fluctuation due to Random Telegraph Noise", Proceedings of IEEE Nano 2010, Seoul Korea, Aug. 17-20, 2010
- [P134] Abhijeet Paul, Gerhard Klimeck, "Atomistic modeling of the thermoelectric power factor in ultra-scaled silicon nanowires", proceedings of 2010 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI, June 13-14, 2010
- [P133] Gerhard Klimeck, Mathieu Luisier, "Scattering in Si-nanowires - Where does it matter?", proceedings of 2010 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI, June 13-14, 2010
- [P132] Hoon Ryu, S. Lee, Bent Weber, Suddhasatta Mahapatra, Michelle Simmons, Lloyd Hollenberg, Gerhard Klimeck, "Quantum transport in ultra-scaled phosphorous-doped silicon nanowires", proceedings of 2010 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI, June 13-14, 2010
- [P131] Mark Rodwell, William Frensley, Sebastian Steiger, E. Chagarov, S. Lee, Hoon Ryu, Y. Tan, Ganesh Hegde, L Wang, J. Law, Timothy Boykin, Gerhard Klimeck, P. Asbeck, A. Kummel, J. Schulman, "III-V FET Channel Designs for High Current Densities and Thin Inversion Layers", proceedings of Device Research Conference (DRC), 21-23 June 2010, pg. 149 - 152
- [P130] Krishna Madhavan, Gerhard Klimeck, Diane Beaudoin, George Adams III., Swaroop Shivarajapura, D.F. Radcliffe, "Bridging engineering practice and learning through cyber-environments", Proceedings of the workshop on Engineering Learning at the International Conference on the Learning Sciences June 28, 2010, Chicago, IL.
- [P129] Gerhard Klimeck, Saumitra Mehrotra, Abhijeet Paul, Mathieu Luisier, "Atomistic simulations for SiGe pMOS devices Bandstructure to Transport", ISDRS 2009, December 9-11, 2009, College Park, MD, USA. Page(s):1-2
- [P128] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Study of Ultra-scaled SiGe/Si Core/Shell Nanowire FETs for CMOS Applications", ISDRS 2009, December 9-11, 2009, College Park, MD, USA. Page(s):1-2
- [P127] Gabriel Lansbergen, Abhijeet Paul, Nadine Collaert, Gerhard Klimeck, Serge Biesemans, Sven Rogge, "Subthreshold Study of Undoped Trigate nFinFET", Thin Solid Films. Page(s):2521-2523
- [P126] Neerav Kharche, Gerhard Klimeck, Dae-Hyun Kim, Jesús. Alamo, Mathieu Luisier, "Performance Analysis of Ultra-Scaled InAs HEMTs", IEDM 2009, Dec. 7-9, 2009. Page(s):1-4
- [P125] Gerhard Klimeck, Mathieu Luisier, "Performance Comparisons of Tunneling Field-Effect Transistors made of InSb, Carbon, and GaSb-InAs Broken Gap Heterostructures", IEDM 2009, Dec. 7-9, 2009. Page(s):1-4
- [P124] Gerhard Klimeck, Neophytos Neophytou, Hans Kosina, "Diameter, orientation, and bias dependence of injection velocity and capacitance in Si nanowires: An atomistic tight-binding study", IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009. Page(s):1-4
- [P123] Gerhard Klimeck, Mathieu Luisier, "Investigation of In_xGa_{1-x}As Ultra-Thin-Body Tunneling FETs using a Full-Band and Atomistic Approach", IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009. Page(s):1-4
- [P122] Mincheol Shin, Sunhee Lee, "k.p-based Quantum Transport Simulation of Silicon Nanowire pMOSFETs", Nanotechnology, 2009. IEEE-NANO 2009. 9th IEEE Conference on Publication Year: 2009, Page(s): 374 - 377
- [P121] Benjamin Haley, Sunhee Lee, Mathieu Luisier, Gerhard Klimeck, Hoon Ryu, Faisal Saied, Steven Clark, Hansang Bae, "Advancing Nanoelectronic Device Modeling through Peta-Scale Computing and Deployment on nanoHUB", Proceedings of the SciDAC Conference, San Diego, June 15-19, 2009, J. Phys.: Conf. Ser. Vol. 180, 012075 (16pp)
- [P120] Gerhard Klimeck, Mathieu Luisier, "Performance limitations of graphene nano ribbon tunneling FETS due to line edge roughness", IEEE Device Research Conference, June 22-24, 2009. Page(s):201-202
- [P119] Kyle Montgomery, Samarth Agarwal, Gerhard Klimeck, Jerry Woodall, "Proposal of ZnSe/GaAs Digital Alloys for High Band Gap Solar Cells and True Green LEDs", 2009 IEEE Nanotechnology Materials and Devices Conference (NMDC 2009), June 2-5, 2009, Traverse City, Michigan, USA. Page(s):217-220
- [P118] Gerhard Klimeck, Dragica Vasileska, "ABACUS and AQME: Semiconductor Device and Quantum Mechanics Education on nanoHUB.org", to appear in IEEE proceedings of the 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009. Page(s): 1-4
- [P117] Sunhee Lee, Hoon Ryu, Zhengping Jiang, Gerhard Klimeck, "Million Atom Electronic Structure and Device Calculations on Peta-Scale Computers", to appear in IEEE proceedings of the 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009. Page(s):1-4
- [P116] Hoon Ryu, Sunhee Lee, Gerhard Klimeck, "A Study of Temperature-dependent Properties of n-type delta-doped Si Band-structures in Equilibrium", to appear in IEEE proceedings of the 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009. Page(s):1-4

- [P115] Muhammad Usman, Hoon Ryu, Gerhard Klimeck, "Quantum Confined Stark Shift and Ground State Optical Transition Rate in [P100] Laterally Biased InAs/GaAs Quantum Dots", to appear in IEEE proceedings of the 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009. Page(s):1-4
- [P114] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "On the validity of the top of the barrier quantum transport model for ballistic nanowire MOSFETs", to appear in IEEE proceedings of the 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009. Page(s):1-4
- [P113] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Surface and Orientation dependence on performance of Trigated Silicon Nanowire pMOSFETs", proceedings of 7th IEEE Workshop on Microelectronics and Electron Devices (WMED 2009), Apr 03, 2009. Page(s):1-4
- [P112] Gabriel Lansbergen, Rajib Rahman, J. Caro, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Transport spectroscopy of a single atom in a FinFET", Journal of Physics: Conference Series 2008, Vol 109, pp 012003
- [P111] Gabriel Lansbergen, Rajib Rahman, J. Caro, Jerry Woodall, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Addressing the charge and spin of a single dopant atom in a nano MOSFET", proceedings of the MRS Fall Meeting, Boston, Dec. 1-4, 2008
- [P110] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, J. Caro, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Atomistic Understanding of a Single Gated Dopant Atom in a MOSFET", proceedings of the MRS Spring meeting 2008 San Francisco 2008
- [P109] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, P.E. Rutten, J. Caro, Jerry Woodall, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Determination of the eigenstates and wavefunctions of a single gated As donor", International Conference on Nanoscience and Nanotechnology, ICONN 2008, Feb. 25-29, 2008, Page(s):164-167
- [P108] Gerhard Klimeck, Mathieu Luisier, "From NEMO1D and NEMO3D to OMEN: moving towards atomistic 3-D quantum transport in nano-scale semiconductors", INVITED paper in IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008
- [P107] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, J. Caro, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Transport-based dopant mapping in advanced FinFETs", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008
- [P106] Mathieu Luisier, Neophytos Neophytou, Neerav Kharche, Gerhard Klimeck, "Full-Band and Atomistic Simulation of Realistic 40 nm InAs HEMT", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008
- [P105] Mathieu Luisier, Gerhard Klimeck, "A multi-level parallel simulation approach to electron transport in nano-scale transistors", Supercomputing 2008, Austin TX, Nov. 15-21 2008. Regular paper - 59 accepted papers, 277 submissions (21%), preprint. Page(s):1-10
- [P104] Hoon Ryu, Gerhard Klimeck, "Contact Block Reduction Method for Ballistic Quantum Transport with Semi-empirical sp³d⁵s* Tight Binding Band Models", IEEE Proceedings of the 2008 International Conference on Solid-State and Integrated-Circuit Technology (ICSICT), Pages 349-352, October 20-23, 2008, Beijing, China.
- [P103] Mathieu Luisier, Gerhard Klimeck, "Full-band and atomistic simulation of n- and p-doped double-gate MOSFETs for the 22nm technology node", 2008 International Conference on Simulation of Semiconductor Processes and Devices, SISPAD 2008, September 9-11, 2008, Yumoto Fujiya Hotel, Hakone, Japan, pages 17-20
- [P102] Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, Timothy Boykin, Gerhard Klimeck, "A parallel sparse linear solver for nearest-neighbor tight-binding problems", 14th International Conference on Parallel and Distributed Computing. August 26-29, Las Palmas de Gran Canaria, Spain, 89 accepted papers out of 264 submissions.
- [P101] Gerhard Klimeck, Michael McLennan, Mark Lundstrom, George Adams III., "nanoHUB.org - online simulation and more materials for semiconductors and nanoelectronics in education and research", 8th IEEE Conference on Nanotechnology, 2008. NANO '08. Aug. 18-21 2008 Page(s):401-404
- [P100] Muhammad Usman, Shaikh Ahmed, Gerhard Klimeck, "Atomistic tight binding study of strain-reduced confinement potentials in identical and non-identical InAs/GaAs vertically stacked quantum dots", 8th IEEE Conference on Nanotechnology, 2008. NANO '08. Aug. 18-21 2008 Page(s):541-544
- [P99] Mathieu Luisier, Gerhard Klimeck, "OMEN an atomistic and full-band quantum transport simulator for post-CMOS nanodevices", 8th IEEE Conference on Nanotechnology, 2008. NANO '08. Aug. 18-21 2008 Page(s):354-357
- [P98] Abhijeet Paul, Neophytos Neophytou, Gerhard Klimeck, "Orientation dependence of the charge distribution and quantum capacitance in silicon nanowire transistors", Proceedings of TECHCON 2008, Austin, TX, September 15 - 16, 2008, 50% acceptance rate.

- [P97] Amritanshu Palaria, Alejandro Strachan, Gerhard Klimeck, "Electronic Structure and Transport in Silicon Nano-Structures with Non-Ideal Bonding Environments", Proceedings of TECHCON 2008, Austin, TX, September 15 - 16, 2008, 50% acceptance rate.
- [P96] Samarth Agarwal, Gerhard Klimeck, "1D hetero-structure tool for atomistic simulation of nano-devices", Austin, TX, September 15 - 16, 2008, 50% acceptance rate.
- [P95] Muhammad Usman, Dragica Vasileska, Gerhard Klimeck, "Strain-Engineered Self Organized InAs/GaAs Quantum Dots for Long Wavelength (1.3-1.5 μ m) Optical Applications", Proceedings of ICPS 2008 (International Conference on the Physics of Semiconductors), Rio de Janeiro, Brazil, July 27-Aug 1, 2008.
- [P94] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Level Spectrum of Single Gated As Donors", Proceedings of ICPS 2008 (International Conference on the Physics of Semiconductors), Rio de Janeiro, Brazil, July 27-Aug 1, 2008 (Oral presentation).
- [P93] Hansang Bae, Steven Clark, Benjamin Haley, Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Mathieu Luisier, Faisal Saied, "A Nano-electronics Simulator for Petascale Computing: From NEMO to OMEN", Proceedings of TeraGrid 2008, June 9-13, 2008, Las Vegas.
- [P92] Clemens Heitzinger, Rick Kennel, Gerhard Klimeck, Norbert Mauser, Michael McLennan, Christian Ringhofer, "Modeling and simulation of field-effect biosensors (BioFETs) and their deployment on the nanoHUB", Journal of Physics: Conference Series, Vol. 107, pg. 012004 (2008).
- [P91] Bhaskaran Muralidharan, Hoon Ryu, Zhen Huang, Gerhard Klimeck, "NEMO-3D based Atomistic Simulation of a Double Quantum Dot Structure for Spin-Blockaded Transport", Proceedings of the 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007. Vol 7, Page(s):403-406
- [P90] Roksana Golizadeh-Mojarad, A.N.M. Zainuddin, Shaikh Ahmed, Gerhard Klimeck, Supriyo Datta, "Atomistic NEGF Simulations of Carbon Nano-Ribbons in Magnetic Fields", Proceedings of The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007
- [P89] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Simulation of nanowire transistors: Atomistic vs. Effective Mass Models", Proceedings of The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007
- [P88] Neerav Kharche, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Electronic Structure and Transmission Characteristics of SiGe Nanowires", Proceedings of The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007
- [P87] Maxim Naumov, Sunhee Lee, Benjamin Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Steven Clark, Gerhard Klimeck, "Eigenvalue Solvers for Atomistic Simulations of Electronic Structures with NEMO-3D", Proceedings of The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007
- [P86] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Self-consistent simulations of nanowire transistors using atomistic basis sets", Proceedings of The 12th International Conference on Simulation of Semiconductor Devices and Processes (SISPAD), Vienna Austria, September 25-27, 2007.
- [P85] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Self-consistent simulations of nanowire transistors using atomistic basis sets", Proceedings of SRC's TECHCON 2007, September 10-12, 2007
- [P84] Hansang Bae, Steven Clark, Gerhard Klimeck, Sunhee Lee, Maxim Naumov, Faisal Saied, "Large Scale Simulations of Nanoelectronic devices with NEMO3-D on the Teragrid", Proceedings of Teragrid 2007 Conference, Madison WI, June 2007.
- [P83] Mark Lundstrom, Jason Clark, Gerhard Klimeck, Arvind Raman, "Nanoelectronics: Metrology and Computation", proceedings of 2007 International Conference on Frontiers of Characterization and Metrology for Nanoelectronics, March 27-29, 2007, National Institutes of Standards and Technology, Gaithersburg, MD. conference proceedings will be published by AIP in a hardback book
- [P82] Shaikh Ahmed, Muhammad Usman, Neerav Kharche, Andrei Schliwa, Gerhard Klimeck, "Atomistic Simulation of Non-Degeneracy and Optical Polarization Anisotropy in Pyramidal Quantum Dots", proceedings of IEEE NEMs Jan 16-19, 2007, pgs. 937-942, Bangkok Thailand. oral presentation, 340 submission, 90% acceptance, 55% oral presentations.
- [P81] Krishna Madhavan, Sebastien Goasguen, Gerhard Klimeck, "The impact of the nanoscale vision on the future of learning and teaching", Proc. SPIE 6328, Nanomodeling II, 63280N (8 September 2006)
- [P80] Eddie Howell, Clemens Heitzinger, Gerhard Klimeck, "Investigation of Device Parameters for Field-Effect DNA-Sensors by Three-Dimensional Simulation", in proceedings of IEEE Nanotechnology Materials and Devices Conference, October 22-25, pg 154, 2006. (about 67% acceptance rate)
- [P79] Clemens Heitzinger, Gerhard Klimeck, "Investigation of Conventional DNAFETs for Genome-wide Detection of Polymorphisms", Proceedings of Eurosensor Conference, Goteborg, Sweden, September 21, 2006

- [P78] Gerhard Klimeck, Timothy Boykin, Mathieu Luisier, Neerav Kharche, Andreas Schenk, "A study of alloyed nanowires from two perspectives: Approximate dispersion and transmission", proceedings of the 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006, AIP Conference Proceedings Volume 893, pp 711-712
- [P77] Shaikh Ahmed, Muhammad Usman, Clemens Heitzinger, Rajib Rahman, Andrei Schliwa, Gerhard Klimeck, "Symmetry Breaking and Fine Structure Splitting in Self-Assembled Zincblende Quantum Dots: Atomistic Simulations of Long-Range Strain and Piezoelectric Field", proceedings of the 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006, AIP Conference Proceedings Volume 893, pg 849
- [P76] Muhammad Usman, Shaikh Ahmed, Marek Korkusinski, Clemens Heitzinger, Gerhard Klimeck, "Strain and electronic structure interactions in realistically scaled quantum dot stacks", proceedings of the 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006, AIP Conference Proceedings Volume 893, pg 849.
- [P75] Gerhard Klimeck, Michael McLennan, Matteo Mannino, Marek Korkusinski, Clemens Heitzinger, Rick Kennel, Steven Clark, "NEMO 3-D and nanoHUB: Bridging Research and Education", proceedings of IEEE-NANO 2006. Sixth IEEE Conference on Nanotechnology, 17-20 June 2006, Vol. 2, pg. 441-444
- [P74] Clemens Heitzinger, Gerhard Klimeck, "Computational aspects of the three-dimensional feature-scale simulation of silicon-nanowire field-effect sensors for DNA detection", Extended Abstract in Proceedings of 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [P73] Mathieu Luisier, Gerhard Klimeck, Andreas Schenk, Wolfgang Fichtner, "Transport Calculation of Semiconductor Nanowires Coupled to Quantum Well Reservoirs", Extended Abstract in Proceedings of 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006
- [P72] Gianluca Fiori, Giuseppe Iannaccone, Gerhard Klimeck, "Coupled mode space vs Real space approach for the simulation of CNT-FETs", Extended Abstract in Proceedings of 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006. Vol 6, Issue:4, Page(s):475-480
- [P71] Neophytos Neophytou, Shaikh Ahmed, M. Anantram, Gerhard Klimeck, "Non-Equilibrium Green's Function (NEGF) Simulation of Metallic Carbon Nanotube Transistors: Impact of Vacancy Defect ", Extended Abstract in Proceedings of 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [P70] Vladimir Mitin, Nizami Vagidov, Mathieu Luisier, Gerhard Klimeck, "Energy dispersion relations for holes in silicon quantum wells and quantum wires", Extended Abstract in Proceedings of 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [P69] Mark Lundstrom, Gerhard Klimeck, "The NCN: Science, Simulation, and Cyber Services", 2006 IEEE Conference on Emerging Technologies - Nanoelectronics, 10-13 Jan. 2006 Page(s):496 - 500
- [P68] Sebastien Goasguen, Krishna Madhavan, Michael McLennan, Mark Lundstrom, Gerhard Klimeck, "The nanoHUB: A science Gateway for nanotechnology", Proceedings in GGF14 - The Fourteenth Global Grid Forum, Science Gateways workshop, June 27-30, 2005 Chicago, IL, USA
- [P67] Jing Wang, Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, "Bandstructure and orientation effects in ballistic Si and Ge nanowire FETs", 2005 IEEE International Electron Devices Meeting, Washington, DC, December 5 - 7, 2005. (One of 27 accepted out 120 submitted Modeling and Simulation abstracts)
- [P66] Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, "Novel channel materials for ballistic nanoscale MOSFETs bandstructure effects", 2005 IEEE International Electron Devices Meeting, Washington, DC, December 5 - 7, 2005. (One of 27 accepted out 120 submitted Modeling and Simulation abstracts)
- [P65] Gianluca Fiori, Giuseppe Iannaccone, Gerhard Klimeck, "Performance of Carbon Nanotube Field Effect Transistors with doped source and drain extensions and arbitrary geometry", Electron Devices Meeting, 2005. IEDM Technical Digest. IEEE International . Page(s):522-525
- [P64] Wei Qiao, David Ebert, Alireza Entezari, Marek Korkusinski, Gerhard Klimeck, "VolQD: direct volume rendering of multi-million atom quantum dot simulations", IEEE Visualization 2005, October 23-28, Minneapolis, Minnesota, USA, one of 88 accepted from 268 submissions
- [P63] Gianluca Fiori, Giuseppe Iannaccone, Mark Lundstrom, Gerhard Klimeck, "Three-dimensional atomistic simulation of Carbon Nanotube FETs with realistic geometry", European Solid-State Device Research Conference, ESSDERC, Grenoble, France, 12 - 16 September 2005, pages 537-540
- [P62] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Atomistic simulations of long-range strain and spatial asymmetry effects in multimillion-atom single and double quantum dot nanostructures", SISPAD 2005, International Conference on Simulation of Semiconductor Processes and Devices, Komaba Eminence, Tokyo, Japan, September 1-3, 2005. pg 335-338
- [P61] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org and Atomistic simulations of multimillion-atom quantum dot nanostructures", Proceedings of the 5th IEEE Conference on Nanotechnology, July 11-15, pg 807, Vol 2 (2005)

- [P60] Richard Terrile, Hrand Aghazarian, Michael Ferguson, W. Fink, Terrance Huntsberger, Didier Keymeulen, Gerhard Klimeck, Mark Kordon, Seungwon Lee, Paul Allmen, "Evolutionary Computation Technologies for the Automated Design of Space Systems", Proceedings. 2005 NASA/DoD Conference on Evolvable Hardware, 2005. 29 June-1 July 2005, pg 131-138
- [P59] Marek Korkusinski, Gerhard Klimeck, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Atomistic Simulations in Nanostructures Composed of Tens of Millions of Atoms: Importance of long-range Strain Effects in Quantum Dots", 2005 NSTI Nanotechnology Conference and Trade Show, Anaheim, CA, May 8-12, 2005.
- [P58] Sebastien Goasguen, Michael McLennan, Gerhard Klimeck, Mark Lundstrom, "What do Mambo, VNC, UML and Grid computing have in common?", 2005 Linux Cluster Institute Conference, Raleigh, NC, April, 2005
- [P57] Marek Korkusinski, Faisal Saied, Haiying Xu, Seungwon Lee, Mohammed Sayeed, Sebastien Goasguen, Gerhard Klimeck, "Large Scale Simulations in Nanostructures with NEMO3-D on Linux Clusters", 2005 Linux Cluster Institute Conference, Raleigh, NC, April, 2005
- [P56] Richard Terrile, Christoph Adami, Hrand Aghazarian, Savio Chau, Van Dang, Michael Ferguson, Wolfgang Fichtner, Terrance Huntsberger, Gerhard Klimeck, Mark Kordon, Seungwon Lee, Paul Allmen, Joseph Xu, "Evolutionary Computation Technologies for the Automated Design of Space Systems", IEEE Aerospace Conference Proceedings, 5-12 March 2005 Page(s):1 - 12 .
- [P55] Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, "Bandstructure Effects in Nanoscale MOSFETs", IEEE IEDM, San Francisco, CA, Dec. 6-8 2004, pgs. 139-142
- [P54] E. Khorenko, W. Prost, F.-J. Tegude, M. Stoffel, R. Duschl, M. Dashiell, O.G. Schmidt, Gerhard Klimeck, "Manufacturability and Electrical Characteristics of Si/SiGe Interband Tunnelling Diodes", ASDAM '04, Proceedings of The Fifth International Conference on Advanced Semiconductor Devices and Microsystems, Smolenice Castle, Slovakia, Oct. 17-21, 2004, IEEE Catalog Number 04EX867, ISBN 0-7803-8535-7, Library of Congress: 2004105360
- [P53] Seungwon Lee, Paul Allmen, Fabiano Oyafuso, Gerhard Klimeck, Timothy Boykin, Susan Coppersmith, Mark Friesen, Mark Eriksson, "Electron Exchange Interaction in Electronically Confined Si Quantum Dots", IEEE proceedings of the 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, 2004. Page(s):115
- [P52] Yun Zheng, Christian Rivas, Roger Lake, Khairul Alam, Timothy Boykin, Gerhard Klimeck, "Electronic Properties of Silicon Nanowires", IEEE proceedings of the 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, 2004
- [P51] Anisur Rahman, Gerhard Klimeck, Nizami Vagidov, Timothy Boykin, Mark Lundstrom, "Nanoscale Device Simulation at the Scaling Limit and Beyond", International Conference on Solid State Devices and Materials (SSDM 2004), Tokyo, Japan, Sept. 14-17, 2004.
- [P50] Gerhard Klimeck, "NEMO 1-D: the first NEGF-based TCAD tool", IEEE SISPAD 2004, Keynote Speaker, Munich, Germany, September 2-4, 2004
- [P49] Ahmet Yanik, Prabhakar Srivastava, Gerhard Klimeck, Supriyo Datta, "Coherent Transport in SWCNTs with Spin-Orbit Coupling", IEEE Nano 2004, pgs. 89-91, Munich, Germany, August 16-19, 2004

Work Performed at JPL (31 Total)

- [P48] Olga Lazarenkova, Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "The effect of the strain relaxation in InAs/GaAs stacked quantum dots and multiple quantum wells on the Raman spectrum", 12-th International Symposium "Nanostructures: Physics and Technology" June 21-25, 2004, St Petersburg, Russia
- [P47] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, Olga Lazarenkova, "Coupled electron and nuclear spin dynamics in InAs quantum dots: impact on single and two-qubit operations", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004
- [P46] Seungwon Lee, Olga Lazarenkova, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Effect of wetting layers on the strain and electronic structure of InAs self-assembled quantum dots", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [P45] Olga Lazarenkova, Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "Atomistic-Level Simulation of the Vibration Spectrum of Quantum Dot Crystals", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [P44] Mark Kordon, Gerhard Klimeck, Dave Hanks, Hook Hua, "Evolutionary Computing for Spacecraft Power Subsystem Design Search and Optimization", Proceedings of IEEE Aerospace Conference, Big Sky, Montana, March 2004, pg 4004-4014.
- [P43] Seungwon Lee, Paul Allmen, Fabiano Oyafuso, Gerhard Klimeck, K. Whaley, "Electron spin dephasing and decoherence by interaction with nuclear spins in self-assembled quantum dots", published in proceedings of Winter International Symposium on Information and Communication Technologies, January 5-8, 2004, Cancun, Mexico.
- [P42] Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, "Conduction band valley splitting in silicon nano-structures", Sixth International

- Conference on New Phenomena in Mesoscopic Structures, Fourth International Conference on Surfaces and Interfaces of Mesoscopic Devices, December 1-5, 2003, Maui, Hawaii.
- [P41] Seungwon Lee, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Numerical surface treatment for finite-extent semiconductor nanostructures", 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona, Spain. October 16-17 2003.
- [P40] Hans Kosina, Gerhard Klimeck, Michail Nedjalkov, Siegfried Selberherr, "Comparison of Numerical Quantum Device Models", International Conference on Simulation of Semiconductor Processes and Devices (SISPAD 2003), September 3-5, 2003, Boston, MA, pages 171 -174
- [P39] Gerhard Klimeck, Gary Yagi, Robert Deen, Michael McAuley, Eric DeJong, Fabiano Oyafuso, "Near Real-Time Parallel Image Processing using Cluster Computers", International Conference on Space Mission Challenges for Information Technology (SMC-IT), Pasadena, CA July 13-16, 2003.
- [P38] Fabiano Oyafuso, Gerhard Klimeck, Timothy Boykin, R. Bowen, Paul Allmen, "Study of Strain Boundary Conditions and GaAs Buffer Sizes in InGaAs Quantum Dots", Extended Abstract in Proceedings of International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [P37] Gerhard Klimeck, Phillip Stout, R. Bowen, "Quantum and semi-classical transport in RTDs using NEMO 1-D", Extended Abstract in Proceedings of International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [P36] Jeremy Green, Corrie Farmer, Michel Garcia, Hock Lee, Colin Stanley, Charles Ironside, Gerhard Klimeck, Roger Lake, "Quantum cascade laser simulation using an sp^3s^* full Brillouin zone tight-binding model", 2003 Conference on Lasers and Electro-Optics Europe, CLEO/Europe. Munich, 22-27 June 2003 Page(s):182
- [P35] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, Paul Allmen, "Study of Alloy Disorder in Quantum Dots Through Multi-million Atom Simulations", Pasadena, CA: Jet Propulsion Laboratory, National Aeronautics and Space Administration, 2003.
- [P34] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, "Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems", SISPAD 2002, Kobe, Japan, Sept. 3-6, pg 163 - 166, 2002
- [P33] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, Paul Allmen, "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", The first International Workshop on Quantum Dots for Quantum Computing and Classical Size Effect Circuits, Kochi, Japan, Jan 26-28, 2002
- [P32] Tom Cwik, Gerhard Klimeck, Michael McAuley, Bob Deen, Eric DeJong, "Applications on High Performance Cluster Computers Production of Mars Panoramic Mosaic Images", Proceedings of the 2001 AMOS Technical Conference September 10-14, 2001, Maui
- [P31] Gerhard Klimeck, "Full Brillouin-Zone, Charge Self-consistent Quantum Transport Simulations Enabled by Parallelization of the Nanoelectronic Modeling Tool (NEMO 1-D) on a Beowulf Cluster", 8th International Workshop on Computational Electronics October 15-18, 2001, Univ. of Illinois, Extended abstract in conference handout.
- [P30] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", 8th International Workshop on Computational Electronics October 15-18, 2001, Univ. of Illinois. Extended abstract in conference handout.
- [P29] Tom Cwik, Gerhard Klimeck, Charles Norton, Thomas Sterling, Frank Villegas, Ping Wang, "The Use of Cluster Computers Systems for NASA/JPL Applications", Proceedings of AIAA Space 2001 Conference and Exposition Albuquerque, New Mexico 28-30 August 2001.
- [P28] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Large-Scale Design and Optimization Using Cluster Computers", Proceedings of IEEE AP-S International Symposium and USNC/URSI National Radio Science Symposium, Boston, MA, July 8-13 (2001)
- [P27] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Atomistic simulation of quantum dots including strain and bandstructure and full band simulation of hole transport in 1-D heterostructures", 7th International Workshop on Computational Electronics, 2000, Univ. of Glasgow, book of abstracts, pages 6-7
- [P26] Didier Keymeulen, Gerhard Klimeck, Ricardo Zebulum, Adrian Stoica, Yili Jin, Carlos Salazar-Lazaro, "EHWPack: an Evolvable Hardware Environment using the Spice Simulator and the Field Programmable Transistor Array", In the Proceedings of ANNIE 2000 (Smart Engineering System Design), St. Louis, MO, November 5-8, 2000
- [P25] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Transverse Momentum Dependence of Electron and Hole Tunneling in a Full Band Tight-Binding Simulation", Proceedings of the 27th international Symposium on Compound Semiconductors (ISCS), IEEE, pg. 257 (2000)
- [P24] Adrian Stoica, Didier Keymeulen, Ricardo Zebulum, Anil Thakor, Taher Daud, Gerhard Klimeck, Yili Jin, R. Tawel, Vu Duong, "Evolution of analog circuits on field programmable transistor arrays", Proceedings of 2nd NASA/DoD Workshop on Evolvable Hardware, July 13-15, pg. 99-108, 2000

- [P23] Didier Keymeulen, Gerhard Klimeck, Ricardo Zebulum, Adrian Stoica, Carlos Salazar-Lazaro, "EHWPack: A Parallel Software/Hardware Environment for Evolvable Hardware", In Whitley Darrell (eds.), Proceedings of the Genetic and Evolutionary Computation Conference (GECCO-2000), July 8-12, 2000, Las Vegas, Nevada USA. San Francisco, CA: Morgan Kaufmann.
- [P22] Adrian Stoica, Gerhard Klimeck, Carlos Salazar-Lazaro, Didier Keymeulen, Anil Thakor, "Evolutionary Design of Electronic Devices and Circuits", Proceedings of the 1999 Congress on Evolutionary Computation, IEEE, CEC 99, Vol. 2, Pages: 1271-1278
- [P21] Tom Cwik, Gerhard Klimeck, "Genetically Engineered Microelectronic Infrared Filters", Proceedings of the First NASA/DoD Workshop on Evolvable Hardware, IEEE 1999 , Page(s): 242 -246.
- [P20] Gerhard Klimeck, Carlos Salazar-Lazaro, Adrian Stoica, Thomas Cwik, "Genetically Engineered Nanoelectronics", Proceedings of the First NASA/DoD Workshop on Evolvable Hardware, IEEE 1999 , Page(s): 247 -248.
- [P19] Tom Cwik, Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", Proceedings of 1999 Aerospace Conference, IEEE Volume: 5 , 1999 , Page(s): 131 -138
- [P18] Gerhard Klimeck, Carlos Salazar-Lazaro, Adrian Stoica, Tom Cwik, "Genetically Engineered Nanostructure Devices", in "Materials in Space Science, Technology, and Exploration" MRS Symposium Proceedings, Vol. 551, pg. 149 (1999).

Work Performed at UTD/TI (14 Total)

- [P17] Daniel Blanks, Gerhard Klimeck, Roger Lake, R. Bowen, Manhua Leng, Chenjing Fernando, William Frensley, Dejan Jovanovic, "NEMO Quantum Device Simulator", 1998 Government Microcircuit Applications Conference Digest of Papers (GOMAC), March 1998, p. 218.
- [P16] R. Bowen, Chenjing Fernando, Gerhard Klimeck, Amitava Chatterjee, Daniel Blanks, Roger Lake, J. Hu, Joseph Davis, M. Kularni, Sunil Hattangady, Cheng-Kok Koh, "Physical Oxide Extraction and Versification using Quantum Mechanical Simulation", Proceedings of IEDM 1997, IEEE, 869 (1997)
- [P15] R. Bowen, Chenjing Fernando, Gerhard Klimeck, Amitava Chatterjee, Daniel Blanks, Roger Lake, Jerry Woodall, Joseph Davis, Mak Kulkarni, Sunil Hattangady, Cheng-Kok Koh, "Dopant Fluctuations and Quantum Effects in Sub-0.1um CMOS", Proceedings of the 1997 International Semiconductor Device Research Symposium, p. 1.
- [P14] Roger Lake, Berinder Brar, Glen Wilks, Alan Seabaugh, Gerhard Klimeck, "Resonant Tunneling in Disordered Materials such as SiO₂/Si/SiO₂", Proceedings of the 24th International Symposium on Compound Semiconductors, September 8-11, San Diego, CA, (1997). Inst. Phys. Conf. Ser. 156: 617-620, 1998
- [P13] Daniel Blanks, Gerhard Klimeck, Roger Lake, Dejan Jovanovic, R. Bowen, Chenjing Fernando, William Frensley, Manhua Leng, "NEMO: General Release of a New Comprehensive Quantum Device Simulator", Proceedings of the Twenty-Forth International Symposium on Compound Semiconductors, IEEE, NJ (1997). Inst. Phys. Conf. Ser. 156: 639-642, 1998
- [P12] J. Wagt, Alan Seabaugh, Gerhard Klimeck, Shaikh Ahmed, Timothy Boykin, R. Bowen, Roger Lake, "Ultralow Current Density RTDs for Tunneling-based SRAM", Proceedings of the 24th International Symposium on Compound Semiconductors, September 8-11, San Diego, CA, (1997). Inst. Phys. Conf. Ser. 156: 601-604, 1998.
- [P11] Daniel Blanks, Gerhard Klimeck, Roger Lake, R. Bowen, William Frensley, Manhua Leng, Chenjing Fernando, "Nanoelectronic Modeling (NEMO): A New Quantum Device Simulator", Proceedings of The Second NASA Device Modeling Workshop, August 7-8, 1997, page 70-84, Edited by Subhash Saini. You can request a copy of this from NAS Library, MS 258-5, NASA Ames research center, Moffett Field, CA 94035-1000.
- [P10] Gerhard Klimeck, Timothy Boykin, R. Bowen, Roger Lake, Daniel Blanks, Ted Moise, Y. Kao, William Frensley, "Quantitative Simulation of Strained InP-Based Resonant Tunneling Diodes", in Proceedings of the 1997 55th IEEE Device Research Conference Digest, IEEE, NJ, p. 92 (1997)
- [P9] Gerhard Klimeck, Daniel Blanks, Bobby Brar, Tom Broekaert, Gary Frazier, Dejan Jovanovic, Roger Lake, Ted Moise, Alan Seabaugh, Glen Wilks, Paul Wagt, Chenjing Fernando, R. Bowen, William Frensley, "Design and Implementation of Resonant Tunneling Devices into Circuits and Applications", in Proceedings of PHASDOM 97, Phantoms Strategic Domain Meetings, Aachen, Germany 10-13 March 1997.
- [P8] Roger Lake, Gerhard Klimeck, "Experimentally Verified Quantum Device Simulations Based on Multiband Models, Hartree Selfconsistency, and Scattering Assisted Charging", in Proceedings of the 1996 54th IEEE Device Research Conference Digest, IEEE, NJ, p. 174, 1996
- [P7] William Frensley, R. Bowen, Chenjing Fernando, Gerhard Klimeck, Roger Lake, "Quantitatively Accurate Simulation of Quantum Semiconductor Devices", Proceedings of International Workshop on Physics and Computer Modeling of Devices Based on Low-Dimensional Structures. IEEE Comp. Soc. Press, Los Alamitos, CA, p.2-5, 1996
- [P6] Gerhard Klimeck, Roger Lake, Chenjing Fernando, R. Bowen, Daniel Blanks, Manhua Leng, Ted Moise, Y. Kao, William Frensley, "Numerical Approximations for Polar Optical Phonon Scattering in Resonant

Tunneling Diodes in Quantum Devices and Circuits", edited by K. Ismail, S. Bandyopadhyay, ed J. P. Leburton, Imperial Press London (1996).

- [P5] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, William Frensley, "Nanoelectronic Modeling (NEMO)", in Proceedings of the 1995 53rd Device Research Conference Digest, IEEE, NJ p. 52, 1995
- [P4] Gerhard Klimeck, R. Bowen, William Frensley, "Efficient I-V simulation of quantum devices using full bandstructure models", Proceeding of IEEE Cornell Conference on Advanced Concepts in High Speed Semiconductor Devices and Circuits, IEEE, New York, NY, p.435, 1995

Work Performed in Graduate School (3 total)

- [P3] Gerhard Klimeck, Roger Lake, Supriyo Datta, M. Anantram, "Resonant Tunneling devices: Effect of Scattering", International Symposium on Compound Semiconductors, San Diego, Sept. 18-24, 1994. Inst. Phys. Conf. Ser. No 141
- [P2] Gerhard Klimeck, Roger Lake, Supriyo Datta, "The Phonon Peak in Resonant Tunneling Diodes", Journal of the Electrochemical Society, (1995)
- [P1] Gerhard Klimeck, Roger Lake, Supriyo Datta, Garnett Bryant, "High Bias Transport through Quantum Dots", Journal of the Electrochemical Society, (1995)

INVITED CONFERENCES (273 +11 TOTAL)**Work Performed at Purdue (237 +11 total)**

- [I285] Gerhard Klimeck, "Quantum transport with NEMO and online simulation with nanoHUB ", Winter School on III-Sb Applications Non-Volatile memories – A modelling perspective, Berlin, Germany, Feb. 27-Mar.3, 2023
- [I284] Gerhard Klimeck, "Atomistic, multi-scale, multi-physics quantum transport models for quantitative, predictive nanoscale device designs", 53rd Winter Colloquium on the Physics of Quantum electronics, Snowbird UT, Jan 8-13, 2023. Attendance by invitation only.
- [I283] Gerhard Klimeck, "Semiconductor workforce development through immersive simulations on nanoHUB.org", Second International Conference on Carbon Chemistry and Materials at Rome, Italy on October 10-12, 2022 (virtual)
- [I282] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", Purdue University Cyberinfrastructure Symposium, Oct. 4, 2022.
- [I286] Gerhard Klimeck, "nanoHUB Integration into Semiconductor Education", Computing in Engineering Forum, University of Wisconsin, Madison (virtual), Sept. 20, 2022.
- [I280] Gerhard Klimeck, Lynn Zentner, Alejandro Strachan, Michael Zentner, Daniel Mejia, Tanya Faltens, "Semiconductor workforce development through immersive simulations on nanoHUB.org", International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), one of four invited presentations, Sept. 5-9, 2022, Granada, Spain.
- [I279] Gerhard Klimeck, "Semiconductor workforce development through immersive simulations on nanoHUB.org", Academia International Webinar on Materials Science & Engineering, August 15 - 16, 2022.
- [I278] Gerhard Klimeck, Lynn Zentner, Alejandro Strachan, Michael Zentner, Daniel Mejia, Tanya Faltens, "Semiconductor Workforce Development Through Immersive Simulations on nanoHUB.org", Keynote Address, Global Web Forum on Applied Science and Engineering, August 4-5, 2022, <https://auragengroup.com/gwfase-2022/index.php>
- [I277] Gerhard Klimeck, "Overview of nanoelectronics modeling – From Obscure theory to Today's Standard", SiNano Summer School, July 12-16, 2022, Glasgow, UK.
- [I276] Gerhard Klimeck, "Atomistic, multi-scale, multi-physics models for quantitative, predictive nanoscale device designs " in session "Quantum Transport Basics and Theory", CECAM Workshop on "Quantum Transport Methods and Algorithms: From Particles to Waves Approaches" (July 6th – 8th 2022) Zurich Switzerland.
- [I275] Gerhard Klimeck, "nanoHUB: serving millions of learners, teachers, and researchers in one overarching platform", Quantum Science Center, 2nd Annual Quantum Summer School, Purdue University, May 8-12, 2022.
- [I274] Gerhard Klimeck, "nanoHUB.org: immersive online semiconductor education and workforce development with broad academic adoption", Education and Workforce Development for the U.S. Microelectronics Industry – Innovative Approaches and Best Practices for Preparing and Expanding the U.S. Semiconductor Workforce, SUNY/MIT/RPI – online, Feb. 3, 2022
- [I273] Gerhard Klimeck, Alejandro Strachan, Tanya Faltens, Lynn Zentner, Michael Zentner, Elif Ertekin, "Using nanoHUB.org in Research and Education – a Hands-on Tutorial", IEEE NMDC Conference, Dec. 12-15, 2021
- [I272] Gerhard Klimeck, Alejandro Strachan, Lynn Zentner, Michael Zentner, "nanoHUB.org – always 'on' - New Paradigms in Global Scientific Knowledge Transfer, Publishing, and Assessment", Virtual Conference Materials Science and Nanotechnology-2021, September 17-18, 2021
- [I271] Gerhard Klimeck, Alejandro Strachan, Lynn Zentner, Michael Zentner, "nanoHUB.org – always 'on' - New Paradigms in Global Scientific Knowledge Transfer, Publishing, and Assessment", Webinar on Nanotechnology, Recent Advancements in the field of Nanoscience and Nanotechnology, August 31, 2021
- [I270] Gerhard Klimeck, "nanoHUB.org – always "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", 3rd Edition of Webinar on Nanotechnology, Nano 2021, Endeavor Conferences, Virtual Event. August 2&3, 2021.
- [I269] Gerhard Klimeck, Alejandro Strachan, Lynn Zentner, Michael Zentner, "nanoHUB.org – always "on" New paradigms in global scientific knowledge transfer, publishing, and assessment", The 3rd International Conference on Computing and Data Science (CONF-CDS), <https://www.confcds.org/> Aug. 12-17, 2021, Stanford University (Online Event)
- [I268] Gerhard Klimeck, Alejandro Strachan, Lynn Zentner, Michael Zentner, "nanoHUB.org – always "ON": New Paradigms in Global Scientific Knowledge Transfer, Publishing, and Assessment" Nano 2021, Endeavor Conferences, Virtual Event. March 23, 2021.
- [I267] Gerhard Klimeck, "The nanoHUB Platform", NITRD Big Data Interagency Virtual Workshop on Pioneering the Future of Federally Supported Data Repositories Wednesday Jan 13th - Friday Jan 15th, 2021 <https://www.orau.gov/bdworkshop21>
- [I266] Gerhard Klimeck, "The nanoHUB Platform", 2021 NNI Strategic Planning Stakeholder Workshop, January 11-13, 2021, National Nanotechnology Coordination Office

- [I265] Gerhard Klimeck, "The nanoHUB Platform", Nanoscientific Symposium, Park Systems, Oct. 10, 2020, Virtual Conference.
- [I264] Gerhard Klimeck, "A Single Atom Transistor: The Ultimate Scaling Limit – Calibration for Atomistic Device Models", 28th International Symposium "Nanostructures: Physics and Technology", Virtual Conference, Oct. 2, 2020, Moscow/St. Petersburg.
- [I263] Jennifer E Hoffman, Jay Deep Sau, James R Williams, Gerhard Klimeck, "Majorana Nanomanipulation for Topological Quantum Computing", OSA, NSF Quantum Leaps Grantees Conference, Sept. 29, 2020.
- [I262] Gerhard Klimeck, "Quantum Computing: Myth or Reality – Computer Aided Design Automation", ESSDRG, Virtual Conference, Sept. 4, 2020, Belgium.
- [I261] Gerhard Klimeck, Alejandro Strachan, "nanoHUB role in nanoinformatics and nanoHUB: online simulation and data", 2019 NSF Nanoscale Science and Engineering Grantees Conference, Dec. 9-10, 2019, Alexandria, VA
- [I260] Gerhard Klimeck, "The Single-Atom Transistor: How it was Created and What it may Mean for the Future", Keynote speech at the 1st International Symposium on Single Atom Electronics, Joint Institute University of Michigan-Shanghai Jiao Tong University Joint Institute (JI), Oct. 13, 2019 in Shanghai, China.
- [I259] Gerhard Klimeck, "nanoHUB.org – always "ON": New Paradigms in Global Scientific Knowledge Transfer, Publishing, and Assessment", 2019 Latin American Optics & Photonics Workshop, Cancún, Mexico, Monday, September 30, 2019
- [I258] Michael Zentner, Stephen Burley, Gerhard Klimeck, Emre Brookes, Mark Miller, Sabine Brunswicker, Dan Stanzione, Sharon Tettegah, "Impact Measurement Strategies for Science Gateways: Present and Future", PEARC Practice & Experience in Advanced Research Computing, Chicago, IL, July 28-August 1
- [I257] Gerhard Klimeck, Gustavo Valencia-Zapata, Nathan Denny, Lynn Zentner, Michael Zentner, "nanoHUB user behavior: moving from retrospective statistics to actionable behavior analysis", 11th International Workshop on Science Gateways (IWSG 2019), Ljubljana, Slovenia, June 12-14, 2019
- [I256] Gerhard Klimeck, "nanoHUB.org – always "ON": New Paradigms in Global Scientific Knowledge Transfer, Publishing, and Assessment", A Day Dedicated to the Issues in Science and Its Funding, The University of Montenegro, Podgorica, Montenegro, Tuesday, June 11, 2019
- [I255] Gerhard Klimeck, "nanoHUB.org – always "ON": New Paradigms in Global Scientific Knowledge Transfer, Publishing, and Assessment", 8th Mediterranean Conference on Embedded Computing MECO2019, Budva, Montenegro, Monday, June 10, 2019
- [I254] Gerhard Klimeck, "nanoHUB - Always ON - Community Repository and Use", ESA NSF PI Workshop on: Creating and Implementing Sustainability Plans for Data Repositories, Alexandria VA, Thursday, January 25 and Friday, January 26, 2018
- [I253] Gerhard Klimeck, "NEMO5 on Blue Waters – A Flexible Package for Nanoelectronics Modeling Problems", Presentation at Blue Waters Symposium 2018, Sunriver, OR, June 3-7, 2018
- [I252] Gerhard Klimeck, Michael Zentner, Lynn Zentner, Tillmann Kubis, "nanoHUB.org – always "on"", 4th Workshop on Supercomputing for Computational Bio/Nano/Materials Science, Korea Institute of Science Technology Information (KISTI), Daejeon, Korea, July 10-11, 2018
- [I251] Gerhard Klimeck, Junzhe Geng, KuangChung Wang, Prasad Sarangapani, Tillmann Kubis, "NEMO5: Multi-Scale, Multi-Physics, Atomistic Modeling of Superlattice LEDs and Global Impact on nanoHUB.org", 19th International Symposium on the Physics of Semiconductors and Applications (ISPSA 2018), Jeju, Korea, July 1- 5, 2018
- [I250] Gerhard Klimeck, Michael Zentner, Lynn Zentner, Tillmann Kubis, "NEMO5: Multi-Scale, Multi-Physics, Atomistic Modeling of Non-Equilibrium Processes in Nanometer-Scaled Compound Materials For Active Devices and Global Impact on nanoHUB.org", Collaborative Conference on Materials Research (CCMR) 2018, 25 - 29 June 2018, Incheon/Seoul, South Korea
- [I249] Gerhard Klimeck, "nanoHUB In a Nutshell: Translating Traditional Research To New Paradigms In Publishing, Computing, Research, and Education", 2018 NSF SI2 PI meeting, April 30 and May 1, 2018, Washington, D.C., The Westin Washington D.C. City Center
- [I248] Gerhard Klimeck, "Leading Future Electronics Into the Nano Regime Using Quantum Atomistic Simulations in NEMO5", Presentation at Blue Waters Symposium 2017, Sunriver, OR, May 16-19, 2017
- [I247] Xinchun Guo, Daniel Lemus, Daniel Mejia, Jim Fonseca, Gerhard Klimeck, Tillmann Kubis, "NEMO5: A Parallelized Multi-Scale and Multi-Physics Nanodevices Simulation Software", Presentation at SIAM Conference on Computational Science and Engineering, Atlanta, GA, February 27-March 3, 2017
- [I246] Gerhard Klimeck, "Keynote - Nanoscale modeling and simulation", 2017 NSF Nanoscale Science and Engineering Grantees Conference, December 12-13, 2017, Westin Hotel - Arlington, VA
- [I245] Gerhard Klimeck, "Single investigator vs centerlevel team research", EVPRP Workshop: Preparing for Large, CenterLevel Research Proposals, Purdue University, March 21, 2017
- [I244] Gerhard Klimeck, "nanoHUB: Going Beyond Specialized Capabilities", FAME Center 5th Annual Review, February 14-15, 2017, Luskin Conference Center, Los Angeles (UCLA Campus)

- [I243] Gerhard Klimeck, "nanoHUB: translating traditional research to new paradigms in publishing, computing, research, & education", National Science Foundation Seminar, Arlington, VA, Feb 8, 2017
- [I242] Junzhe Geng, Prasad Sarangapani, Carl Wordelman, Erik Nelson, Ben Browne, Tillmann Kubis, Gerhard Klimeck, "NEMO5: realistic and efficient NEGF simulations of GaN light-emitting diodes", Invited talk, SPIE Photonics West OPTO 2017 (Physics and Simulation of Optoelectronic Devices XXV conference), January 30 – February 2, San Francisco, CA
- [I241] Tillmann Kubis, Gerhard Klimeck, Michael Povolotskyi, Jim Fonseca, Xinchun Guo, Daniel Lemus, Daniel Mejia, James Charles, Prasad Sarangapani, KuangChung Wang, "Post-Moore Nanoscale Logic Devices", ALCF Aurora Early Science Program, 2016
- [I240] Gerhard Klimeck, "Knowledge Transfer in nanoHUB^[SEP]World's Largest Nanotech User Facility", 2016 NSF Nanoscale Science and Engineering Grantees Conference, Arlington, VA, Dec 12-13, 2016
- [I239] Gerhard Klimeck, "Success Examples and Challenges of ^[SEP]Multi-Scale and Multi-Expertise ^[SEP]Modeling and Simulations (nanoHUB/NEMO5)", MRS Conference, Boston, Nov. 28, 2016
- [I238] Gerhard Klimeck, "Myth busting knowledge generation and transfer with nanoHUB ", DP Open House, Purdue, Sept 23, 2016
- [I237] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Workshop on Emerging Electronic Materials and Devices (EEMD2016), University of Science and Technology of China (USTC), Hefei, China, July 9-11, 2016
- [I236] Gerhard Klimeck, "Single investigator vs centerlevel team research", EVPRP Workshop: Making the Transition to Strategies for Large, CenterLevel Research Proposals, Purdue University, March 22, 2016
- [I235] Hesameddin Ilatikhameneh, "Novel steep transistors", StarNET E-Workshop, Purdue University, IN, USA (2016)
- [I234] Gerhard Klimeck, "nanoHUB: always ON 24/7", CHiMaD Data, Databases & Discovery Workshop II, Northwestern University, Evanston, IL, May 2, 2016
- [I233] Gerhard Klimeck, "Myth busting knowledge generation and transfer with nanoHUB and NEMO", Workshop on Emerging and timely capabilities and research objectives: High Entropy Materials, Ultra-strong Molecules, and Nanoelectronics, Defense Materials Manufacturing and Infrastructure (DMMI), The National Academies of Sciences, Engineering, Medicine, Keck Center Washington D.C. February 10-11 (Wednesday-Thursday) 500 Fifth Street, NW Washington D.C. 20001
- [I232] Gerhard Klimeck, "Mythbusting Nanotechnology Knowledge Transfer through Novel Cyberinfrastructure", Dawn or Doom conference, Purdue University, West Lafayette, IN, Sept. 24, 2015
- [I231] Gerhard Klimeck, "nanoHUB.org: Novel Knowledge Transfer: What is it? Some History. Future?", Purdue University: Birck Nanotechnology Center - 10th Anniversary Celebration, MRGN 121, October 30, 2015
- [I230] Hesameddin Ilatikhameneh, Fan Chen, Saima Sharmin, Tarek Ameen, Yaohua Tan, Pengyu Long, Jun Huang, Zhengping Jiang, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, Joerg Appenzeller, zhihong chen, Patrick Fay, Mark Rodwell, "STEEP Transistor Modeling with NEMO5", Steep Transistors Workshop, University of Notre Dame, Notre Dame, IN, October 5-6, 2015
- [I229] Mark Rodwell, Cheng-Ying Huang, J. Rode, P. Choudhary, Sanghoon Lee, Arthur Gossard, Pengyu Long, Evan Wilson, Saumitra Mehrotra, Michael Povolotskyi, Gerhard Klimeck, M. Urteaga, B. Brar, Varistha Chobpattana, S. Stemmer, "Transistors for VLSI, for Wireless: A View Forwards Through Fog", 73rd Device Research Conference (DRC), Ohio State University, June 21-24, 2015
- [I228] Mehdi Salmani-Jelodar, Hesameddin Ilatikhameneh, Prasad Sarangapani, Saumitra Mehrotra, SungGeun Kim, Kwok Ng, Gerhard Klimeck, "Tunneling: The Major Issue in Ultra-scaled MOSFETs", IEEE Nano, Rome, Italy, July 26-30, 2015
- [I227] Gerhard Klimeck, "Using Nanohub.Org in Research and Education – A Hands-on Workshop", IEEE Nano, Rome, Italy, July 26-30, 2015
- [I226] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org ", CECD/ME Symposium on Computation-Enabled Materials, 20 May 2015, University of Maryland College Park, MD
- [I225] Michael Zentner, Gerhard Klimeck, Nathan Denny, Dwight McKay, Steve Snyder, Gustavo Valencia, Swaroop Samek, "nanoHUB: the Growth of a United States Cyberinfrastructure into a Global Learning and Research Community", The Eleventh International Nanotechnology Conference on Communication and Cooperation (INC 11), Hilton Fukuoka Sea Hawk, Fukuoka, Japan, May 11-13, 2015.
- [I224] Gerhard Klimeck, "Marching Towards The End of The Transistor Roadmap with NEMO: From MOS devices to Tunneling Devices and Single Atom Transistors", Workshop: Current Topics in Nano Simulations (CT-NanoSim2014), Tsukuba, Japan, March 11, 2014
- [I223] Gerhard Klimeck, "NEMO - Nanoelectronic Modeling: for HPC, Industry, Research and for everyone on nanoHUB.org", EPASA2014, Tsukuba, Japan, March 6-8, 2014

- [I222] Krishna Madhavan, Gerhard Klimeck, "Next generation cyberinfrastructure for the nanoscale science and engineering community: nanoHUB.org.", Nanoscale Science and Engineering Education Workshop, Arlington, VA. (2014).
- [I221] Krishna Madhavan, Gerhard Klimeck, "nanoHUB in Education", Annual Technical Meeting of the Society of Engineering Sciences, West Lafayette, IN. (2014).
- [I220] Gerhard Klimeck, "Non Equilibrium Greens Function NEGF (quantum transport, nanowires, ballistic effects etc.)", 2014 International Conference on Computer Aided Design, November 3-6, 2014, San Jose, California
- [I219] Gerhard Klimeck, Krishna Madhavan, Michael Zentner, Lynn Zentner, Victoria Farnsworth, Michael McLennan, "nanoHUB.org: Redefining research and learning in nanoscale engineering and science", University of the Future Workshop Purdue University, West Lafayette, Indiana, USA, 28-29 October, 2014
- [I218] Gerhard Klimeck, "Elevating nanoHUB to the Next Level Vision and Status 2014", Program of the International CECAM-Tutorial, Bremen Center for Computational Materials Science – BCCMS University of Bremen, October 5th – 6th, 2014
- [I217] Gerhard Klimeck, "Development of the NEMO tool suite: from basic physics to real industrial devices and to global impact on nanohub.org", Program of the International CECAM-Tutorial, Bremen Center for Computational Materials Science – BCCMS University of Bremen, October 5th – 6th, 2014
- [I216] Gerhard Klimeck, "Introduction to nanoHUB", SES Annual Technical Meeting; October 1-2, 2014, Purdue University
- [I215] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org ", KEYNOTE: Mechanics in Material Science, SES Annual Technical Meeting; October 1-2, 2014, Purdue University
- [I214] Gerhard Klimeck, "Elevating nanoHUB to the Next Level - Vision and Status 2014", eScience workshop, MURPA, Melbourne, Australia, Sept 24, 2014 (remote)
- [I213] Gerhard Klimeck, Parijat Sengupta, Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, "Topological Insulator Modeling within Atomistic Nanoelectronic Modeling", NEMO Representations, Workshop on the modeling of Topological Insulators and Majorana Systems, Delft Technical University, Sept 22-23, 2014
- [I212] Gerhard Klimeck, "Mythbusting today's Nanotechnology and Knowledge Transfer through nanoHUB.org", Dawn or Doom, Purdue University, Sept 18, 2014
- [I211] Gerhard Klimeck, "NEMO5 Overview", QuantumHagen, Modeling of Electronic Devices and Materials at the Nanoscale, workshop in Copenhagen, Denmark on July 1-3, 2014
- [I210] Gerhard Klimeck, "Scientific Simulation Software as a Service", Session: "Outsourcing Science: Will the Cloud Transform Research?", AAAS Annual Meeting, 14 February, 2014, Chicago
- [I209] Michael Zentner, Gerhard Klimeck, "On Safari in nanoHUB: The Hunt for Prototypical Users", HUBbub13, Indianapolis, IN, 2013.
- [I208] Gerhard Klimeck, "Short Course on NanoHub", 2013 NSF Nanoscale Science and Engineering Grantees Conference, December 4-6, 2013 Westin Hotel - Arlington, VA
- [I207] Gerhard Klimeck, Mehdi Salmani-Jelodar, Saumitra Mehrotra, Abhijeet Paul, Hoon Ryu, Sunhee Lee, Yu He, Daniel Lemus, Bozidar Novakovic, Tillmann Kubis, Michael Povolotskyi, "Development of the NEMO Tool Suite From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Embedded tutorial on FinFET: A Multifaceted Perspective for CAD Engineers , International Conference on Computer Aided Design, Nov 18-21, 2013, San Jose, CA
- [I206] Gerhard Klimeck, Krishna Madhavan, Michael Zentner, Lynn Zentner, Victoria Farnsworth, Michael Povolotskyi, Tillmann Kubis, Jim Fonseca, Bozidar Novakovic, "Taking Nanoelectronics to the Next Level Through NEMO and nanoHUB.org", CMSI International Symposium 2013: Extending the power of computational materials sciences with K-computer, Tokyo, Japan, Oct 21 -22, 2013
- [I205] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", Second KredibleNet workshop on Reputation, Trust, and Authority at Stanford University, Oct 18, 2013
- [I204] Gerhard Klimeck, "nanoHUB.org – A Science Gateway with global usage and impact CENIC", Corporation of Education network Initiatives in California, Big Data, Big Network Workshop, Oct 10, 2013
- [I203] Gerhard Klimeck, "Development of the NEMO Tool Suite From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", KEYNOTE at The International Conference on Simulation of Semiconductor Processes and Device, Glasgow, UK, Sept 3-5, 2013
- [I202] Gerhard Klimeck, "nanoHUB tutorial", IEEE Nano Conference, Beijing, Aug 5-10, 2013
- [I201] Gerhard Klimeck, "Short Course on NanoHUB", INC9, The Ninth International Nanotechnology Conference on Communication and Cooperation, Berlin, Germany, May 13-16, 2013
- [I200] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", eScience workshop, Melbourne, Australia, March 20, 2013 (remote)
- [I199] Gerhard Klimeck, "Mythbusting scientific knowledge transfer with nanoHUB.org: Collaborative research and dissemination with quantifiable impact on research and education", 245th ACS National Meeting, New Orleans, LA, April 8, 2013

- [I198] Gerhard Klimeck, Rajib Rahman, Hoon Ryu, Sunhee Lee, Yui-Hong Tan, "Nanoelectronic Modeling (NEMO) for Si-based Quantum Electronics", International workshop on Silicon Quantum electronics Villard-de-Lans 7-8 February 2013
- [I197] Gerhard Klimeck, "Multi-Million Atom Simulations for Single Atom Transistor Structures", Foresight Institute Technical Conference, Illuminating Atomic Precision, January 11-13, 2013, Palo Alto, CA
- [I196] Gerhard Klimeck, "Mythbusting Knowledge Transfer Mechanisms through Science Gateways", Foresight Institute Technical Conference, Illuminating Atomic Precision, January 11-13, 2013, Palo Alto, CA
- [I195] Krishna Madhavan, Gerhard Klimeck, "nanoHUB.org: Democratizing Nanoscale Modeling, Simulations, and Education through a Cloud-based Science Gateway.", Invited lecture at the CI Days, Michigan State University, Lansing, MI. (October 2012).
- [I194] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", HUBbub conference, Indianapolis, Sept 24-25, 2012
- [I193] Gerhard Klimeck, "nanoHUB Nanoscale Modeling & Simulation Workshop", TechConnect World, Santa Clara, CA, June 18-21, 2012
- [I192] Gerhard Klimeck, "High-Performance Computing for Atomistic Materials Modeling", NSTI Nanotechnology Conference, TechConnect World, Santa Clara, CA, June 18-21, 2012
- [I191] Gerhard Klimeck, "Tutorial: Atomistic Modeling of Band-to-Band-Tunneling Transistors and nanoHUB tools", Device Research Conference, Penn State, June 17, 2012
- [I190] Gerhard Klimeck, "nanoHUB.org: Mythbusting Scientific Knowledge Transfer", International Workshop "Novel Ideas in Optics: From Advanced Materials to Revolutionary Applications", Purdue University, May 31-June 1, 2012
- [I189] Gerhard Klimeck, "Mythbusting Knowledge Transfer with nanoHUB.org", Purdue Preside3nt Council's Back to School, Purdue University, Oct. 5, 2012
- [I188] Gerhard Klimeck, "Mythbusting Knowledge Transfer with nanoHUB.org: A software as a service cloud focused on end-to-end application users, application developers, and 24/7 service", IEEE International Conference on eScience 2012, Chicago, Oct. 8-12, 2012
- [I187] Gerhard Klimeck, "The Single Atom Transistor", (substituted for a missing speaker), IEEE Central Indiana Section, Latest Trends in Emerging Topics for Practicing Engineers, Indianapolis, Nov. 10, 2012
- [I186] Gerhard Klimeck, "nanohub.org - An Online Virtualization Tool Supporting Experiments in Nanotechnology", IEEE Central Indiana Section, Latest Trends in Emerging Topics for Practicing Engineers, Indianapolis, Nov. 10, 2012.
- [I185] Gerhard Klimeck, "nanoHUB Demo", 2012 NSF Nanoscale Science and Engineering Grantees Conference, Dec. 3-4, 2012
- [I184] Jim Fonseca, "NEMO5 and nanoHUB", Quantum Technology: Computational Models for Quantum Device Design, Banff International Research Station, Banff, Canada, January 2012
- [I183] Gerhard Klimeck, Michael McLennan, "nanoHUB User Session", 2012 NSF Nanoscale Science and Engineering Grantees Conference, Dec. 3-4, 2012
- [I182] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer via nanoHUB.org", Challenges in PV Science, Technology, and Manufacturing: A workshop on the role of theory, modeling and simulation, Purdue University, August 2 & 3, 2012
- [I181] Gerhard Klimeck, "Simulation of ultrasmall structures and devices", ICSNN 2012, Dresden, July 22-27, 2012
- [I180] Gerhard Klimeck, "Mythbusting with nanoHUB.org the first science gateway software as a service cloud focused on end to end application users AND application developers", XSEDE12, Chicago, July 18, 2012
- [I179] Gerhard Klimeck, "Modeling devices in the No MOS regime", No MOS Workshop, Washington DC, NIST, June 7 & 8, 2012
- [I178] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", workshop on Building the Materials Innovation Infrastructure: Data and Standards, Washington DC, May 14-15, 2012
- [I177] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Yui-Hong Tan, Neerav Kharche, Zhengping Jiang, Lloyd Hollenberg, Michelle Simmons, Martin Fuechsle, Bent Weber, Jill Miwa, Suddhasatta Mahapatra, Andrea Morello, Andrew Dzurak, "Atomistic, Multi-Scale, Multi-Physics Modeling of Extended Si Quantum Devices – Outreach Opportunities for CQCT", CQCT Workshop, Chowder Bay, Sydney, Feb 15-16, 2012.
- [I176] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Yui-Hong Tan, Rajib Rahman, Seung Park, Neerav Kharche, Gabriel Lansbergen, Jan Verduijn, Bent Weber, Lloyd Hollenberg, Sven Rogge, Michelle Simmons, Richard Muller, "Million-Atom Electronic Structure Simulations for Realistically Large Si-Based Quantum Devices", International Workshop On Silicon Quantum Electronics, Chowder Bay, Sydney, Feb 13-14, 2012.
- [I175] Bent Weber, Suddhasatta Mahapatra, Thomas Watson, Michelle Simmons, Hoon Ryu, Sunhee Lee, Yui-Hong Tan, Gerhard Klimeck, Lloyd Hollenberg, "Silicon at the Fundamental Scaling Limit: Atomic-scale Donor-based Quantum Electronics", ICYRAM 2012 Session EM1: Inorganic Semiconductor (and Metal) Nanoelectronics

- [I174] Krishna Madhavan, Gerhard Klimeck, "nanoHUB.org: Platforms based strategy for global impact in nanoscale engineering and science research and education", Invited presentation at the NSF EEC Grantees Conference, Washington, DC. (2012).
- [I173] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Yui-Hong Tan, Lloyd Hollenberg, Michelle Simmons, Martin Fuechsle, Bent Weber, Jill Miwa, Suddhasatta Mahapatra, "Atomistic, Multi-Scale, Multi-Physics Modeling of Single Impurity Devices", International Workshop on Silicon Quantum Electronics, Sydney, Feb 13-14, 2012
- [I172] Seung Park, Saumitra Mehrotra, Tillmann Kubis, Gerhard Klimeck, Mark Lundstrom, "What is different below 10 nm?", Invited presentation at the NNIN Symposium on Frontiers in Nanoscale Transistors and Electronics, Santa Barbara, CA, February 6, 2012.
- [I171] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Yui-Hong Tan, Neerav Kharche, Zhengping Jiang, Lloyd Hollenberg, Michelle Simmons, Martin Fuechsle, Bent Weber, Jill Miwa, Suddhasatta Mahapatra, Andrea Morello, Andrew Dzurak, "Atomistic, Multi-Scale, Multi-Physics Modeling of Extended Si Quantum Devices", Center for Quantum Computing (CQCT) 2011 Annual Workshop, The Seargents Mess, Chowder Bay, Sydney, Feb 15-16, 2011.
- [I170] Krishna Madhavan, Gerhard Klimeck, "Deriving deep insights about the impact of e-Science research", Keynote talk presented at the Workshop on Measuring the Impact of e-Science Research, 7th IEEE International Conference on e-Science 2011, Stockholm, Sweden, December 5 - 8, 2011
- [I169] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer: nanoHUB usage Scenarios and Impact", Nanoinformatics 2011, Arlington, VA, Dec 8th, 2011
- [I168] Gerhard Klimeck, "Second Annual NanoHUB.org User Forum 2011", NSF Nanoscale Science and Engineering Grantees Conference, Education Networks and Programs, Dec. 6, 2011
- [I167] Gerhard Klimeck, "NCN: Global Initiative About 'Electronics from the Bottom-up'", 2011 NSF Nanoscale Science and Engineering Grantees Conference, Education Networks and Programs, Dec. 6, 2011
- [I166] Gerhard Klimeck, "nanoHUB.org powered by HUBzero® – A Platform for Collaborative Research and Dissemination with Quantifiable Impact on Research and Education", Palmer Commons, Cyberinfrastructure (CI) Days 2011, Nov. 29 - Dec. 1, 2011, Ann Arbor, MI
- [I165] Gerhard Klimeck, Krishna Madhavan, Diane Beaudoin, Michael Zentner, Lynn Zentner, Swaroop Shivarajapura, Nathan Denny, Victoria Farnsworth, George Adams III., "Knowledge Transfer via a Global Cyberinfrastructure for over 170,000 Annual nanoHUB.org Users", Invited to participated at the National Academies Keck Futures Initiative, Ecosystem Services: Charting a Path to Sustainability, Irvine CA, Nov. 10-13, 2011
- [I164] Gerhard Klimeck, "nanoHUB.org: A Global Cyberinfrastructure Centered at Old Purdue", Purdue West Coast Partnership Center, Discovery with Delivery Symposium, Friday Oct. 28, 2011, Vineyard Conference Center, Cisco Systems, San Jose, CA.
- [I163] Gerhard Klimeck, "Nanoelectronic Modeling and nanoHUB.org: where new devices and new materials meet at the atomic scale", IEEE Nanotechnology Materials and Devices Conference (IEEE NMDC 2011), Oct. 18-21, 2011 at The Shilla Jeju, Korea
- [I162] Gerhard Klimeck, "Cyberinfrastructure serving over 170,000 users in 172 countries", Nanoelectronics: Physics and Devices Workshop, in Honor of Prof. Dr. Ulrich Kunze, Ruhr University Bochum, Oct. 14, 2011
- [I161] Gerhard Klimeck, "nanoHUB - a nanotechnology cyberinfrastructure serving over 170,000 users in 172 countries", Nanoelectronics: Physics and Devices Workshop, 14. Oktober 2011, Ruhr University, Bochum.
- [I160] Gerhard Klimeck, "nanoHUB.org Cyberinfrastructure: Innovating Knowledge Transfer", ICTPI: The International Conference on Technology Policy and Innovation, Bogota, Colombia, September 8-9, 2011
- [I159] Lynn Zentner, Saumitra Mehrotra, Gerhard Klimeck, "Introduction to nanoHUB.org – online simulation and more", Tutorial at IEEE nano conference, Portland, Aug, 2011.
- [I158] Gerhard Klimeck, Krishna Madhavan, Lynn Zentner, George Adams III., Victoria Farnsworth, Michael Zentner, Nathan Denny, Mathieu Luisier, Sebastian Steiger, Michael Povolotskyi, Hong-Hyun Park, Tillmann Kubis, "High Performance Computational Nanotechnology for Research and Education on nanoHUB.org", TeraGrid Conference, July 18-22, 2011, Salt Lake City.
- [I157] Gerhard Klimeck, "Quantitative multi-million atom simulations for quantum dots and single impurities in Si", CMOS Emerging Technologies, June 15-17, 2011, Whistler, British Columbia.
- [I156] Gerhard Klimeck, "nanoHUB.org Tutorial 1) nanoHUB impact 2) Semiconductor and Quantum Mechanics Education", proceedings of the IEEE Device Research Conference (DRC), June 20-22 2011.
- [I155] Gerhard Klimeck, George Adams III., Krishna Madhavan, Nathan Denny, Michael Zentner, Swaroop Shivarajapura, Lynn Zentner, Diane Beaudoin, "Social Networks of Researchers and Educators on nanoHUB.org", proceedings of the 11th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, CCGrid 2011, Newport Beach, CA, USA, May 23-26, 2011.
- [I154] Gerhard Klimeck, George Adams III., Krishna Madhavan, Nathan Denny, Michael Zentner, Swaroop Shivarajapura, Lynn Zentner, Diane Beaudoin, "Social Networks of Researchers and Educators on

- nanoHUB.org", proceedings of the 11th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, CCGrid 2011, Newport Beach, CA, USA, May 23-26, 2011.
- [I153] Gerhard Klimeck, "nanoHUB.org - Future Cyberinfrastructure serving over 170,000 users today", NNIN-C Workshop, Advanced Modeling and Simulation of NEMS/MEMS and Nano/Microfluidic Devices, Ann Arbor, Michigan, April 19-20 2011
- [I152] Gerhard Klimeck, George Adams III., Krishna Madhavan, Nathan Denny, Michael Zentner, Swaroop Shivarajapura, Lynn Zentner, Diane Beaudoin, Mehdi Salmani-Jelodar, "Exploring the Impact of nanoHUB.org on Research and Education", HUBbub 2011, the HUBzero conference, April 5-6, 2011, Indianapolis. Presentation online at <http://hubzero.org/resources/429>
- [I151] Lynn Zentner, Gerhard Klimeck, Krishna Madhavan, George Adams III., "Success Criteria for Establishing a Thriving HUBzero Based Site: A Model for Science 2.0", HUBbub 2011, the HUBzero conference, April 5-6, 2011, Indianapolis. Presentation online at <http://hubzero.org/resources/408>
- [I150] Gerhard Klimeck, "Success examples and challenges of multi-scale and multi-expertise modeling and simulations", Conference on Materials for Energy Applications — Experiment, Modeling and Simulations, March 30 - April 1, 2011, Terranea Resort, Rancho Palos Verdes, CA
- [I149] Gerhard Klimeck, "Device Modeling for Si Spin Qubits", Centre for Quantum Computation and Communication Technology, Inaugural Kick-Off Meeting, Sydney Australia, Jan 19-21, 2011.
- [I148] Sebastian Steiger, Michael Povolotskyi, Hong-Hyun Park, Tillmann Kubis, Ganesh Hegde, Denis Areshkin, Benjamin Haley, Jean Sellier, Mark Rodwell, Gerhard Klimeck, "The Nanoelectronic Modeling Tool NEMOS: Capabilities, Validation, and Application to Sb-Heterostructures", Device Research Conference (DRC) 2011, Santa Barbara CA
- [I147] Michael McLennan, Gerhard Klimeck, "Atomistic Modeling and Simulation Tools for Nanoelectronics and their Deployment on nanoHUB.org", US-India Network Enabled Research Collaboration Workshop, Lalit Hotel, New Delhi, India, Dec. 5 - 7, 2010
- [I146] Gerhard Klimeck, "Keynote: The NCN and Modeling and Simulation of Nanosystems", 2010 NSF Nanoscale Science and Engineering Grantees Conference, Dec. 6-8, 2010, The Westin Arlington Gateway - Arlington, VA
- [I145] Michael McLennan, Gerhard Klimeck, "Introducing the Rappture Toolkit", Building a Collaborative Framework for Nanoscale Simulations Joint NNIN/NCN Fall Workshop, Cornell University, Nov 14-16, 2010
- [I144] Gerhard Klimeck, "nanoHUB.org: Sociology and Cybertechnology to enable Multidisciplinary Research and Education for over 160,000 Annual Users", Building a Collaborative Framework for Nanoscale Simulations Joint NNIN/NCN Fall Workshop, Cornell University, Nov 14-16, 2010
- [I143] Mark Rodwell, William Frensley, Sebastian Steiger, E. Chagarov, S. Lee, Hoon Ryu, Y. Tan, Ganesh Hegde, L Wang, J. Law, Timothy Boykin, Gerhard Klimeck, P. Asbeck, A. Kummel, J. Schulman, "III-V FET Channel Designs for High Current Densities and Thin Inversion Layers", Device Research Conference (DRC), 21-23 June 2010
- [I142] Gerhard Klimeck, Mathieu Luisier, Timothy Boykin, Xueping Jiang, Neerav Kharche, Yu Zhou, Saroj K. Nayak, "Atomistic Graphene Transistors - New Device or New Material?", University of Minnesota Nanotech Conference, Oct 7 and 8, 2010
- [I141] Gerhard Klimeck, "Nano-Scale Simulations", Second Annual Nano-Link Conference, October 5-6, 2010, Minneapolis
- [I140] Gerhard Klimeck, Mathieu Luisier, Timothy Boykin, Xueping Jiang, Neerav Kharche, Yu Zhou, Saroj K. Nayak, "Atomistic Graphene Transistors - New Device or New Material ?", NRI Workshop on Carbon Based Electronics, Albany NY, Sept. 21-22, 2010
- [I139] Tillmann Kubis, Gerhard Klimeck, Peter Vogl, "Non-equilibrium Green", International Workshop for Computational Electronics, October 27th-29th, Pisa, Italy (2010)
- [I138] Gerhard Klimeck, "Success Examples and Challenges of Multi-Scale and Multi-Expertise Modeling and Simulations", ARL
- [I137] Gerhard Klimeck, "HUBzero: Future Sociology and Cybertechnology that empowers over 137,000 Annual Users in Research, Education, and Industry Today", SME/OEM Midwest Pilot for Modeling and Simulation Summit & Workshop, August 31, 2010, Gleacher Center, University of Chicago Booth School of Business
- [I136] Gerhard Klimeck, Krishna Madhavan, "nanoHUB tutorial", IEEE Nano 2010, Seoul Korea, Aug. 17-20, 2010
- [I135] Gerhard Klimeck, Sunhee Lee, Hoon Ryu, Suddhasatta Mahapatra, Michelle Simmons, Lloyd Hollenberg, "Equilibrium Bandstructure of a Phosphorus δ -doped Layer in Silicon using a Tight-binding Approach", IEEE Nano 2010, Seoul Korea, Aug. 17-20, 2010.
- [I134] Gerhard Klimeck, "Interactive Online Curricula and Resources for 125,000 nanoHUB.org Users", Spring University Materials Council Meeting Workshop on Computational Materials Education, June 23-24, Northwestern University, Evanston IL, (2010)

- [I133] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 125,000 users today", International Association of Technological University Libraries (IATUL), 31st Annual IATUL Conference, Purdue University, June 20-14, 2010.
- [I132] Gerhard Klimeck, Dragica Vasileska, "Semiconductor Device and Quantum Mechanics Education on nanoHUB.org", ASEE IN/IL section meeting, Purdue University, April 9-10, 2010
- [I131] Mathieu Luisier, Gerhard Klimeck, "Atomistic Simulations of Nanoelectronic Devices", International Conference on Computational and Experimental Engineering and Sciences (ICCES'10), Las Vegas, Nevada, 28 March – 1 April 2010
- [I130] George Adams III., Gerhard Klimeck, "nanoHUB.org Gateway for Computational Nanotechnology", International Conference on Computational and Experimental Engineering and Sciences (ICCES'10), Las Vegas, Nevada, 28 March – 1 April 2010.
- [I129] Gerhard Klimeck, Mathieu Luisier, Hoon Ryu, Sunhee Lee, Rajib Rahman, Lloyd Hollenberg, Bent Weber, Michelle Simmons, "Atomistic Electronic Structure and Transport Modeling of Realistically Extended Nanoelectronic Devices", 2010 International Conference On Nanoscience and Nanotechnology (ICONN), Sydney, 22-26th Feb. 2010.
- [I128] Gerhard Klimeck, Mathieu Luisier, Hoon Ryu, Sunhee Lee, Rajib Rahman, Lloyd Hollenberg, Bent Weber, Michelle Simmons, "Atomistic Electronic Structure and Transport Modeling of Si:P devices", Center for Quantum Computing (CQCT) 2010 Annual Workshop, Harbours Edge, Darling Harbour, Sydney. Feb 15-17, 2010.
- [I127] Gerhard Klimeck, "Keynote: Conceptual Challenges for Simulation in Nanotechnology", 2009 NSF Nanoscale Science and Engineering Grantees Conference, December 7-9, 2009, Arlington, VA
- [I126] Gerhard Klimeck, "Participant at National Academy of Engineering", 2009 U.S. Frontiers of Engineering Program, Irvine, CA, Sept. 9-12, 2009, ~240 suggested applicants, ~80 invited participants.
- [I125] Gerhard Klimeck, Mathieu Luisier, Benjamin Haley, Sunhee Lee, Hoon Ryu, Neerav Kharche, Faisal Saied, Steven Clark, Hansang Bae, "NEMO 3-D and OMEN: Nanoelectronic Modeling for Advanced Semiconductor Device Studies and their Deployment on nanoHUB.org", TeraGrid Conference, Crystal City, June 21-26, 2009.
- [I124] Gerhard Klimeck, Mathieu Luisier, Benjamin Haley, Sunhee Lee, Hoon Ryu, Faisal Saied, Steven Clark, Hansang Bae, "Advancing Nanoelectronic Devices through Peta-Scale Computing and Deployment on nanoHUB", SciDAC Conference, San Diego, June 15-19, 2009.
- [I123] Gerhard Klimeck, Mathieu Luisier, "From NEMO1D and NEMO3D to OMEN: moving towards atomistic 3-D quantum transport in nano-scale semiconductors", NRI e-Workshop, April 28, 2009.
- [I122] Mathieu Luisier, Gerhard Klimeck, "Full-Band and Atomistic Modeling of Nanoelectronic Devices", Nanotech Conference and Expo, Houston, TX, May 7-9, 2009.
- [I121] George Adams III., Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "nanoHUB.org: An Example of Cyberinfrastructure for Simulation-Driven Science", CI Days at UT Pan American, March 27, 2009.
- [I120] Gerhard Klimeck, Mathieu Luisier, Rajib Rahman, Muhammad Usman, Neerav Kharche, Hoon Ryu, Sunhee Lee, Dragica Vasileska, "NEMO 3-D and OMEN: Nanoelectronic modeling tools for advanced semiconductor device studies and their deployment on nanoHUB.org", American Chemical Society meeting, Salt Lake City, Utah, 22-26 March 2009
- [I119] Gerhard Klimeck, "Modeling and Simulation Tools for Nanoelectronics", Winter Meeting of the American Association of Physics Teachers, Chicago, USA, Jan 12-16, 2008.
- [I118] Gerhard Klimeck, Mathieu Luisier, "From NEMO1D and NEMO3D to OMEN: moving towards atomistic 3-D quantum transport in nano-scale semiconductors", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008.
- [I117] Mathieu Luisier, Gerhard Klimeck, "Full-Band Simulation of Realistic Nanoelectronic Devices at the Atomic Scale", 4th International Workshop on High Performance Computing for Nanoscience and Technology, HPCNano08, in conjunction with Supercomputing 2008, Purdue University Exhibition Booth, Nov 21, 2008, Austin, TX.
- [I116] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 75,000 users today", Supercomputing 2008, Purdue University Exhibition Booth, Nov 18, 2008, Austin, TX.
- [I115] Gerhard Klimeck, Hoon Ryu, "Contact Block Reduction Method for Ballistic Quantum Transport with Semi-empirical sp³d⁵s* Tight Binding Band Models.", International Conference on Solid State and Integrated Circuit Technology (ICSICT 2008), Beijing, October 20-23, 2008.
- [I114] Gerhard Klimeck, Neerav Kharche, Muhammad Usman, Timothy Boykin, "Multi-Million Atom Simulations of Strain and Electronic Structure with NEMO 3-D", Materials Science and Technology Conference and Exhibition (MS&T), Pittsburgh, October 5-9, 2008.
- [I113] Gerhard Klimeck, Michael McLennan, Mark Lundstrom, George Adams III., "nanoHUB.org - future cyberinfrastructure serving over 75,000 users today", IEEE Symposium on Massive Storage Systems and Technologies (MSST), Baltimore, September 22-24, 2008.

- [I112] Gerhard Klimeck, Michael McLennan, Mark Lundstrom, George Adams III., "nanoHUB.org - online simulation and more materials for semiconductors and nanoelectronics in education and research", IEEE nano 2008, Arlington, TX, August 18-21, 2008.
- [I111] Gerhard Klimeck, representing Committee, "The Next Generation Research Grid: A Path Forward", Presentation to the TeraGrid Science Advisory Board Meeting, TeraGrid 2008, June 9, 2008, Las Vegas.
- [I110] Gerhard Klimeck, Michael McLennan, Mark Lundstrom, George Adams III., "nanoHUB.org - serving over 58,000 researchers, educators, and students", Ohio Nanotechnology Summit, Mason, OH, April 10-11, 2008.
- [I109] Barbara Fossum, Gerhard Klimeck, Michael McLennan, Mark Lundstrom, George Adams III., "nanoHUB.org - Future Cyberinfrastructure - serving over 60,000 users today", Workshop on Designing cyberinfrastructure to enable US-China collaboration in tobacco research, Beijing, March 28-29, 2008.
- [I108] Gerhard Klimeck, "Connecting Scientists Through nanoHUB", National Academy of Sciences E-Journal Summit, March 18, 2008.
- [I107] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, George Adams III., "Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D", ICONN 2008, Melbourne, Australia, Feb 25-29, 2008.
- [I106] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, George Adams III., "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", NSF CMMI Grantee Conference, Knoxville TN, Jan 7-9, 2008.
- [I105] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", thermalHUB Community Planning Workshop, Purdue University, Dec. 10, 2007.
- [I104] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, George Adams III., "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", NSF nanotechnology grantee's meeting, Washington DC, Dec. 3-6, 2007.
- [I103] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today with online simulations and more", invited software demonstration, BIRS Workshop 07w5057 (Banff International Research Station), Physics-Based Mathematical Models of Low-Dimensional Semiconductor Nanostructures: Analysis and Computation, Banff, Canada, Nov. 18-23 2007.
- [I102] Gerhard Klimeck, "Atomistic NanoElectronic Modeling (NEMO): for Predictive Resonant Tunneling Diode Simulation and Disordered 3-D Systems", Plenary / Keynote Address, BIRS Workshop 07w5057 (Banff International Research Station), Physics-Based Mathematical Models of Low-Dimensional Semiconductor Nanostructures: Analysis and Computation, Banff, Canada, Nov. 18-23 2007.
- [I101] Gerhard Klimeck, "nanoHPC NEMO: Scaling to Over 23,000 Cores", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [I100] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [I99] Alejandra Magana, Alissa Nedossekina, Gerhard Klimeck, "nano-based education through generation-nano.org", Supercomputing 2007, Education Program to Middle School, High School, and College Teachers, Nov 10, 2007, Reno, NV.
- [I98] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", Supercomputing 2007, Education Program to Middle School, High School, and College Teachers, Nov 10, 2007, Reno, NV.
- [I97] Gerhard Klimeck, "NanoElectronic MOdeling (NEMO)", Workshop on Excellence in Modeling and Simulation, University of California at Berkeley, Nov. 6, 2007.
- [I96] Gerhard Klimeck, "Nanoelectronics: is it a new device or a new material?", Keynote at Project review meeting. Meeting the materials challenges of nano-CMOS electronics. Prof. Asen Asenov, University of Glasgow, Prof. Alexander Shluger, University College London, London, UK, Oct. 22, 2007.
- [I95] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure used by over 24,000 users today", Keynote: International Multi-Symposiums on Computer and Computational Sciences 2007 (IMSCCS'07), The University of Iowa, Iowa City, Iowa, USA, August 13 - 15, 2007.
- [I94] Gerhard Klimeck, "nanoHUB, a Fully Operational Science Gateway", Science Gateways TeraGrid Planning Process Workshop, University of Wisconsin Memorial Union, Madison, Wisconsin, June 7, 2007.
- [I93] Gerhard Klimeck, "Atomistic Modeling of Nanoelectronic devices", Si nanoelectronics, Leiden, Netherlands, May 21-25, 2007.
- [I92] Gerhard Klimeck, "Multi-million Atom Simulations of Strain and Electronic Structure with NEMO 3-D and its Deployment on nanoHUB.org as a Community Code and Service", 2007 Nanomaterials for Defense Applications Symposium, April 23-26, 2007, San Diego CA.
- [I91] Mark Lundstrom, J.C. Clark, Gerhard Klimeck, Arvind Raman, "Nanoelectronics: Metrology and Computation", 2007 International Conference on Frontiers of Characterization and Metrology for Nanoelectronics, March 27-29, 2007, National Institutes of Standards and Technology, Gaithersburg, MD. conference proceedings will be published by AIP in a hardback book.

- [I90] Gerhard Klimeck, Michael McLennan, "nanoHUB.org and High Performance Computing", Purdue-Industry High-Performance Computing Workshop, March 20, 2007, Purdue Computing Research Institute (CRI).
- [I89] Michael McLennan, Gerhard Klimeck, "Who wants to be a nanoscientist?", After dinner gameshow for the demonstration of nanoHUB capabilities. Forum on the Frontiers in Computational Nanoelectronics February 20-21, 2007, Indianapolis, IN.
- [I88] Gerhard Klimeck, "Atomistic Nanoelectronic Modeling", Forum on the Frontiers in Computational Nanoelectronics February 20-21, 2007, Indianapolis, IN.
- [I87] Gerhard Klimeck, Michael McLennan, "nanoHUB tutorial - overview, usage scenarios, vision", IEEE International Conference on Nano/Micro Engineered and Molecular Systems (IEEE-NEMS) Jan 16-19, 2007, Bangkok Thailand.
- [I86] Mark Lundstrom, Gerhard Klimeck, "The Network for Computational Nanotechnology: Shared Infrastructure for the NNI", NSF Grantees, Conference, Washington, D.C., Dec. 4-6, 2006.
- [I85] Michael McLennan, Gerhard Klimeck, "nanoHUB - overview and usage scenarios", FutureTECH Conference Nov 18, 2006, Norfolk State University.
- [I84] Gerhard Klimeck, Michael McLennan, "nanoHUB - overview", Supercomputing 2006, Two Presentations in the TeraGrid Booth, Nov 11-17, 2006, Tampa, FL.
- [I83] Gerhard Klimeck, "Multi-million Atom Simulations of Strain and Electronic Structure in NEMO 3-D Enabled by HPC and TeraGrid and Deployment on nanoHUB.org", Supercomputing 2006, Presentation in the Purdue Booth, Nov 11-17, 2006, Tampa, FL.
- [I82] Gerhard Klimeck, Michael McLennan, Wei Qiao, David Ebert, Rick Kennel, "nanoVIZ Server", Supercomputing 2006, Presentation in the Purdue Booth, Nov 11-17, 2006, Tampa, FL.
- [I81] Gerhard Klimeck, Michael McLennan, Mathew Potrawski, "nanoHUB - HUB Technologies: A Fully Operational Collaborative Cyberinfrastructure for Research, Education, and Outreach", Supercomputing 2006, Two Presentations in the Purdue Booth, Nov 11-17, 2006, Tampa, FL.
- [I80] Gerhard Klimeck, Rick Kennel, Michael McLennan, Steven Clark, Clemens Heitzinger, Shaikh Ahmed, Wei Qiao, David Ebert, Sebastien Goasguen, Krishna Madhavan, "nanoHUB.org - A fully operational Science Gateway for the nano Science Community", Supercomputing 2006, The Second IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology (HPCNano06), Nov 11-17, 2006, Tampa, FL.
- [I79] Gerhard Klimeck, Michael McLennan, "nanoHUB overview and usage scenarios", Supercomputing 2006, Education Program to Middle School and High School Teachers, Nov 11-17, 2006, Tampa, FL.
- [I78] Gerhard Klimeck, "nanoHUB - a community website for online simulation and more", Short Course at IEEE-NMDC, IEEE Nanotechnology Materials and Devices Conference, October 22-25, 2006, www.ieee-nmdc.org
- [I77] Gerhard Klimeck, Shaikh Ahmed, Clemens Heitzinger, Neerav Kharche, Muhammad Usman, Mathieu Luisier, Raseong Kim, Neophytos Neophytou, Michael McLennan, Timothy Boykin, "Quantum Dot, Nanowire, ad Bandstructure Modeling and Deployment on nanoHUB.org", International Topical Workshop "Tera- and Nano-Devices: Physics and Modeling", University of Aizu, Aizu-Wakamatsu, Japan in October 16-19, 2006.
- [I76] Gerhard Klimeck, "Quantum Transport in Resonant Tunneling Diodes", Si-nano summer school, Bologna, Italy, Aug 20-25, 2006.
- [I75] Gerhard Klimeck, "NEMO 3-D and nanoHUB: Bridging Research and Education", IEEE Nano 2006, Cincinnati, July 18, 2006.
- [I74] Gerhard Klimeck, "NCN / nanoHUB.org: An infrastructure to accelerate the transformation of Nanoscience to Nanotechnology in research and education: Atomistic simulations of long-range strain and close-range electronic structure in self-assembled quantum dot systems", Synergy Between Experiment and Computation in Nanoscale Science, Harvard University, May 31-June 3, 2006.
- [I73] Mark Lundstrom, Gerhard Klimeck, "The Network for Computational Nanotechnology", International Nanotechnology Conference on Communication and Cooperation: NSF/NNI Symposium, Arlington, VA, May, 15, 2006.
- [I72] Krishna Madhavan, Gerhard Klimeck, Sebastien Goasguen, Michael McLennan, Mark Lundstrom, "New frontiers in nano-education through the nanoHUB", Annual ECE Department Heads Association, Oahu, HI, March 10-14, 2006.
- [I71] Krishna Madhavan, Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, "IMS e-learning standard compliance and learning object use on the nanoHUB", IMS Quarterly Meeting, Boston, MA, Feb. 6-10, 2006.
- [I70] Krishna Madhavan, Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, "Integrating nanoHUB content with MERLOT", MERLOT Mid-year Directors Conference, San Diego, CA, Jan 27 - 29, 2006.
- [I69] Mark Lundstrom, Gerhard Klimeck, "The NCN: Science, Simulation, and Cyber Services", NanoSingapore 2006, IEEE Conference on Emerging Technologies, January 10-13, 2006. (KEYNOTE Talk).

- [I68] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Krishna Madhavan, "The Network for Computational Nanotechnology", 2005 Nanoscale Science and Engineering Grantee Conference, Washington DC, December 12-15, 2005.
- [I67] Mark Lundstrom, Gerhard Klimeck, Sebastien Goasguen, Jose Fortes, "Network for Computational Nanotechnology", Presentation in the SC05 Purdue Booth, Supercomputing 2005, Nov 12-18, 2005, Seattle, WA.
- [I66] Gerhard Klimeck, Sebastien Goasguen, Michael McLennan, Faisal Saied, Krishna Madhavan, Mark Lundstrom, "nanoHUB.org – A Service-Oriented Gateway for the nano Science Community", HPCNano2005 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2005, Nov 12-18, 2005, Seattle, WA
- [I65] Gerhard Klimeck, Sebastien Goasguen, Michael McLennan, Faisal Saied, Krishna Madhavan, Mark Lundstrom, "Network for Computational Nanotechnology - software deployment on the nanoHUB using the NSF Teragrid", Presentation in the SC05 Argonne Booth, Supercomputing 2005, Nov 12-18, 2005, Seattle, WA
- [I64] Gerhard Klimeck, "Introduction to the Integration of High Performance Computing: Nanotechnology. Physics, Chemistry, Chemical Engineering", Supercomputing 2005, Education Program to Middle School and High School Teachers, Nov 12-18, 2005, Seattle, WA
- [I63] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Atomistic simulations of long-range strain and close-range electronic structure in self-assembled quantum dot systems and quantum dot nanostructures and Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org", IPAM Workshop II: Multiscale Modeling in Condensed Matter and Materials Sciences, including MiniWorkshop: Time Acceleration Methods in Atomistic Simulations, October 17 - 22, 2005, UCLA.
- [I62] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org and Atomistic simulations of multimillion-atom quantum dot nanostructures", 5th IEEE Conference on Nanotechnology, July 11-15, 2005, Nagoya Congress Center, Nagoya, Japan.
- [I61] Shaikh Ahmed, Gerhard Klimeck, Sebastien Goasguen, Faisal Saied, Marek Korkusinski, Haiying Xu, Seungwon Lee, "Building and Deploying Nanotechnology Community Software tools on nanoHUB.org, Atomistic Simulations of multimillion-atom quantum dot nanostructures", I-light Symposium, September 2005, Indianapolis, IN.
- [I60] Sebastien Goasguen, Mark Lundstrom, Gerhard Klimeck, Michael McLennan, Jose Fortes, Renato Figueiredo, "The nanoHUB a portal to TeraGrid and OSG for nanotechnology", Open Science Grid Application workshop, SLAC June 1-2, 2005
- [I59] Mark Lundstrom, Gerhard Klimeck, "The NCN: A Vision for Theory, Simulation and Networking", First International Nanotechnology Conference on Communication and Cooperation, San Francisco, CA, June 1-3, 2005.
- [I58] Gerhard Klimeck, Mark Lundstrom, Sebastien Goasguen, Michael McLennan, "nanoHUB.org - a resource for students and educators NCN - Network for Computational Nanotechnology", GNN 2005, 3rd International Workshop to Develop a Global Nanotechnology Network, May 25-27, 2005, Saarbrücken, Germany.
- [I57] Sebastien Goasguen, Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "The nanoHUB a Cyberinfrastructure for Computational Nanotechnology", Gridchem Computational Chemistry Workshop, April 17-19, 2005.
- [I56] Gerhard Klimeck, Marek Korkusinski, Fabiano Oyafuso, Seungwon Lee, Timothy Boykin, Paul Allmen, R. Bowen, Olga Lazarenkova, Mark Friesen, Susan Coppersmith, Mark Eriksson, Anisur Rahman, Mark Lundstrom, "NEMO 3D Atomistic Modeling of Realistic Heterostructures Containing Tens of Millions of Atoms", DARPA Workshop on Quantum Computer Modeling: From Devices to Systems, St. Augustine, FL, April 7-8, 2005.
- [I55] Gerhard Klimeck, Mark Lundstrom, Marek Korkusinski, Haiying Xu, Faisal Saied, Sebastien Goasguen, Timothy Boykin, Fabiano Oyafuso, S. Lee, H Hua, Olga Lazarenkova, R. Bowen, Paul Allmen, "nanoHUB.org - Towards On-Line Simulation for Materials and Nanodevices by Design", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [I54] Eric Jakobson, Narayan Aluru, Jeff Brinker, Gerhard Klimeck, "National Center for Design of Biomimetic Nanoconductors", NIH Nanomedicine Concept Development Plan Meeting, Gaithersburg, March 9-10, 2005
- [I53] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, "The Network for Computational Nanotechnology", Inaugural NWICG HPC Workshop, Envision Center, Purdue University, W. Lafayette, March 8-9, 2005
- [I52] Marek Korkusinski, Gerhard Klimeck, Fabiano Oyafuso, Seungwon Lee, Timothy Boykin, Paul Allmen, R. Bowen, Olga Lazarenkova, "Development of the Nanoelectronic Modeling tool (NEMO-3D) for multimillion atom quantum dots", CQCT Annual Workshop, Avoca Beach, Australia, Feb 8-11, 2005.

- [I51] Gerhard Klimeck, "Nanoelectronic Modeling (NEMO): Is it Device or Material Modeling?", Materials Modeling for Emerging Research Materials Workshop (2005 ITRS), Motorola/Freescale Semiconductor, Austin, TX, June 8, 2004.
- [I50] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, "The Network for Computational Nanotechnology", 2004 Nanoscale Science and Engineering Grantee Conference, Washington DC, December 13-15, 2004.
- [I49] Gerhard Klimeck, Sebastien Goasguen, Haiying Xu, Faisal Saied, Mohammed Sayeed, Hook Hua, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Paul Allmen, "HPC simulations of quantum dots consisting of multi-million atoms using NEMO 3-D", Workshop on Large-Scale Nano Simulation at Supercomputing 2004, Pittsburgh, Nov. 7-12, 2004.
- [I48] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Mohammed Sayeed, Faisal Saied, Sebastien Goasguen, Anisur Rahman, Seungwon Lee, Timothy Boykin, Paul Allmen, R. Bowen, Olga Lazarenkova, "Nanoelectronic Modeling (NEMO-3D) for multimillion atom quantum dot simulations", Invited Presentation at the Purdue and Notre Dame Booth at Supercomputing 2004, Pittsburgh, Nov. 7-12, 2004.
- [I47] Gerhard Klimeck, Anisur Rahman, Nizami Vagidov, Timothy Boykin, Mark Lundstrom, "Nanoscale Device Simulation at the Scaling Limit and Beyond", International Conference on Solid State Devices and Materials (SSDM 2004), Tokyo, Japan, Sept. 14-17, 2004
- [I46] Gerhard Klimeck, "NEMO 1-D: the first NEGF-based TCAD tool", IEEE SISPAD 2004, Keynote Speaker, Munich, Germany, September 2-4, 2004,
- [I45] Gerhard Klimeck, Mark Lundstrom, Sebastien Goasguen, "The Network for Computational Nanotechnology: Cyber-Infrastructure and Grid Computing for Nanotechnology Exploration and Education", Grid Forum Korea (GFK) Summer Workshop, Seoul, Korea, Aug. 26-27, 2004.
- [I44] Gerhard Klimeck, Ahmet Yanik, Prabhakar Srivastava, Supriyo Datta, "Coherent Transport in SWCNTs with Spin-Orbit Coupling", IEEE Nano 2004, Munich, Germany, August 16-19, 2004
- [I43] Gerhard Klimeck, Fabiano Oyafuso, Seungwon Lee, Timothy Boykin, Paul Allmen, R. Bowen, Olga Lazarenkova, Mark Friesen, Susan Coppersmith, Mark Eriksson, Anisur Rahman, Mark Lundstrom, K. Whaley, "Development of the Nanoelectronic Modeling tool (NEMO-3D) for multimillion atom quantum dots", CECAM workshop, Modeling of self-assembled semiconductor nanostructures Lyon, France, June 28-30, 2004.
- [I42] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Susan Coppersmith, Mark Friesen, "Empirical Atomic Level Simulations for QC Applications", CQDT Workshop, Potsdam, NY, May 17-21, 2004.
- [I41] Mark Lundstrom, Gerhard Klimeck, "The Network for Computational Nanotechnology", National Nanotechnology Initiative: From Vision to Commercialization, Keynote Address, Washington DC, March 31-April 2, 2004.
- [I40] Mark Lundstrom, Gerhard Klimeck, "The Network for Computational Nanotechnology", Nanotech 2004, Keynote Address, Boston, MA, March 8-11, 2004.
- [I39] Mark Lundstrom, Gerhard Klimeck, "Network for Computational Nanotechnology", Supercomputing Conference 2003, Birds of a Feather Session on HPC Innovation for Nanotechnology, Phoenix, AZ, November 16-21, 2003.
- [I38] Mark Lundstrom, Gerhard Klimeck, "Device Simulation at the Molecular Scale", Silicon Nanoelectronics and Beyond Workshop, Panel Session IV - Tools and Methodologies for Nanoelectronic Design, Hillsboro, OR, October 29-30, 2003, sponsored by NSF, SRC, Intel.

Work Performed at JPL (22 Total)

- [I37] Gerhard Klimeck, Fabiano Oyafuso, Seungwon Lee, Timothy Boykin, Paul Allmen, R. Bowen, Olga Lazarenkova, "Development of the Nanoelectronic Modeling tool (NEMO-3D) for multimillion atom quantum dots", Computational Approaches Toward the Electronic Properties of Quantum Dots Workshop, Chicago, September 22-24, 2003, sponsored by DARPA.
- [I36] Gerhard Klimeck, Fabiano Oyafuso, Paul Allmen, Timothy Boykin, R. Bowen, "Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations", CERION II Workshop Bilbao (Spain) September 2-6, 2003.
- [I35] Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul Allmen, Seungwon Lee, K. Whaley, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 18-22, 2003.
- [I34] Gerhard Klimeck, Roger Lake, R. Bowen, Timothy Boykin, Daniel Blanks, William Frensley, Fabiano Oyafuso, Seungwon Lee, Paul Allmen, Olga Lazarenkova, Thomas Cwik, "Key elements in NEMO to quantitative nano-scale carrier transport analysis in semiconductors", Workshop on molecular conduction, Purdue University, July 8-11, 2003.

- [I33] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, Timothy Boykin, "Empirical Atomic Level Simulations for QC Applications", THINQC, June 9-10, 2003, Harpers Ferry.
- [I32] Gerhard Klimeck, Gary Yagi, Robert Deen, Michael McAuley, Eric DeJong, Fabiano Oyafuso, "Near Real-Time Parallel Image Processing using Cluster Computers", Quality Mission Software Workshop, May 13-15, 2003, Rehoboth Beach, Delaware.
- [I31] Gerhard Klimeck, Fabiano Oyafuso, Paul Allmen, Timothy Boykin, R. Bowen, "Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations", Nanotech2003 (including MSM 2003 and ICCN 2003), February 23-27, 2003, San Francisco.
- [I30] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, Paul Allmen, "Development of a 3-D tight binding-based electronic structure simulator for multi-million atom systems (NEMO 3-D)", Advanced Heterostructure Workshop, Hapuna Beach, HI, Dec. 1-6, 2002.
- [I29] Gerhard Klimeck, Fabiano Oyafuso, Paul Allmen, Timothy Boykin, R. Bowen, "Nanoelectronic Modeling: NEMO 1-D: Design, Optimization, Synthesis, NEMO 3-D: Fundamental Limits", Nanoelectronics Planet Fall 2002, Conference and Expo, NY, NY, Nov. 18-19, 2002.
- [I28] Paul Allmen, Gerhard Klimeck, "Transport Simulation of Precessing Spin Distribution across Semiconductor Heterojunctions", DARPA Spintronics Workshop, Delray Beach, FL, Sep 30 - Oct 4, 2002.
- [I27] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, Paul Allmen, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 19-23, 2002.
- [I26] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, Paul Allmen, "NEMO 3-D: Electronic Structure Simulations Including over Ten Million Atoms", Nanospace 2002, Galveston, TX, June 24-28, 2002.
- [I25] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, Paul Allmen, "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", The first International Workshop on Quantum Dots for Quantum Computing and Classical Size Effect Circuits, Kochi, Japan, Jan 26-28, 2002
- [I24] Nikzad Toomarian, Amir Fijani, Gerhard Klimeck, Rosa Leon, Yuming Qiu, "Quantum Dots Based Rad-Hard Computing and Sensors", Keynote, CMP Cientifica, Sept 3-7, 2001.
- [I23] Gerhard Klimeck, "Applications of quantum transport in devices", Advanced Research Workshop on Quantum Transport in Semiconductors, Maratea, Italy, June 17-22 (2001)
- [I22] Gerhard Klimeck, "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001)
- [I21] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Atomistic 3-D Simulation of Nanoelectronic Structures", 2nd Workshop on Computational Materials and Electronics, Motorola University, Tempe, Arizona, Nov 9-10, (2000).
- [I20] Gerhard Klimeck, R. Bowen, Thomas Cwik, Timothy Boykin, "Development of a 3-D Nanoelectronic Device Modeling Tool (NEMO 3-D)", DARPA Workshop on Gigascale Integration, Washington DC, May 5, 2000.
- [I19] Gerhard Klimeck, R. Bowen, Timothy Boykin, Carlos Salazar-Lazaro, Thomas Cwik, Adrian Stoica, "Simulator Development for Nanoelectronic Device", 3rd NASA Workshop on Device Modeling, NASA Ames Research Center, August 26-29, 1999.
- [I18] Gerhard Klimeck, R. Bowen, Timothy Boykin, Fabiano Oyafuso, Carlos Salazar-Lazaro, Adrian Stoica, Tom Cwik, "Nanoelectronic Modeling at JPL", DARPA Ultra Electronics Program Review, Oct 18-21, 1998, Estes Park, CO.
- [I17] Gerhard Klimeck, R. Bowen, Timothy Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", ICSDT 98 - 6th International Conference on Simulation of Devices and Technologies, Cape Town, South Africa, Oct 14-16, 1998.
- [I16] Gerhard Klimeck, Carlos Salazar-Lazaro, Adrian Stoica, Tom Cwik, "Structural Analysis Using Quantum Mechanical Electron Transport Simulations Driven by a Genetic Algorithm", Second Workshop on Characterization, Future Opportunities and Applications of 6.1Å III-V Semiconductors, Organized by ONR, NRL, and DARPA, August 24-26, 1998 Naval Research Laboratory, Washington, DC.

Work Performed at TI/UTD (12 Total)

- [I15] Gerhard Klimeck, Daniel Blanks, Roger Lake, "NEMO: A Novel 1-D Quantum Device Simulator", DARPA/Rome Lab Composite CAD Program Principal Investigator Meeting, Huntsville, AL, December 1-3, 1998
- [I14] Gerhard Klimeck, Roger Lake, Daniel Blanks, "NEMO: Quantitative Resonant Tunneling Diode Simulation", 1997 DARPA ULTRA Electronics and Advanced MicroElectronics Program Review, October 26-31, Santa Fe, NM (1998).
- [I13] R. Bowen, Chenjing Fernando, Gerhard Klimeck, Amitava Chatterjee, Daniel Blanks, Roger Lake, Jerry Woodall, Joseph Davis, Mak Kulkarni, Sunil Hattangady, Cheng-Kok Koh, "Dopant Fluctuations and Quantum

- Effects in Sub-0.1 μ m CMOS", 1997 International Semiconductor Device Research Symposium, Virginia, Dec. 11-12, 1997.
- [I12] Gerhard Klimeck, Daniel Blanks, Roger Lake, R. Bowen, William Frensley, Manhwa Leng, Chenjing Fernando, "Nanoelectronic Modeling (NEMO): A New Quantum Device Simulator", The Second NASA Device Modeling Workshop, Aug. 7-8 1997, NASA Ames Research Center, Moffett Field, CA.
- [I11] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, Manhwa Leng, Chenjing Fernando, William Frensley, Dejan Jovanovic, Paul Sotirelis, "The NEMO Project or Writing Software in a Large Research Group", International Workshop on Computational Electronics, South Bend, IN, May 1997.
- [I10] Gerhard Klimeck, Daniel Blanks, R. Bowen, Bobby Brar, Tom Broekaert, Gary Frazier, Dejan Jovanovic, Roger Lake, Ted Moise, Alan Seabaugh, Glen Wilks, Paul Wagt, "Design and Implementation of Resonant Tunneling Devices into Circuits and Applications", Phantoms Strategic Domain Meetings, Aachen, Germany, March 10-13, 1997.
- [I9] William Frensley, R. Bowen, Chenjing Fernando, Gerhard Klimeck, Manhwa Leng, Daniel Blanks, Ted Moise, "Resonant Tunneling as a Probe of Electron Transport in Semiconductor Heterostructures", First International Conference on Open Problems in Charged Particle Transport, Paris, France, June 1996.
- [I8] Roger Lake, Gerhard Klimeck, R. Bowen, Chenjing Fernando, Ted Moise, Daniela Francovicchio, Y. Kao, "Transport Physics of Tunnel Devices", Third International Symposium on Nanostructures and Mesoscopic Structures, Santa Fe, NM, May 19-24, 1996.
- [I7] Roger Lake, Gerhard Klimeck, Chenjing Fernando, R. Bowen, Ted Moise, Y. Kao, Daniela Francovicchio, "Interface Roughness and Polar Optical Phonon Scattering in RTDs: theory, modeling and experiment", 23rd Conference on the Physics and Chemistry of Semiconductor Interfaces, La Jolla, CA, Jan. 21-25, 1996.
- [I6] William Frensley, James Hellums, Chenjing Fernando, R. Bowen, Gerhard Klimeck, Roger Lake, Daniel Blanks, "Quantitative Accurate Simulation of Quantum Semiconductor Devices", Workshop on Physics and Computer Modeling of Devices Based on Low Dimensional Structures, University of Aizu, Aizu-Wakamatsu, Japan, Nov. 1995.
- [I5] William Frensley, James Hellums, Chenjing Fernando, R. Bowen, Gerhard Klimeck, "Open System Boundary Conditions for the Time-Dependent and Steady State Schrödinger Equations", Workshop on Density Matrix Methods at the Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, Aug. 1995.
- [I4] William Frensley, Chenjing Fernando, R. Bowen, Gerhard Klimeck, "Modeling Tools for the Development of Quantum and Conventional Semiconductor Heterostructure Devices", Government Microcircuit Applications Conference (GOMAC), San Diego, CA, Nov. 1994.

Work Performed in graduate school (3 Total)

- [I3] Supriyo Datta, Gerhard Klimeck, Roger Lake, Yong Lee, Michael McLennan, "Quantum Device Simulation Including Interactions", International Workshop on Computational Electronics, Portland, May 18-20 1994.
- [I2] Supriyo Datta, Gerhard Klimeck, Roger Lake, "Resonant tunneling diodes: Effects of Scattering on the Valley Current", International Symposium on Compound Semiconductors, San Diego, Sept. 18-24, 1994. Inst. Phys. Conf. Ser. 141: 770-775, 1995.
- [I1] Supriyo Datta, Roger Lake, Gerhard Klimeck, "Quantum Device Simulation", Microwave Theory and Techniques Symposium, Workshop on Combined Self-Consistent Particle Transport Simulation and Full Wave Dynamic Field Simulation for Monolithic Solid State Device and Circuit Calculations, Atlanta, June 18, 1993.

CONTRIBUTED CONFERENCES (513 + 7 TOTAL)**Work Performed at Purdue (395 + 6 Total)**

- [C520] Gerhard Klimeck¹, Tanya Faltens¹, Daniel Mejia¹, Alejandro Strachan¹, Lynn Zentner¹, Michael Zentner², “nanoHUB.org: How to enable Rapid Curriculum Innovation through Translation of Research-Based Simulation Tools into Apps”, WINDS 2022 Conference, Kauai, HI, Dec. 12, 2022.
- [C519] Gerhard Klimeck, Tillmann Kubis, Michael Povolotskyi, James E. Fonseca, Bozidar Novakovic, Rajib Rahman, Tarek Ameen, James Charles, Junzhe Geng, Kaspar Haume, Yu He, Ganesh Hegde, Yuling Hsueh, Hesam Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Lemus, Daniel Mejia, Kai Miao, Samik Mukherjee, Seung Hyun Park, Ahmed Reza, Mehdi Salmani, Parijat Sengupta, Saima Sharmin, Yaohua Tan, Archana Tankasala, Daniel Valencia, Evan Wilson, “NEMO5, a Multiscale, Multiphysics Nanoelectronics Modeling Tool used for Ultra-Scaled CMOS, 2D Transistor, Topological Materials, and Quantum Computing Devices”, WINDS 2022 Conference, Kauai, HI, Dec. 12, 2022.
- [C518] Jay Alameda, Claire Stirn, Gregory Bauer, Timothy Boerner, Brett Bode, Maytal Dahan, William Gropp, Marlon Pierce, Cynthia Yewdall, Michael Zentner, Meghna Babbar-Sebens, Michael Barton, Daniele Bianchi, Michael Bell, Michel Boufadel, Michael Cianfrocco, Sean Cleveland, Cosan Daskiran, Kjersten Fagnan, Geoffrey Fox, Eleftherios Garyfallidis, Jerome Hajjar, Gerhard Klimeck, Mark Miller, Mark Perri, Victor Pinks II, Mohan Ramamurthy, Michel Regenwetter, Amy Roberts, Aldo Romero, Carol Song, Alejandro Strachan, Ellad Tadmor and Gregory Tucker, “The Delta Gateway: Exploring Community Use of GPU Resources through a Science Gateway”, Science Gateways Conference, San Diego, Oct. 18, 2022
- [C517] Gerhard Klimeck, Lynn Zentner, Alejandro Strachan, Michael Zentner, “Driving Sustainability of a Gateway with a Customer Relationship Management (CRM) System”, Science Gateways Conference, San Diego, Oct. 18, 2022
- [C516] Yuanchen Chu, Shang-Chun Lu, Michael Povolotskyi, Gerhard Klimeck, Umberto Ravaioli, Tomás Palacios, and Mohamed Mohamed, "Assessment of Lateral and Vertical Tunneling FETs Based on 2D Material for Ultra-Low Power Logic Applications", International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Sept. 5-9, 2022, Granada, Spain.
- [C515] Gerhard Klimeck, “nanoHUB for Workforce Development”, Workshop on Workforce development, The Ohio State University, April 6, 2023.
- [C514] Sandra Gesing, Claire Stirn, Gerhard Klimeck, Lynn Zentner, S. Wang, B.M. Martinez, Diaz, C. Donovan, L. Zhao, Carol Song, I.L. Kim, Alejandro Strachan, Michael Zentner, R. Kalyanam, "Open Science via HUBzero: Exploring Five Science Gateways Supporting and Growing their Open Science Communities", HICSS-55 (55th Hawaii International Conference on System Sciences), January , 5, 2022
- [C513] Gerhard Klimeck, ""nanoHUB", Heterogeneous data, Federated data, and Interoperability, Pioneering the Future of Federally Supported Data Repositories", A NITRD Big Data Interagency Working Group Virtual Workshop, Wednesday Jan 13th - Friday Jan 15th, 2021
- [C512] Veljko Milutinovic, Miljan Đorđević, Erfan Azer, Kristy Yoshimoto, Ivan Ratković, Gerhard Klimeck, Milos Kotlar, Miroslav Bojovic, Bozidar Miladinovic, Nenad Korolija, Stevan Stankovic, Nenad Filipović, Zoran Babović, Miroslav Kosanic, Akira Tsuda, Mateo Valero, Massimo Santo, Erich Neuhold, Jelena Skoručak, Laura Dipietro, "The Ultimate DataFlow for Ultimate SuperComputers-on-a-Chip, for Scientific Computing, Geo Physics, Complex Mathematics, and Information Processing", MECO'2021 and CPS'2021, Budva, Montenegro, June 07-10, 2021
- [C511] Tanya Faltens, Lynn Zentner, Michael Zentner, Alejandro Strachan, "Network for Computational Nanotechnology Cyber Platform (NCN-CP)", Poster at the biennial NSF ERC Meeting, Washington DC, Oct. 25, 2019
- [C510] Nathan Denny, Michael Zentner, Daniel Mejia, Gerhard Klimeck, ""Instant On" Science Gateways: An Introduction to Caching Simulation Results and a Path Towards Data Exploration", Gateways 2019, Sept. 23–25, 2019, San Diego, California
- [C509] Claire Stirn, Sandra Gesing, Michael Zentner, Gerhard Klimeck, Lynn Zentner, Carly Dearborn, "HUBzero's Variations of Sustainability: From Simulation/Modeling Tools to Communities", 11th International Workshop on Science Gateways, Ljubljana, Slovenia, June 12-14, 2019
- [C508] Lynn Zentner, Gerhard Klimeck, Stuti Magar, Louis Tay, "Understanding your Science Gateway Users – A case study of who, how, and why", 11th International Workshop on Science Gateways, Ljubljana, Slovenia, June 12-14, 2019
- [C507] Gerhard Klimeck, Gustavo Valencia-Zapata, Nathan Denny, Lynn Zentner, Michael Zentner, "nanoHUB user behavior: moving from retrospective statistics to actionable behavior Analysis", 11th International Workshop on Science Gateways, Ljubljana, Slovenia, June 12-14, 2019

- [C506] Gerhard Klimeck, Alejandro Strachan, Tanya Faltens, Brad Hallberg, Lynn Zentner, Michael Zentner, Martin Hunt, "Using nanoHUB.org in Research and Education—A Hands-on Tutorial", IWCN 2019 - International Workshop on Computational Nanotechnology, May 20-24, 2019 Evanston, IL, USA
- [C505] Nathan Denny, Michael Zentner, Gerhard Klimeck, "Visualizing User Interactions with Simulation Tool", Gateways 2018: The 13th Gateway Computing Environments Conference, September 25-27, 2018, Austin, TX
- [C504] Michael Zentner, Nathan Denny, Krishna Madhavan, Swaroop Samek, George Adams III., Gerhard Klimeck, "Using Automatic Detection and Characterization to Measure Educational Impact of nanoHUB", Gateways 2018: The 13th Gateway Computing Environments Conference, September 25-27, 2018, Austin, TX
- [C503] Dwight McKay, Michael Zentner, Gerhard Klimeck, "Clustering Download Events to Identify Classrooms", Gateways 2018: The 13th Gateway Computing Environments Conference, September 25-27, 2018, Austin, TX
- [C502] Daniel Valencia, K. Wang, Y. Chu, Gerhard Klimeck, Michael Povolotskyi, "Surface and grain boundary effects on copper interconnects thin films modeling with an atomistic basis", International Conference on Simulation of Semiconductor Processes and Devices, September 24-26, 2018, Austin, TX
- [C501] Shang-Chun Lu, Yuanchen Chu, Youngseok Kim, Mohamed Mohamed, Gerhard Klimeck, Thomas Palacios, Umberto Ravaioli, "Design Guidelines and Limitations of Multilayer Two-dimensional Vertical Tunneling FETs for Ultra-Low Power Logic Applications", International Conference on Simulation of Semiconductor Processes and Devices, September 24-26, 2018, Austin, TX
- [C500] Yuanchen Chu, Prasad Sarangapani, James Charles, Gerhard Klimeck, Tillmann Kubis, "Electron-only explicit screening quantum transport model for semiconductor nanodevices", International Conference on Simulation of Semiconductor Processes and Devices, September 24-26, 2018, Austin, TX
- [C499] Lynn Zentner, Gerhard Klimeck, "Abstract: The Role of Analytics in Science Gateway Communities", Presented at the 10th International Workshop on Science Gateways, Edinburgh, Scotland, June 13-15, 2018
- [C498] Patrick Fay, W. Li, D. Digiovanni, L. Cao, H. Ilatikhameneh, Fan Chen, Tarek Ameen, Rajib Rahman, Gerhard Klimeck, C. Lund, S. Keller, S.M. Islam, A. Chaney, Y. Cho, Debdeep Jena, "III-N heterostructure devices for low-power logic", 2017 China Semiconductor Technology International Conference (CSTIC), Shanghai, China, March 12-13, 2017
- [C497] Prasad Sarangapani, Cory Weber, Jiwon Chang, Stephen Cea, Roksana Golizadeh-Mojarad, Michael Povolotskyi, Gerhard Klimeck, Tillmann Kubis, "Assessment of Si/SiGe PMOS Schottky contacts through atomistic tight binding simulations: Can we achieve the $10\text{--}9\Omega\cdot\text{cm}^2$ target?", 2017 IEEE 17th International Conference on Nanotechnology (IEEE-NANO), Pittsburgh, PA, July 25-28, 2017
- [C496] Jun Huang, Pengyu Long, Michael Povolotskyi, Gerhard Klimeck, Mark Rodwell, "Sb- and Al-free ultra-high-current tunnel FET designs", 2017 Fifth Berkeley Symposium on Energy Efficient Electronic Systems & Steep Transistors Workshop (E3S), Berkeley, California, October 19-20, 2017
- [C495] Pengyu Long, Michael Povolotskyi, Jun Huang, James Charles, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, "A high-current InP-channel triple heterojunction tunnel transistor design", 75th Device Research Conference (DRC), University of Notre Dame (Indiana, USA) from June 25-28, 2017
- [C494] Lynn Zentner, Gerhard Klimeck, "Abstract: Strategies for Community Building in Science Gateways", Presented at the 9th International Workshop on Science Gateways, Poznan, Poland, June 19-21, 2017
- [C493] Xinchun Guo, James Charles, Junzhe Geng, Daniel Valencia, Daniel Lemus, Tillmann Kubis, Gerhard Klimeck, "Nanoelectronic Modeling on Blue Waters with NEMO5", Presentation at Blue Waters Symposium 2017, Sunriver, OR, May 16-19, 2017
- [C492] KuangChung Wang, Teodor Stanev, Daniel Valencia, James Charles, Prasad Sarangapani, Alex Henning, Vinod Sangwan, Aritra Lahiri, Michael Povolotskyi, A. Afzalian, Gerhard Klimeck, Mark Lundstrom, Mark Hersam, Lincoln Lauhon, Nathaniel Stern, Tillmann Kubis, "Stark effect in the photoluminescence of transition metal dichalcogenide structures", International Workshop on Computational Nanotechnology (IWCN), Leeds, United Kingdom, 5-9 June, 2017
- [C491] Prasad Sarangapani, Yuanchen Chu, James Charles, Gerhard Klimeck, Tillmann Kubis, "Non-equilibrium Green's function method: Band tail formation in non-local polar optical phonon scattering", International Workshop on Computational Nanotechnology (IWCN), Leeds, United Kingdom, 5-9 June, 2017
- [C490] Gerhard Klimeck, "NanoHUB.org - Always on enabling global scientific knowledge transfer", International Workshop on Computational Nanotechnology (IWCN), Leeds, United Kingdom, 5-9 June, 2017
- [C489] Junzhe Geng, Prasad Sarangapani, Ben Browne, Carl Wordelman, Erik Nelson, Tillmann Kubis, Gerhard Klimeck, "Multi-scale nonequilibrium green's function method for LEDs: Balance of thermalization and tunneling", International Workshop on Computational Nanotechnology (IWCN), Leeds, United Kingdom, 5-9 June, 2017
- [C488] Yuanchen Chu, Prasad Sarangapani, James Charles, Michael Povolotskyi, Gerhard Klimeck, Tillmann Kubis, "Nonequilibrium Green's function method: Performance prediction of band-to-band tunneling devices in electron-only representation", International Workshop on Computational Nanotechnology (IWCN), Leeds, United Kingdom, 5-9 June, 2017

- [C487] James Charles, Prasad Sarangapani, Yuanchen Chu, Gerhard Klimeck, Tillmann Kubis, "Non-local scattering with a new recursive nonequilibrium green's function method", International Workshop on Computational Nanotechnology (IWCN), Leeds, United Kingdom, 5-9 June, 2017
- [C486] Junzhe Geng, KuangChung Wang, Prasad Sarangapani, Ben Browne, Carl Wordelman, Erik Nelson, Tillmann Kubis, Gerhard Klimeck, "New insights into III-Nitride LED designs through quantitative modeling", E-MRS ICNS 12 Meeting, symposium B : Optical devices, Congress Center in Strasbourg (France), July 24-28, 2017
- [C485] Jun Huang, Pengyu Long, Michael Povolotskyi, Gerhard Klimeck, Mark Rodwell, "Sb- and Al- Free Ultra-High-Current Tunnel FET Design", Fifth Berkeley Symposium on Energy Efficient Electronic Systems and Steep Transistors Workshop October 19-20, 2017 University of California, Berkeley, California, USA
- [C484] Chin-Yi Chen, Tarek Ameen, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, "Optimizing the Device Structure of 2D Material Tunnel FETs", TECHCON 2017, Renaissance Hotel in Austin, Texas, September 10-12, 2017
- [C483] Rifat Ferdous, Kok , Menno Veldhorst, Jason Hwang, Henry Yang, Gerhard Klimeck, Andrea Morello, Andrew Dzurak, Rajib Rahman, "Interface induced spin-orbit interaction in silicon quantum dots and anisotropic dephasing time", 2017 Silicon Quantum Electronics Workshop, August 18-21, 2017, Intel Jones Farm Conference Center, Hillsboro, Oregon
- [C482] Chin-Yi Chen, Archana Tankasala, Rifat Ferdous, Rajib Rahman, "Exchange coupling in silicon quantum dots from atomistic configuration interaction", 2017 Silicon Quantum Electronics Workshop, August 18-21, 2017, Intel Jones Farm Conference Center, Hillsboro, Oregon
- [C481] Harshad Sahasrabudhe, Saeed Fallahi, James Nakamura, Michael Povolotskyi, Bozidar Novakovic, Rajib Rahman, Michael Manfra, Gerhard Klimeck, "Electrostatic and Quantum Transport Simulations of Quantum Point Contacts in the Integer Quantum Hall Regime", APS March Meeting 2017 Volume 62, March 13-17, 2017, New Orleans, Louisiana
- [C480] Rifat Ferdous, Kok , Menno Veldhorst, Jason Hwang, Henry Yang, Gerhard Klimeck, Andrew Dzurak, Rajib Rahman, "Interface induced spin-orbit interaction in silicon quantum dots and prospects of scalability", APS March Meeting 2017 Volume 62, March 13-17, 2017, New Orleans, Louisiana
- [C479] KuangChung Wang, Daniel Valencia, James Charles, Yu He, Michael Povolotskyi, Gerhard Klimeck, Jesse Maassen, Mark Lundstrom, Tillmann Kubis, "NEMO5: Predicting MoS2 Heterojunctions", International Conference on Simulation of Semiconductor Processes and Devices 2016, Nuremberg, Germany, September 6-8
- [C478] Daniel Valencia, Evan Wilson, Prasad Sarangapani, Gustavo Valencia, Gerhard Klimeck, Michael Povolotskyi, Zhengping Jiang, "Grain Boundary Resistance in Nanoscale Copper Interconnections", International Conference on Simulation of Semiconductor Processes and Devices 2016, Nuremberg, Germany, September 6-8
- [C477] Patrick Fay, W. Li, L. Cao, K. Pourang, S.M. Islam, C. Lund, Saima Sharmin, Hesameddin Ilatikhameneh, Tarek Ameen, Jun Huang, Rajib Rahman, Debdeep Jena, S. Keller, Gerhard Klimeck, "Novel III-N heterostructure devices for low-power logic and more", 2016 IEEE 16th International Conference on Environment and Electrical Engineering, Florence, Italy, 2016
- [C476] Lynn Zentner, Michael Zentner, Gerhard Klimeck, "Extended Abstract: Analysis of nanoHUB.org from a Business Perspective", Presented at the 11th Gateway Computing Environments Conference, San Diego, CA, November 2-3, 2016
- [C475] Lynn Zentner, Gerhard Klimeck, "nanoHUB: Experiences and Insights on Care and Feeding of a Successful, Engaged Science Gateway Community", Presented at the 8th International Workshop on Science Gateways, Rome, Italy, June 8-10, 2016
- [C474] Xinchun Guo, Daniel Lemus, Daniel Mejia, Jim Fonseca, Gerhard Klimeck, Tillmann Kubis, "MPI + hStreams in NEMO5: Partitioning Xeon Phi", Presentation at the Intel Xeon Phi User Group 2016 Annual Meeting, Chicago, IL
- [C473] Xinchun Guo, KuangChung Wang, James Charles, Junzhe Geng, Daniel Mejia, Daniel Valencia, Daniel Lemus, Jim Fonseca, Gerhard Klimeck, Tillmann Kubis, "NEMO5, Xeon Phi and hStreams: Physics of Ultrascaled 2D Nanotransistors", Poster session presented at SC '16 the International Conference for High Performance Computing, Networking, Storage and Analysis, Salt Lake City, UT, 2016
- [C472] Pengyu Long, Jun Huang, Michael Povolotskyi, Devin Verreck, James Charles, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, B. Calhoun, "A Tunnel FET Design for High-Current, 120 mV Operation", IEEE International Electron Devices Meeting, December 3-7, 2016, San Francisco
- [C471] Junzhe Geng, Prasad Sarangapani, Erik Nelson, Carl Wordelman, Ben Browne, Tillmann Kubis, Gerhard Klimeck, "Multi-Scale, Multi-Physics NEGF Quantum Transport for Nitride LEDs", 16th International Conference on Numerical Simulation of Optoelectronic Devices, July 11-15, 2016, Sydney, Australia
- [C470] Rifat Ferdous, Gerhard Klimeck, Rajib Rahman, Erika Kawakami, Pasquale Scarlino, Michal Nowak, Lieven Vandersypen, Mark Friesen, Susan Coppersmith, Mark Eriksson, "Valley dependent anisotropic spin splitting

- in silicon quantum dots", Poster Session, ARO Quantum computing program review, Alexandria, VA, 18-21 July, 2016
- [C469] Sara Fathipour, Hesameddin Ilatikhameneh, Jun Park, Cristobal Alessandri, Rajib Rahman, Gerhard Klimeck, Susan Fullerton-Shirey, Alan Seabaugh, "2D crystal TFETs", LEAST review, August 10 & 11, 2016, University of Notre Dame
- [C468] Chin-Sheng Pang, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, zhihong chen, "Double Gated TMD p/n Junctions for TFET Applications", LEAST review, August 10 & 11, 2016, University of Notre Dame
- [C467] Hesameddin Ilatikhameneh, Fan Chen, Tarek Ameen, Rajib Rahman, Gerhard Klimeck, "Atomistic modeling of 2D material devices", US-EU workshop on 2D layered materials and devices, Arlington, Virginia, April 22, 2015
- [C466] Jun Huang, Pengyu Long, Hesameddin Ilatikhameneh, Tarek Ameen, Rajib Rahman, Michael Povolotskyi, Mark Rodwell, Gerhard Klimeck, "Multiscale Transport Simulation of Nanoelectronic Devices with NEMO5", Progress In Electromagnetics Research Symposium (PIERS), August, 2016, Shanghai, China
- [C465] Jun Huang, Yu Wang, Pengyu Long, Yaohua Tan, Michael Povolotskyi, Gerhard Klimeck, "Computational Study of Strain-Engineered III-V Tunneling Transistors", Progress In Electromagnetics Research Symposium (PIERS), August, 2016, Shanghai, China
- [C464] Pengyu Long, Jun Huang, Michael Povolotskyi, Devin Verreck, Gerhard Klimeck, Mark Rodwell, "High-Current InP-Based Triple Heterojunction Tunnel Transistors", 28th International Conference on Indium Phosphide and Related Materials (IPRM), June, 2016, Toyama, Japan
- [C463] Pengyu Long, Michael Povolotskyi, Jun Huang, Hesameddin Ilatikhameneh, Tarek Ameen, Rajib Rahman, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, "Extremely high simulated ballistic currents in triple-heterojunction tunnel transistors", Device Research Conference (DRC), June, 2016, Newark, Delaware, USA
- [C462] Jun Huang, Pengyu Long, Michael Povolotskyi, Mark Rodwell, Gerhard Klimeck, "Exploring Channel Doping Designs for High-Performance Tunneling FETs", Device Research Conference (DRC), June, 2016, Newark, Delaware, USA
- [C461] Tarek Ameen, Hesameddin Ilatikhameneh, Jun Huang, Michael Povolotskyi, Gerhard Klimeck, Rajib Rahman, "The Influence Of Carrier Thermalization On The Performance Of Nitride Tunneling Hetero-Structures", TECH CON 2016, Sept. 11 - Tuesday, Sept. 13, 2016, Renaissance Austin Hotel, Austin, TX, United States
- [C460] Hesameddin Ilatikhameneh, Tarek Ameen, Fan Chen, Jun Huang, Rajib Rahman, Gerhard Klimeck, "Why Do We Need Novel Steep Transistors?", TECH CON 2016, Sept. 11 - Tuesday, Sept. 13, 2016, Renaissance Austin Hotel, Austin, TX, United States
- [C459] Fan Chen, Hesameddin Ilatikhameneh, Yaohua Tan, Daniel Valencia, Gerhard Klimeck, Rajib Rahman, "Transport in vertically stacked hetero-structures from 2D materials", 33rd International Conference on the Physics of Semiconductors, Beijing, China on July 31- August 5, 2016
- [C458] Fan Chen, Hesameddin Ilatikhameneh, Yaohua Tan, Daniel Valencia, Gerhard Klimeck, Rajib Rahman, "Atomistic Modeling of Interlayer TFETs", 2016 LEAST review, August 10 & 11, 2016, University of Notre Dame
- [C457] Fan Chen, Hesameddin Ilatikhameneh, Yaohua Tan, Daniel Valencia, Gerhard Klimeck, Rajib Rahman, "Atomistic Modeling of WTe-MoS₂ Interlayer TFETs", TECH CON 2016, Sept. 11 - Tuesday, Sept. 13, 2016, Renaissance Austin Hotel, Austin, TX, United States
- [C456] Rifat Ferdous, Erika Kawakami, Pasquale Scarlino, Michal Nowak, Gerhard Klimeck, Mark Friesen, Susan Coppersmith, Mark Eriksson, Lieven Vandersypen, Rajib Rahman, "Valley dependent electron spin resonance in a silicon quantum dot with integrated micro-magnets", Silicon Quantum Electronics Workshop, 13 & 14 June 2016, Science Centre of TU Delft, The Netherlands
- [C455] Rifat Ferdous, Erika Kawakami, Pasquale Scarlino, Michal Nowak, Gerhard Klimeck, Mark Friesen, Susan Coppersmith, Mark Eriksson, Lieven Vandersypen, Rajib Rahman, "Valley dependent g-factor anisotropy in Silicon quantum dots", APS March Meeting 2016, March 14-18, 2016; Baltimore, Maryland
- [C454] Yasuyuki Maeda, Tetsuya Sakurai, James Charles, Michael Povolotskyi, Gerhard Klimeck, Jose Roman, "Numerical Integral Eigensolver for a Ring Region on the Complex Plane", Presented at the International Workshop on Eigenvalue Problems: Algorithms; Software and Applications, in Petascale Computing
- [C453] Daniel Valencia, Evan Wilson, Mark Rodwell, Gerhard Klimeck, Michael Povolotskyi, "Effect of the High-k Dielectric/Semiconductor Interface on Electronic Properties in Ultra-thin Channels", IWCE 2015
- [C452] Saima Sharmin, Tarek Ameen, Junzhe Geng, Hesameddin Ilatikhameneh, Wenjun Li, Patrick Fay, Rajib Rahman, Gerhard Klimeck, "Transport characteristics of Nitride TFETs: Ballistic versus scattering", 2015 LEAST (Center for Low Energy Systems Technology) Annual Review, August 12 & 13, 2015, University of Notre Dame.
- [C451] Zhengping Jiang, Michael Povolotskyi, Nicolas Onofrio, David Guzman, Daniel Lemus, Santiago Rubiano, Jose Bermeo, Alejandro Strachan, Gerhard Klimeck, "Multi-Scale Quantum Simulations of Conductive

- Bridging RAM", Oral presentation, 18th International Workshop on Computational Electronics, West Lafayette, Indiana, September 2-4, 2015
- [C450] Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "Transferable tight binding model for strained group IV and III-V heterostructure", International Workshop on Computational Electronics (IWCE), West Lafayette, USA, 2015
- [C449] Bozidar Novakovic, Gerhard Klimeck, "Atomistic quantum transport approach to time-resolved device simulations", 20th International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Washington DC, 9-11 Sep. 2015.
- [C448] Rifat Ferdous, Chin-Yi Chen, Archana Tankasala, Rajib Rahman, Gerhard Klimeck, Erika Kawakami, Pasquale Scarlino, Michal Nowak, Lieven Vandersypen, Mark Friesen, Susan Coppersmith, Mark Eriksson, "Valley dependent spin and charge properties of silicon quantum dots", Poster Session, ARO Quantum computing program review, San Diego, Aug 10-12, 2015
- [C447] Rifat Ferdous, Yu Wang, Yuling Hsueh, Rajib Rahman, Gerhard Klimeck, Menno Veldhorst, C.H. Yang, J.C.C. Hwang, Fahd Mohiyaddin, Andrew Dzurak, R. Ruskov, C. Tahan, "Atomistic modeling of spin qubits hosted in realistic silicon quantum dots", Poster Session, ARO Quantum computing program review, San Diego, Aug 10-12, 2015
- [C446] Archana Tankasala, Yu Wang, Joe Salfi, Juanita Bocquel, Benoit Voisin, Muhammad Usman, Sven Rogge, Michelle Simmons, Lloyd Hollenberg, Rajib Rahman, Gerhard Klimeck, "Modeling exchange interaction in bulk and sub-surface donor pairs in silicon for two-qubit gates", Poster Session, ARO Quantum computing program review, San Diego, Aug 10-12, 2015
- [C445] Juanita Bocquel, Benoit Voisin, Joe Salfi, Archana Tankasala, Muhammad Usman, Rajib Rahman, Bret Johnson, Jeffrey McCallum, Lloyd Hollenberg, Michelle Simmons, Sven Rogge, "Modeling exchange interaction in bulk and sub-surface donor pairs in silicon for two-qubit gates", CQC2T Workshop at Kingscliff, New South Wales (NSW), Australia, February 18 - 20, 2015
- [C444] Fan Chen, Hesameddin Ilatikhameneh, Tao Chu, zhihong chen, Rajib Rahman, Gerhard Klimeck, "High Performance Bilayer graphene transistors", LEAST review, student poster, South Bend, IN, Aug. 2015
- [C443] Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, "Challenges and Solutions for 2D Material Tunnel Transistors", TECHCON 2015, Sept. 20-22, 2015, Austin, TX, United States.
- [C442] Yu Wang, Archana Tankasala, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, Rajib Rahman, "Engineering inter-qubit exchange coupling between donor bound electrons in silicon", Silicon Quantum Electronics Workshop, Poster session, Takamatsu Japan, Aug. 3-4, 2015
- [C441] Bozidar Novakovic, Gerhard Klimeck, "Time-Resolved Computational Method for Atomistic Open System Simulations", 18th International Workshop on Computational Electronics (IWCE), West Lafayette, Indiana, 2-4 Sep. 2015.
- [C440] Yasuyuki Maeda, Tetsuya Sakurai, James Charles, Michael Povolotskyi, Gerhard Klimeck, Jose Roman, "A parallel eigensolver using numerical quadrature for annular regions", International Workshop on Eigenvalue Problems: Algorithms; Software and Applications (EPASA 2015), in Petascale Computing, September 14-16, 2015, Tsukuba International Congress Center EPOCHAL TSUKUBA, Tsukuba, Ibaraki, Japan
- [C439] Samik Mukherjee, Gerhard Klimeck, "Electron and Phonon Dispersion Calculation on nanoHUB: Bandstructure Lab", The Second Annual nanoHUB User Conference, Purdue University on August 31 - September 1, 2015
- [C438] Prasad Sarangapani, Daniel Mejia, James Charles, Woody Gilbertso, Hesameddin Ilatikhameneh, Tarek Ameen, Andrew Roche, Jim Fonseca, Gerhard Klimeck, "Quantum Dot Lab: An Online Platform for Quantum Dot Simulations", The Second Annual nanoHUB User Conference, Purdue University on August 31 - September 1, 2015
- [C437] Prasad Sarangapani, Daniel Mejia, James Charles, Woody Gilbertso, Hesameddin Ilatikhameneh, Tarek Ameen, Andrew Roche, Jim Fonseca, Gerhard Klimeck, "Quantum Dot Lab: An Online Platform for Quantum Dot Simulations", International Workshop on Computational Electronics (IWCE 2015) September 2, 2015 West Lafayette, Indiana USA
- [C436] Hesameddin Ilatikhameneh, Gerhard Klimeck, Rajib Rahman, "2D Tunnel Transistors for Ultra-Low Power Applications: Promises and Challenges", Fourth Berkeley Symposium on Energy Efficient Electronic Systems (2015)
- [C435] Yui-Hong Tan, Hoon Ryu, Bent Weber, Michelle Simmons, Gerhard Klimeck, "Atomistic Modelling of Metallic Conduction Limits in Quasi 1-D Silicon Wires", Silicon Quantum Electronics Workshop, August 3-4, 2015, Takamatsu, Japan
- [C434] Hanjun Xian, Daniel Mejia, Krishna Madhavan, Lynn Zentner, Swaroop Shivarajapura, Victoria Farnsworth, Gerhard Klimeck, "Interactive analytic systems for understanding the scholarly impact of large-scale e-Science cyber-environments", eScience 2015, Aug 31 - Sep 4, Munich Germany
- [C433] Fan Chen, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, "Transport properties of bilayer graphene field effect transistor", TECHCON 2015, Sept. 20-22, 2015, Austin, TX, United States

- [C432] Hesameddin Ilatikhameneh, Fan Chen, Joerg Appenzeller, Rajib Rahman, Gerhard Klimeck, "Electrically Doped 2D Material Tunnel Transistors", International Workshop on Computational Electronics (IWCE 2015) September 2, 2015 West Lafayette, Indiana USA
- [C431] Hesameddin Ilatikhameneh, Rajib Rahman, Joerg Appenzeller, Gerhard Klimeck, "Atomistic Simulation of Electrically Doped WTe₂ Tunnel Transistor", The International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Washington DC, USA, September 9-11, 2015
- [C430] Fan Chen, Michael Manfra, Gerhard Klimeck, Tillmann Kubis, "NEMO5: Why must we treat topological insulator nanowires atomically?", International Workshop on Computational Electronics (IWCE 2015) September 2, 2015 West Lafayette, Indiana USA
- [C429] Fan Chen, Hesameddin Ilatikhameneh, Tao Chu, Joerg Appenzeller, zhihong chen, Gerhard Klimeck, Rajib Rahman, "Achieving a higher ON/OFF ratio in Bilayer Graphene FET-- Strain Engineering", The International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Washington DC, USA, September 9-11, 2015
- [C428] Gustavo Valencia-Zapata, Gerhard Klimeck, Michael Zentner, "Discovering Usage Patterns of nanoHUB Tools Through Association Rules", The Eleventh International Nanotechnology Conference on Communication and Cooperation (INC 11), Hilton Fukuoka Sea Hawk, Fukuoka, Japan, May 11-13, 2015.
- [C427] Andrea Morello, Arne Laucht, Juha Muhonen, Fahd Mohiyaddin, Rachpon Kalra, Juan Dehollain, Solomon Freer, Fay Hudson, Menno Veldhorst, Andrew Dzurak, Kohei Itoh, Rajib Rahman, Gerhard Klimeck, Jeffrey McCallum, David, "Local electrical control of a single-atom spin qubit in a continuous microwave field", APS March Meeting 2015, Volume 60, Number 1 March 2-6, 2015; San Antonio, Texas
- [C426] Archana Tankasala, Yu Wang, Gerhard Klimeck, Rajib Rahman, "Atomistic configuration interaction simulations of two-electron states of donors in silicon", APS March Meeting, San Antonio TX, March 2-6, 2015
- [C425] Rifat Ferdous, Yuling Hsueh, Gerhard Klimeck, Rajib Rahman, "Interface roughness mediated phonon relaxation rates in Si quantum dots", APS March Meeting 2015, Volume 60, Number 1, March 2-6, 2015; San Antonio, Texas
- [C424] Saima Sharmin, Hesameddin Ilatikhameneh, Yaohua Tan, Bozidar Novakovic, Tarek Ameen, J. Lyons, C. Walle, Wenjun Li, Patrick Fay, Rajib Rahman, Gerhard Klimeck, "Atomistic Tight-binding Modeling of III-Nitride Materials and Field Effect Transistors", 2014 LEAST (Center for Low Energy Systems Technology) Annual Review, August 12 - 14, 2014, University of Notre Dame.
- [C423] Rajib Rahman, Yu Wang, Yuling Hsueh, Yui-Hong Tan, Gerhard Klimeck, "Atomistic modeling of STM patterned donor devices for Si quantum computing", 17th International Workshop on Computational Electronics (IWCE), Paris, France, 2014
- [C422] Archana Tankasala, Yu Wang, Joe Salfi, Juanita Bocquel, Benoit Voisin, Michelle Simmons, Lloyd Hollenberg, Sven Rogge, Rajib Rahman, Gerhard Klimeck, "Many-particle states in Coulomb confined quantum dots from atomistic tight-binding calculations", Poster Session, ARO/LPS Quantum computing program review, Washington DC, Aug 11-15, 2014
- [C421] Jim Fonseca, Gerhard Klimeck, "NanoElectronic Modeling with the NEMO toolkit on nanoHUB", HUBBUB 2014, 08 Oct 2014; <https://hubzero.org/resources/1241>.
- [C420] Gerhard Klimeck, "Mythbusting Today's Nanotechnology and Knowledge Transfer through nanoHub.org", 2014 Dawn or Doom Conference, September 18, 2014, Loeb Playhouse, Purdue University
- [C419] Yu Wang, Holger Buch, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, Rajib Rahman, "A metrology technique for phosphorus-donor clusters in silicon based on hyperfine splittings", Poster Session, APS march meeting, Denver CO, March 3-7, 2014
- [C418] Rifat Ferdous, Rajib Rahman, Gerhard Klimeck, "Atomistic analysis of valley-orbit hybrid states and inter-dot tunnel rates in a Si double quantum dot", APS march meeting, Denver CO, March 3-7, 2014
- [C417] Yuling Hsueh, Holger Buch, Lloyd Hollenberg, Michelle Simmons, Gerhard Klimeck, Rajib Rahman, "Phonon induced spin relaxation times of single donors and donor clusters in silicon", APS march meeting, Denver CO, March 3-7, 2014
- [C416] Tarek Ameen, Hesameddin Ilatikhameneh, James Charles, Yuling Hsueh, Sicong Chen, Jim Fonseca, Michael Povolotskyi, Rajib Rahman, "Optimization of the Anharmonic Strain Model to Capture Realistic Strain Distributions in Quantum Dots", IEEE Nano, Toronto, 2014
- [C415] Rajib Rahman, Archana Tankasala, Yu Wang, Gerhard Klimeck, "Atomistic simulations of multi-electron states for donor qubits in silicon", Silicon Quantum Electronics Workshop, Albuquerque, NM, Aug 18-19, 2014
- [C414] Hesameddin Ilatikhameneh, Bozidar Novakovic, Yaohua Tan, Tillmann Kubis, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, "Transport properties of 2D material transistors", 17th International Workshop on Computational Electronics (IWCE), Paris, France, 2014
- [C413] Hesameddin Ilatikhameneh, Bozidar Novakovic, Yaohua Tan, Mehdi Salmani-Jelodar, Tillmann Kubis, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, "Transport Properties of 2D Material Transistors", TECHON 2014, October 1-3, 2014, Santa Clara, CA

- [C412] Hesameddin Ilatikhameneh, Bozidar Novakovic, Yaohua Tan, Mehdi Salmani-Jelodar, Tillmann Kubis, Michael Povolotskyi, Rajib Rahman, Gerhard Klimeck, "Atomistic Simulation of Steep Subthreshold Slope Bi-layer MoS₂ Transistors", Poster Session, 2014 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI USA June 8-9, 2014
- [C411] Fahd Mohiyaddin, Rajib Rahman, Rachpon Kalra, Sunhee Lee, Gerhard Klimeck, Lloyd Hollenberg, C.H. Yang, A. Rossi, Andrew Dzurak, Andrea Morello, "Designing a Large Scale Quantum Computer with Atomistic Simulations", Poster Session, 2014 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI USA June 8-9, 2014
- [C410] Y. Tan, Hoon Ryu, Bent Weber, Sunhee Lee, Rajib Rahman, Lloyd Hollenberg, Michelle Simmons, Gerhard Klimeck, "Statistical Modeling of Ultra-Scaled Donor-Based Silicon Phosphorus Devices", Poster Session, 2014 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI USA June 8-9, 2014
- [C409] Bent Weber, Y. Tan, Suddhasatta Mahapatra, T.F. Watson, Hoon Ryu, Sunhee Lee, Rajib Rahman, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, "Silicon at the Fundamental Scaling Limit - Atomic-Scale Donor-Based Quantum Electronics", 2014 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI USA June 8-9, 2014
- [C408] Mehdi Salmani-Jelodar, S. Kim, K. Ng, Gerhard Klimeck, "Performance Degradation due to Thick Physical Layer of High-k Oxide in Ultra-scaled MOSFETs and Mitigation through Electrostatics Design", 2014 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI USA June 8-9, 2014
- [C407] Xueping Jiang, Neerav Kharche, Paul Kohl, Timothy Boykin, Gerhard Klimeck, Mathieu Luisier, Pulickel Ajayan, Saroj K. Nayak, "Quasiparticle Band Gap modulation in Graphene Nanoribbons Supported on Weakly interacting Surfaces", APS March Meeting, March 18-22, 2013, Baltimore, Maryland.
- [C406] Somaia Sylvia, M. Khayer, Khairul Alam, Seung Park, Gerhard Klimeck, Roger Lake, "Discrete random distribution of source dopants in nanowire tunnel transistors (TFETs)", APS March Meeting, March 18-22, 2013, Baltimore, Maryland.
- [C405] Mehdi Salmani-Jelodar, SungGeun Kim, Kwok Ng, Gerhard Klimeck, "On the Scaling Issues and Solutions for Double Gate MOSFETs at the end of ITRS Roadmap", accepted for ISDRS 2013
- [C404] Yu He, Yu Wang, Gerhard Klimeck, Tillmann Kubis, "Nonequilibrium Green's function method: Algorithm for regular and irregular leads", TECHCON, Sep 8-11 September, 2013, Austin, TX
- [C403] Ganesh Hegde, Saumitra Mehrotra, Ravi Vedula, Yu He, Yu Wang, Zhengping Jiang, Michael Povolotskyi, Tillmann Kubis, Jim Fonseca, Alejandro Strachan, Gerhard Klimeck, "Atomistic Modeling of CBRAM Switching Behavior", 2013 FAME (Function Accelerated nanoMaterial Engineering) Annual Review, poster presentation, Oct. 15 & 16, 2013, Los Angeles, CA
- [C402] Zach Schaffter, Gerhard Klimeck, "Next Generation Crystal Viewing Tool", Summer Undergraduate Research Fellowship (SURF) Symposium, July 31, 2013, Neil Armstrong Hall of Engineering, Purdue University
- [C401] Kevin Margatan, Gerhard Klimeck, "nanoHUB - Crystal Viewer 2.0", Summer Undergraduate Research Fellowship (SURF) Symposium, July 31, 2013, Neil Armstrong Hall of Engineering, Purdue University
- [C400] Osiris Ntarugera, Gerhard Klimeck, "Developing a Crystal Viewer Tool for nanoHUB", Summer Undergraduate Research Fellowship (SURF) Symposium, July 31, 2013 at Neil Armstrong Hall of Engineering, Purdue University
- [C399] Victoria Farnsworth, Mark Lundstrom, Supriyo Datta, Ron Reifengerger, Arvind Raman, Timothy Fisher, Alejandro Strachan, Michael McLennan, Swaroop Shivarajapura, Lynn Zentner, Krishna Madhavan, Gerhard Klimeck, "nanoHUB-U: A Science Gateway Ventures into Structured Online Education", 13th IEEE International Conference on Nanotechnology, August 5-8, 2013, Shangri-La Hotel, Beijing, China
- [C398] Yaohua Tan, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, "Tight Binding modeling of monolayer MoS₂ and ilayer graphene devices", 2013 LEAST (Center for Low Energy Systems Technology) Annual Review, August 14 & 15, 2013, University of Notre Dame.
- [C397] Hesameddin Ilatikhameneh, Saima Sharmin, Parijat Sengupta, Junzhe Geng, Rajib Rahman, Gerhard Klimeck, "Atomistic Modeling of Nitride Devices", 2013 LEAST (Center for Low Energy Systems Technology) Annual Review, August 14 & 15, 2013, University of Notre Dame.
- [C396] SungGeun Kim, Mehdi Salmani-Jelodar, Kwok Ng, Gerhard Klimeck, "Quantum Mechanical Modifications of Drift-diffusion Simulators for Ultra-scaled MOSFETs", TECHCON, 2013
- [C395] Zhengping Jiang, Marcelo Kuroda, Yaohua Tan, Dennis Newns, Glenn Martyna, Michael Povolotskyi, Timothy Boykin, Tillmann Kubis, Gerhard Klimeck, "Tight-Binding Modeling of Intermediate Valence Compound SmSe for Piezoelectronic Devices", 16th International Workshop on Computational Electronics (IWCE), June 2013, Nara, Japan
- [C394] Gerhard Klimeck, Jim Fonseca, Rajib Rahman, Neerav Kharche, Gabriel Lansbergen, Sven Rogge, "Metrology Studies with NEMO, a Multimillion Atom Simulation Tool", The 2013 International Conference on Frontiers of Characterization and Metrology for Nanoelectronics, March 25-28, 2013, at the National Institute of Standards and Technology (NIST), Gaithersburg, Maryland, USA

- [C393] Mehdi Salmani-Jelodar, SungGeun Kim, Kwok Ng, Gerhard Klimeck, "On the Scaling Issues and Possible Solutions for Double Gate MOSFETs at the End of ITRS", accepted for TECHCON 2013
- [C392] Mehdi Salmani-Jelodar, Behtash Behin-Aein, Saumitra Mehrotra, Gerhard Klimeck, Zoran Krivokapic, "PMOS FinFETs Enhanced through Transport in SiGe Cladding", submitted to IEDM2013.
- [C391] Rajib Rahman, Jan Mol, Sven Rogge, Gerhard Klimeck, "Electronic structure of sub-surface Boron acceptors in silicon for potential qubits", APS March Meeting, March 18-22, 2013, Baltimore, Maryland.
- [C390] Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Spin-dependent Peltier effect in 3D topological insulators", Accepted for presentation at 2013 APS March meeting, Baltimore MD
- [C389] Masamichi Yamanishi, Kazuue Fujita, Shinichi Furuta, Kazunori Tanaka, Tadataka Edamura, Tillmann Kubis, Gerhard Klimeck, "Indirect Pumping THz InGaAs/InAlAs Quantum-Cascade Lasers with Coupled-Well Injectors grown by MOVPE", Presented at the International Quantum Cascade Laser School and Workshop 2012
- [C388] Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Atomistic simulation of electronic and transport properties of topological insulator based devices", TECHCON, September 10-11 2012, Austin TX
- [C387] Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Atomistic Simulation of current-voltage characteristics of topological insulator Bi₂Te₃ ultra-thin bodies", TECHCON, September 10-11 2012, Austin, TX
- [C386] Jean Sellier, Jim Fonseca, Tillmann Kubis, Michael Povolotskyi, Yu He, Hesameddin Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Mejia, Parijat Sengupta, Yaohua Tan, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool", SISPAD 2012, International Conference on Simulation of Semiconductor Processes and Devices, Denver, CO, Sept. 2012
- [C385] Behtash Behin-Aein, Abhijeet Paul, Saumitra Mehrotra, Bhagawan Sahu, Kerem Akarvardar, Ajey Jacob, Zoran Krivokapic, Gerhard Klimeck, "Atomistic Analysis of Electrical Performance of Highly Scaled Si_{1-x}Gex p-FinFETs", SISPAD 2012, International Conference on Simulation of Semiconductor Processes and Devices, Denver, CO, Sept. 2012
- [C384] Zhengping Jiang, Yu He, Kai Miao, Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Quantum Transport in Tunneling Field Effect Transistors", MIND review, student poster, South Bend, IN, Aug. 2012
- [C383] Zhengping Jiang, Yeqing Lu, Yaohua Tan, Yu He, Michael Povolotskyi, Tillmann Kubis, Alan Seabaugh, Patrick Fay, Gerhard Klimeck, "Atomistic Simulation of GaSb/InAs Tunneling Field Effect Transistor", TECHCON ,September 10-11 2012, Austin TX
- [C382] Fahd Mohiyaddin, Rajib Rahman, Rachpon Kalra, Gerhard Klimeck, Lloyd Hollenberg, Jarryd Pla, Andrew Dzurak, Andrea Morello, "Advanced Simulation of a Donor Spin Qubit Device", International Workshop on Silicon Quantum Electronics, Sydney Australia, February 13-14, 2012
- [C381] Yosef Borga, Michael Povolotskyi, Jim Fonseca, Gerhard Klimeck, "Crystal Viewer Tool v2.0 Using NEMO5", Purdue Summer Undergraduate Research Fellowship 2012 Research Symposium, 1 Aug. 2012
- [C380] Ravi Vedula, Saumitra Mehrotra, Gerhard Klimeck, Alejandro Strachan, "Theoretical prediction of performance enhancements in asymmetric strain relaxed Ge-PMOS nanowires", MRS Fall Meeting 2012, Boston, Massachusetts, November 25 - 30, 2012
- [C379] Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, Hoon Ryu, Sunhee Lee, Oliver Warschkow, Lloyd Hollenberg, Gerhard Klimeck, Michelle Simmons, "Spectroscopy of a deterministic single-donor device in silicon", Conference on Quantum Information and Computation X; doi:10.1117/12.919763
- [C378] Hoon Ryu, Sunhee Lee, Yui-Hong Tan, Bent Weber, Suddhasatta Mahapatra, Michelle Simmons, Lloyd Hollenberg, Gerhard Klimeck, "Full-band study of ultra-thin Si:P nanowires ", Computational Electronics (IWCE) International Workshop on, Page(s): 1 - 4 , May 21-22, 2012; doi:10.1109/IWCE.2012.6242857
- [C377] Saumitra Mehrotra, Michael Povolotskyi, Jeremy Law, Tillmann Kubis, Gerhard Klimeck, Mark Rodwell, "Design of high-current L-valley GaAs/AlAs_{0.56}Sb_{0.44}/InP (111) ultra-thin-body nMOSFETs", International Conference on Indium Phosphide and Related Materials, University of California at Santa Barbara, Aug 27-30 2012
- [C376] Saumitra Mehrotra, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Modelling of Ge/InGaAs FinFETs", MSD Annual Review , MIT (Boston) MA, May 1-2 2012
- [C375] Saumitra Mehrotra, Tillmann Kubis, Michael Povolotskyi, Mark Lundstrom, Gerhard Klimeck, "MOSFETs near end of the roadmap ", MSD Annual Review , MIT (Boston) MA, May 1-2 2012
- [C374] Seung Park, Yang Liu, Neerav Kharche, Mehdi Salmani-Jelodar, Gerhard Klimeck, Mark Lundstrom, Mathieu Luisier, "Performance Comparison of InGaAs and strained-Si in Planar and Non-planar FETs at Ultra-short Gate Length (12nm)",
- [C373] Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy Boykin, Gerhard Klimeck, "Generation of Empirical Tight Binding Parameters from ab-initio simulations", IWCE 2012, May 21-22, 2012, University of Wisconsin - Madison

- [C372] Junzhe Geng, Sunhee Lee, Hoon Ryu, Gerhard Klimeck, "Atomistic Modeling of a Tunable Single-Electron Quantum Dot in Silicon using NEMO3D-peta", IWCE 2012, May 21-22, 2012, University of Wisconsin - Madison
- [C371] Yu He, Lang Zeng, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Efficient solution algorithm of non-equilibrium Green's functions in atomistic tight binding representation", IWCE 2012, May 21-22, 2012, University of Wisconsin - Madison
- [C370] Tillmann Kubis, Jim Fonseca, Michael Povolotskyi, Jean Sellier, Gerhard Klimeck, "From Atoms to Devices: NEMO5", Focus Center Research Program (FCRP) Proposers' Conference, Dallas, TX May, 2012.
- [C369] Bent Weber, Gerhard Klimeck, "Towards Scalable Donor-Based QC Architectures", International Workshop on Silicon Quantum Electronics on February 2012, Sydney, Australia
- [C368] SungGeun Kim, Mathieu Luisier, Timothy Boykin, J. Geng, Jim Fonseca, Gerhard Klimeck, "Atomistic Simulation of Graphene Transistors", MSD review May 2012, Boston.
- [C367] Mehdi Salmani-Jelodar, Seung Park, Zhengping Jiang, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Contact-to-channel Resistance Modeling in HEMT Devices", MSD review May 2012, Boston.
- [C366] Fahd Mohiyaddin, Rajib Rahman, Rachpon Kalra, Gerhard Klimeck, Lloyd Hollenberg, Jarryd Pla, Andrew Dzurak, Andrea Morello, "Advanced Simulation Methods for a Single Donor Spin Qubit Device", CQC2T Workshop, Feb 15- 16, 2012
- [C365] Fahd Mohiyaddin, Rajib Rahman, Rachpon Kalra, Gerhard Klimeck, Lloyd Hollenberg, Jarryd Pla, Andrew Dzurak, Andrea Morello, "Advanced Simulation Methods for a Single Donor Spin Qubit Device", International Workshop On Silicon Quantum Electronics, Chowder Bay, Sydney, Feb 13-14, 2012.
- [C364] Saumitra Mehrotra, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Double Gate Ge p-FinFET Performance: Dependence on Orientation, Strain and Fin Width Thickness", TECHCON 2012, Austin TX, Sept 10-11 2012
- [C363] Timothy Boykin, Mathieu Luisier, Gerhard Klimeck, Xueping Jiang, Neerav Kharche, Yu Zhou, Saroj K.Nayak, "Six-band nearest-neighbor tight-binding model for the π -bands of bulk graphene and graphene nanoribbons", APS March 2012 Meeting, Boston, MA
- [C362] Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Geometric effects on surface states of 3D-TI Bismuth Telluride quantum wells", APS March Meeting, Feb 27th - March 2nd, 2012
- [C361] Zhengping Jiang, Yu He, Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Quantum Transport in GaSb/InAs Nanowire TFET with Semiclassical Charge Density", IWCE 2012, May 21-22, 2012, University of Wisconsin - Madison
- [C360] Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Full band electron band structure calculation with empirical tight binding for topological insulators and broken gap devices", IWCE 2012, May 21-22, 2012, University of Wisconsin - Madison
- [C359] Timothy Boykin, Mathieu Luisier, Neerav Kharche, Xueping Jiang, Saroj K.Nayak, A. Martins, Gerhard Klimeck, "Multiband Tight-Binding Model for Strained and Bilayer Graphene from DFT Calculations", IWCE 2012, May 21-22, 2012, University of Wisconsin - Madison
- [C358] Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Electric tuning of topological insulator states and their surface scattering", APS March Meeting 2012, Boston, US
- [C357] Timothy Boykin, Mathieu Luisier, Gerhard Klimeck, Xueping Jiang, Neerav Kharche, Yu Zhou, Saroj K.Nayak, "Six-band nearest-neighbor tight-binding model for the π -bands of bulk graphene and graphene nanoribbons", APS March Meeting 2012, Boston, US
- [C356] Yui-Hong Tan, Hoon Ryu, Gerhard Klimeck, "Modeling of charge stability diagrams and lead density of states fluctuations in donor-based (Si:P) quantum dot devices-based", International Conference on quantum Dots (QD2012), May 13-18 2012, Santa Fe, New Mexico, USA
- [C355] Muhammad Usman, Yui-Hong Tan, Gerhard Klimeck, "Theoretical correlation between quantum dot composition and polarization properties", International Conference on quantum Dots DOTS (QD2012), May 13-18 2012, Santa Fe, New Mexico, USA
- [C354] Yui-Hong Tan, Hoon Ryu, Sunhee Lee, Gerhard Klimeck, "Modeling of charge stability diagrams and lead density of states fluctuations in a single phosphorus donor transistor", International Workshop on Silicon Quantum Electronics, oral presentation, Sergeants Mess, Chowder Bay, Sydney, Australia, Feb 13-14, 2012.
- [C353] Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Geometric effects on surface states in topological insulator Bi_2Te_3 nanowire", APS March Meeting 2012, Boston, US
- [C352] Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Geometric effects on surface states of Bismuth Telluride nanowires", submitted to APS March Meeting, Feb 27 - Mar 2 2012, Boston, MA
- [C351] Mehdi Salmani-Jelodar, Abhijeet Paul, Timothy Boykin, Gerhard Klimeck, "Phonon Spectrum and Thermal Properties of free standing Si and InGaAs alloy nanowires", APS March Meeting 2012, Boston, US

- [C350] R. Pipes, Gerhard Klimeck, Mark Pipes, "The Composite Materials Manufacturing HUB – Crowd Sourcing as the Norm", The composite exhibition and convention (COMPOSITES 2012), Feb. 21-23, 2012 at Las Vegas, Nevada
- [C349] Muhammad Usman, Susannah Heck, Edmund Clarke, Peter Spencer, Ray Murray, Gerhard Klimeck, Eoin O'Reilly, "Polarization-resolved Optical Transitions from InAs QDs at Telecommunication Wave-lengths", Quantum Dot Day Workshop January 10, 2011, University of Bristol, UK
- [C348] Mehdi Salmani-Jelodar, Sebastian Steiger, Abhijeet Paul, Gerhard Klimeck, "Model development for lattice properties of gallium arsenide using parallel genetic algorithm", Evolutionary Computation (CEC), 2011 IEEE Congress on, Page(s): 2429 - 2435; doi: 10.1109/CEC.2011.5949918
- [C347] Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Topological Insulator Application: All-Electrical Switching of Conductance", Presented at MRS Fall Meeting 2011, Boston, MA
- [C346] "Tight-binding Simulations on a Deterministic Single Atom Transistor", International Workshop On Silicon Quantum Electronics, August 14-15, 2011, Grand Hyatt Denver, Denver, Colorado, USA
- [C345] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Role of alloy scattering in strained SiGe nano MOSFET", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 10-11, 2011
- [C344] Sunhee Lee, Hoon Ryu, Gerhard Klimeck, F. Mohiyaddin, Wee Lim, Andrea Morello, Andrew Dzurak, "Valley splitting in the highly tunable silicon quantum dot at the single-electron regime", International Workshop on Silicon Quantum Electronics, oral presentation, Denver, CO, Aug. 14-15, 2011
- [C343] Hoon Ryu, Sunhee Lee, Yui-Hong Tan, Gerhard Klimeck, Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, Michelle Simmons, Lloyd Hollenberg, "Tight-binding Simulations on a Deterministic Single Donor Transistor", International Workshop on Silicon Quantum Electronics, oral presentation, Denver, CO, Aug. 14-15, 2011
- [C342] Zhengping Jiang, Woo-Suhl Cho, Hong-Hyun Park, Mathieu Luisier, Tillmann Kubis, Gerhard Klimeck, Y. Lu, R. Li, G. Zhou, Alan Seabaugh, Patrick Fay, Supriyo Datta, Dheeraj Mohata, T. Mayer, David Pawlik, Sean Rommel, "Atomistic Quantum Transport Modeling in Band-to-band Tunneling Transistors", MIND review, student poster, South Bend, IN, Aug. 2011
- [C341] Timothy Boykin, Zhengping Jiang, Neerav Kharche, Gerhard Klimeck, "Effects of disorder on the valley-splitting in Si/SiGe quantum wells", International Workshop on Silicon Quantum Electronics, oral presentation, Denver, CO, Aug. 14-15, 2011
- [C340] F. Mohiyaddin, Rajib Rahman, Gerhard Klimeck, Jarryd Pla, Andrew Dzurak, Andrea Morello, "Advanced Simulation of a Donor Spin Qubit Device", NSA / IARPA / ARO Quantum Computing Technology Workshop, Denver, August 11-12, 2011.
- [C339] Hoon Ryu, Sunhee Lee, Zhengping Jiang, Yui-Hong Tan, Michael Povolotskyi, Neerav Kharche, Mark Eriksson, Timothy Boykin, Gerhard Klimeck, Bent Weber, Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, W. Lim, H. Yang, N. Lai, F. Mohiyaddin, Andrea Morello, Andrew Dzurak, Michelle Simmons, Lloyd Hollenberg, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / IARPA / ARO Quantum Computing Technology Workshop, Denver, August 11-12, 2011
- [C338] Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, Wolfgang Fichtner, "Atomistic nanoelectronic device engineering with sustained performances up to 1.44 PFlop/s", IEEE and ACM Supercomputing 2011, Nov 12-18, 2011, , Gordon Bell Prize Finalist
- [C337] Parijat Sengupta, Yaohua Tan, Tillmann Kubis, Michael Povolotskyi, Gerhard Klimeck, "Tunability of the critical width of a 2D Topological Insulator", Presented at MRS Fall Meeting 2011, SYMPOSIUM L, Boston, MA
- [C336] Seung Park, Hong-Hyun Park, Mehdi Salmani-Jelodar, Sebastian Steiger, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Contact Modeling and Analysis of InAs HEMT Transistors", IEEE proceedings of IEEE Nanotechnology Materials and Devices Conference (IEEE NMDC 2011), Oct. 18-21, 2011 at The Shilla Jeju, Korea
- [C335] SungGeun Kim, Saumitra Mehrotra, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Effects of Interface Roughness Scattering on RF Performance of Nanowire Transistors", International Semiconductor Device Research Symposium (ISDRS 2011), Dec 7-11, Univ of Maryland;doi:10.1109/ISDRS.2011.6135299
- [C334] Saumitra Mehrotra, Abhijeet Paul, Gerhard Klimeck, "Ballistic hole injection velocity analysis in Ge UTB pMOSFETs: Dependence on body thickness, orientation and strain", 2011 International Semiconductor Device Research Symposium (ISDRS 2011), Dec 7-11, Univ of Maryland
- [C333] Lynn Zentner, Steven Clark, Preston Smith, Swaroop Shivarajapura, Victoria Farnsworth, Krishna Madhavan, Gerhard Klimeck, "Practical Considerations in Cloud Utilization for the Science Gateway nanoHUB.org", IEEE/ACM International Conference on Utility and Cloud Computing (UCC 2011), 5-8 Dec. 2011
- [C332] Mehdi Salmani-Jelodar, Yaohua Tan, Gerhard Klimeck, "Single Layer MoS2 Band Structure and Transport", 2011 International Semiconductor Device Research Symposium (ISDRS 2011), Dec 7-11, Univ of Maryland

- [C331] Mehdi Salmani-Jelodar, Seung Park, Hong-Hyun Park, Sebastian Steiger, Gerhard Klimeck, "Contact Modeling in HEMT Devices", MSD/ FCRP Annual Review, Student Poster, MIT, Boston, MA, May 10-11, 2011.
- [C330] Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Atomistic nanoelectronic device simulations with sustained performances up to 1.44 PFlop/s", Gordon Bell Prize Competition (6 finalists) Supercomputing Nov. 2011, E-ISBN : 978-1-4503-0771-0
- [C329] Tillmann Kubis, Gerhard Klimeck, "Terahertz quantum cascade lasers: Conceptual design improvements", Nanoelectronic Devices for Defense and Security Conference, Aug 29 to Sept. 1, 2011.
- [C328] Gerhard Klimeck, George Adams III., Krishna Madhavan, Nathan Denny, Michael Zentner, Swaroop Shivarajapura, Lynn Zentner, Diane Beaudoin, "Social Networks of Researchers and Educators on nanoHUB.org", 11th IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing, Social Network (SN4CCGridS) Workshop, CCGrid 2011, Newport Beach, CA, USA, May 23-26, 2011;doi:10.1109/CCGrid.2011.33
- [C327] Mark Lundstrom, Changwook Jeong, Gerhard Klimeck, "Computational Study of the Electronic Performance of Cross-Plane Superlattice Peltier Devices", Proceedings of the MRS Spring Meeting, March 2011, 2011;doi:10.1557/opl.2011.509
- [C326] Tillmann Kubis, Gerhard Klimeck, "Conceptual design improvements for terahertz quantum cascade lasers needed for molecule detection", Nanoelectronic Devices for Defense & Security (NANO-DDS) conference, August 31
- [C325] Lynn Zentner, Steven Clark, Krishna Madhavan, Swaroop Shivarajapura, Victoria Farnsworth, Gerhard Klimeck, "Automated Grid-Probe System to Improve End-To-End Grid Reliability for a Science Gateway", Proceedings of the 2011 TeraGrid Conference, July 18-21, 2011, Salt Lake City, To appear in ACM proceedings;doi:10.1145/2016741.2016789
- [C324] Parijat Sengupta, Sebastian Steiger, Sunhee Lee, Hoon Ryu, Gerhard Klimeck, "Multiscale Modeling of a Quantum Dot Heterostructures", presented at MRS Spring Meeting 2011, YY10.2, San Francisco CA,
- [C323] Saumitra Mehrotra, Lynn Zentner, Gerhard Klimeck, Dragica Vasileska, "nanoHUB.org – The ABACUS Tool Suite as a Framework for Semiconductor Education Courses", 2011 IEEE Nanotechnology Conference, Portland, Oregon, USA Aug 15-18;doi:10.1109/NANO.2011.6144581
- [C322] Seung Park, Gerhard Klimeck, "Contact Modeling and Performance Analysis of InAs HEMT Architecture", accepted for presentation at TECHCON 2011
- [C321] Abhijeet Paul, Kai Miao, Ganesh Hegde, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Enhancement of thermoelectric efficiency by uniaxial tensile stress in n-type GaAs nanowires", 2011 IEEE Nanotechnology Conference, Portland, Oregon, USA, Aug 15-18, 2011;doi:10.1109/NANO.2011.6144525
- [C320] SungGeun Kim, Mathieu Luisier, Abhijeet Paul, Timothy Boykin, Gerhard Klimeck, "Full 3D Quantum Transport Simulation of Atomistic Interface Roughness in Silicon Nanowire FETs", accepted for presentation at TECHCON 2011;doi:10.1109/TED.2011.2118213
- [C319] Abhijeet Paul, Saumitra Mehrotra, Gerhard Klimeck, Mark Rodwell, "Performance enhancement of GaAs UTB pFETs by strain, orientation and body thickness engineering", Device Research Conference, 2011, 20-22 June 2011;doi:10.1109/DRC.2011.5994511
- [C318] Abhijeet Paul, Kai Miao, Mathieu Luisier, Gerhard Klimeck, "Tuning lattice thermal conductance in ultra-scaled hollow SiNW: Role of porosity size, density and distribution", MRS Spring Meeting, 2011. SanFrancisco, April 25th - 29th;doi:10.1557/opl.2011.1464
- [C317] Mehdi Salmani-Jelodar, Sebastian Steiger, Abhijeet Paul, Gerhard Klimeck, "Parameter Fitting for Lattice Properties of Gallium Arsenide using Parallel Genetic Algorithm", 2011 IEEE Congress on Evolutionary Computation, 5-8 June 2011;doi:10.1109/CEC.2011.5949918
- [C316] Ali Razavieh, Navab Singh, Abhijeet Paul, Gerhard Klimeck, David Janes, Joerg Appenzeller, "A New Method to Achieve RF Linearity in SOI Nanowire MOSFETs", IEEE 2011 RFIC Symposium
- [C315] Abhijeet Paul, Kai Miao, Mathieu Luisier, Gerhard Klimeck, "Strain Engineering of the thermal conductance in Si nanowires", APS March Meeting, Dallas, Texas, March 24, 2011
- [C314] Saumitra Mehrotra, Abhijeet Paul, Gerhard Klimeck, "Tight-binding based alloy scattering calculations in $\text{Si}_{1-x}\text{Ge}_x$ ", APS March Meeting, Dallas, Texas, March 23, 2011.
- [C313] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Fullband Study of Ultra-Scaled Electron and Hole SiGe Nanowire FETs", Microelectronics and Electron Devices (WMED), 2010 IEEE Workshop on, Page(s): 1 - 4; doi: 10.1109/WMED.2010.5453756
- [C312] Bent Weber, Suddhasatta Mahapatra, Michelle Simmons, Hoon Ryu, Sunhee Lee, Gerhard Klimeck, "Transport in atomic-scale Si:P doping wires", 2010 International conference on Nanoscience and Nanotechnology (ICONN2010), Sydney Convention Centre, Darling Harbour, Sydney, Australia
- [C311] Bent Weber, Suddhasatta Mahapatra, W. Clarke, Michelle Simmons, Hoon Ryu, Sunhee Lee, Gerhard Klimeck, Lloyd Hollenberg, "Transport in Atomic-Scale Doped Silicon Nanowires", 2010 IEEE Silicon Nanoelectronic Workshop (SNW), Honolulu, HI, US.

- [C310] Neophytos Neophytou, Hans Kosina, Gerhard Klimeck, "A comprehensive atomistic analysis of bandstructure velocities in si nanowires", Computational Electronics (IWCE), 2010 14th International Workshop, Pisa, Italy, 26-29 Oct. 2010, Page(s): 1-4; doi : 10.1109/IWCE.2010.5678007
- [C309] Mathieu Luisier, Gerhard Klimeck, "Phonon-limited mobility and injection velocity in n- and p-doped ultrascaled nanowire field-effect transistors with different crystal orientations", IEDM, San Francisco, Dec. 6-10, 2010
- [C308] Ganesh Hegde, Gerhard Klimeck, Alejandro Strachan, "First Principles Study of the Energetics of Ideal GaAs Surfaces and Adsorption of Al and O as a Function of Surface Orientation", 41st IEEE Semiconductor Interface Specialists Conference, The Catamaran Hotel, San Diego, CA, December 2-4, 2010
- [C307] Zhengping Jiang, Neerav Kharche, Gerhard Klimeck, "Valley Degeneracy in (110) Si Quantum Wells - Strain and Misorientation Effects", International Workshop for Computational Electronics, Pisa, Italy, October 2010
- [C306] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Atomistic modeling of the phonon dispersion in free-standing <100> Si nanowires", International Workshop for Computational Electronics, Pisa, Italy, October 2010
- [C305] George Adams III., Krishna Madhavan, Michael Zentner, Nathan Denny, Swaroop Shivarajapura, Gerhard Klimeck, "User Flow Informatics to Personalize Learning in Engineering Cyber-environments - nanoHUB.org A Case Study", at the ASEE 9th Global Colloquium on Engineering Education in Singapore on October 18 - 21, 2010
- [C304] Dragica Vasileska, Gerhard Klimeck, Alejandra Magana, S. Goodnick, "Tool-Based Curricula and Visual Learning", European Conference on Electronic Learning, Porto, Portugal, Nov. 4-5 2010
- [C303] Zhengping Jiang, Neerav Kharche, Gerhard Klimeck, "Valley Degeneracy in (110) Si Quantum Wells: Strain and Misorientation Effects", International Workshop for Computational Electronics, October 27th-29th, 2010, Pisa, Italy
- [C302] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Atomistic modeling of the phonon dispersion in free-standing Si nanowires", International Workshop for Computational Electronics, October 27th-29th, 2010, Pisa, Italy
- [C301] Saumitra Mehrotra, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "A Tight-Binding approach for SiGe Bandstructure Calculations", TECHCON, Austin, Texas, Sept. 13-14, 2010
- [C300] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Strain Engineering of Trigated Silicon Nanowire FinFETs for Improved Device Performance", TECHCON, Austin, Texas, Sept. 13-14, 2010
- [C299] Woo-Suhl Cho, Mathieu Luisier, Gerhard Klimeck, "Full-band Simulations of Band-to-Band Tunneling Diodes", TECHCON, Austin, Texas, Sept. 13-14, 2010
- [C298] Nabil Ashraf, Dragica Vasileska, Gerhard Klimeck, "Modeling Fluctuations in the Threshold Voltage and ON-Current and Threshold Voltage Fluctuation due to Random Telegraph Noise", IEEE Nano 2010, Seoul Korea, Aug. 17-20, 2010; doi:10.1109/NANO.2010.5697821
- [C297] Abhijeet Paul, Gerhard Klimeck, "Atomistic modeling of the thermoelectric power factor in ultra-scaled silicon nanowires", 2010 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI, June 13-14, 2010; doi:10.1109/SNW.2010.5562583
- [C296] Gerhard Klimeck, Mathieu Luisier, "Scattering in Si-nanowires - Where does it matter?", 2010 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI, June 13-14, 2010; doi:10.1109/SNW.2010.5562586
- [C295] Hoon Ryu, S. Lee, Bent Weber, Suddhasatta Mahapatra, Michelle Simmons, Lloyd Hollenberg, Gerhard Klimeck, "Quantum transport in ultra-scaled phosphorous-doped silicon nanowires", 2010 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI, June 13-14, 2010
- [C294] Bent Weber, Suddhasatta Mahapatra, W. Clarke, Hoon Ryu, S. Lee, Gerhard Klimeck, Lloyd Hollenberg, Michelle Simmons, "Quantum transport in atomic-scale silicon nanowires", 2010 IEEE Silicon Nanoelectronics Workshop, Hilton Hawaiian Village, Honolulu, HI, June 13-14, 2010
- [C293] Krishna Madhavan, Gerhard Klimeck, Diane Beaudoin, George Adams III., Swaroop Shivarajapura, D.F. Radcliffe, "Bridging engineering practice and learning through cyber-environments", Workshop on Engineering Learning at the International Conference on the Learning Sciences June 28, 2010, Chicago, IL
- [C292] Sunhee Lee, Hoon Ryu, Gerhard Klimeck, Suddhasatta Mahapatra, Michelle Simmons, Lloyd Hollenberg, "Equilibrium Bandstructure of a Phosphorus δ -doped Layer in Silicon using a Tight-binding Approach", Proceedings of IEEE Nano 2010, Seoul Korea, Aug. 17-20, 2010.
- [C291] Neerav Kharche, Mathieu Luisier, S. Lee, Sebastian Steiger, Gerhard Klimeck, "Study on Ultra-scaled InAs Channel Devices", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 5-6, 2010
- [C290] Amritanshu Palaria, Yumi Park, Gerhard Klimeck, Alejandro Strachan, "Atomic and electronic structure properties of Si/Ge heterostructures", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 5-6, 2010

- [C289] Abhijeet Paul, Saumitra Mehrotra, Zhengping Jiang, Mathieu Luisier, Gerhard Klimeck, "Modeling of SiGe material for ultra-scaled CMOS device applications", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 5-6, 2010
- [C288] SungGeun Kim, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, Timothy Boykin, "Full 3D Quantum Transport Simulation of Interface Roughness in Nanowire FETs", American Physical Society, March Meeting, March 15–19, 2010; Portland, Oregon (2010)
- [C287] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Atomistic approach to study charge and current distribution in ultra-scaled SiGe/Si core/shell nanowire FETs", American Physical Society, March Meeting, March 15–19, 2010; Portland, Oregon (2010)
- [C286] Muhammad Usman, Gerhard Klimeck, "Wavelength engineered InAs quantum dots", American Physical Society, March Meeting, March 15–19, 2010; Portland, Oregon (2010)
- [C285] Abhijeet Paul, Gerhard Klimeck, "Atomistic Modeling of the Thermoelectric Properties in Silicon Nanowires", American Physical Society, March Meeting, March 15–19, 2010; Portland, Oregon (2010)
- [C284] Suddhasatta Mahapatra, Tang Wei, Hoon Ryu, Gerhard Klimeck, Michelle Simmons, "Towards a single P donor in Si", American Physical Society, March Meeting, March 15–19, 2010; Portland, Oregon (2010)
- [C283] "A TeraGrid MATLAB Cluster - Exploring New Services for an XD Future", SDCI/STCI as the Software Supply Chain of the National Cyberinfrastructure Workshop, January 28, 29, 2010, National Science Foundation.
- [C282] Gerhard Klimeck, George Adams III., Michael McLennan, "Instant-On Simulation Delivery: Helping TeraGrid Achieve Its Wide and Open Strategic Goals", SDCI/STCI as the Software Supply Chain of the National Cyberinfrastructure Workshop, January 28, 29, 2010, National Science Foundation.
- [C281] Michael McLennan, Gerhard Klimeck, Dongyan Xu, "SDCI NMI Improvement: nanoHUB.org Middleware", SDCI/STCI as the Software Supply Chain of the National Cyberinfrastructure Workshop, January 28, 29, 2010, National Science Foundation.
- [C280] Bent Weber, Suddhasatta Mahapatra, Hoon Ryu, Sunhee Lee, Gerhard Klimeck, Michelle Simmons, "Atomic-scale Si:P dopant wires", 2010 International Conference On Nanoscience and Nanotechnology (ICONN), Sydney, 22-26th Feb. 2010.
- [C279] Christopher Escott, Andrea Morello, Jarryd Pla, Rajib Rahman, Gerhard Klimeck, Andrew Dzurak, Lloyd Hollenberg, "Tunnelling rates in silicon qubit devices", 2010 International Conference On Nanoscience and Nanotechnology (ICONN), Sydney, 22-26th Feb. 2010.
- [C278] Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Rajib Rahman, Benjamin Haley, S.H Park, Neerav Kharche, Zhengping Jiang, Timothy Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabriel Lansbergen, Sven Rogge, Bent Weber, Michelle Simmons, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", International Symposium on Advanced Nanodevices and Nanotechnology (ISANN), Kaanapali, Maui, Nov. 29-Dec. 4, 2009.
- [C277] Saumitra Mehrotra, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Atomistic simulations for SiGe pMOS devices Bandstructure to Transport", ISDRS 2009, December 9-11, 2009, College Park, MD, USA.
- [C276] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Study of Ultra-scaled SiGe/Si Core/Shell Nanowire FETs for CMOS Applications", ISDRS 2009, December 9-11, 2009, College Park, MD, USA.
- [C275] Neerav Kharche, Gerhard Klimeck, Dae-Hyun Kim, Jesús. Alamo, Mathieu Luisier, "Performance Analysis of Ultra-Scaled InAs HEMTs", IEDM 2009, Dec. 7-9, 2009;doi:10.1109/IEDM.2009.5424315
- [C274] Mathieu Luisier, Gerhard Klimeck, "Performance Comparisons of Tunneling Field-Effect Transistors made of InSb, Carbon, and GaSb-InAs Broken Gap Heterostructures", IEDM 2009, Dec. 7-9, 2009;doi:10.1109/IEDM.2009.5424280
- [C273] Jan Verduijn, Gabriel Lansbergen, Giuseppe Tettamanzi, Rajib Rahman, Serge Biesemans, Nadine Collaert, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Electronic Transport Properties of Single Donors in Nanoscale Si MOSFETs", 2009 Silicon Nanoelectronics Workshop, Rihga Royal Hotel Kyoto, Kyoto, Japan, June 13-14, 2009.
- [C272] Giuseppe Tettamanzi, Gabriel Lansbergen, Abhijeet Paul, P. Deosarran, Nadine Collaert, Gerhard Klimeck, Serge Biesemans, Sven Rogge, "Subthreshold Study of Undoped Trigate nFinFET", 2009 Silicon Nanoelectronics Workshop, Rihga Royal Hotel Kyoto, Kyoto, Japan, June 13-14, 2009;doi:10.1016/j.tsf.2009.10.114
- [C271] Giuseppe Tettamanzi, Gabriel Lansbergen, Abhijeet Paul, P. Deosarran, Nadine Collaert, Gerhard Klimeck, Serge Biesemans, Sven Rogge, "Subthreshold Study of Undoped Trigate nFinFET", E-MRS (European Materials Research Society) Conference, Strasbough, France, June 8-12, 2009.
- [C270] Woo-Suhl Cho, Hoon Ryu, Seung Park, Gerhard Klimeck, "B-field verification in OMEN-3D", TECHCON 2009 to be held at the Renaissance Hotel in Austin, Texas, September 14 - 15, 2009.

- [C269] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "On the Validity of Top of the Barrier Quantum Transport Model for Ballistic Nanowire MOSFETs", TECHCON 2009 to be held at the Renaissance Hotel in Austin, Texas, September 14 - 15, 2009;doi:10.1109/IWCE.2009.5091134
- [C268] Neophytos Neophytou, Gerhard Klimeck, Hans Kosina, "Diameter, orientation, and bias dependence of injection velocity and capacitance in Si nanowires: An atomistic tight-binding study", IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009;doi:10.1109/SISPAD.2009.5290245
- [C267] Mathieu Luisier, Gerhard Klimeck, "Investigation of In_xGa_{1-x}As Ultra-Thin-Body Tunneling FETs using a Full-Band and Atomistic Approach", IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009
- [C266] W. Pok, G. Scappucci, W. C. T. Lee, Bent Weber, Suddhasatta Mahapatra, Lloyd Hollenberg, Michelle Simmons, Hoon Ryu, S. Lee, Gerhard Klimeck, Mark Friesen, Mark Eriksson, "Precision control of tunneling in STM-patterned Si:P devices", Silicon Qubit Workshop, University of California Berkeley, Aug. 24-25, 2009.
- [C265] Rajib Rahman, Richard Muller, Andrew Greentree, Gerhard Klimeck, Malcolm Carroll, Lloyd Hollenberg, "Coherent electron transport by adiabatic passage in a triple donor system with imperfect donor placement", University of California Berkeley, Aug. 24-25, 2009;doi:10.1103/PhysRevB.82.155315
- [C264] Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Rajib Rahman, Benjamin Haley, S.H Park, Neerav Kharche, Zhengping Jiang, Timothy Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabriel Lansbergen, Sven Rogge, Bent Weber, Michelle Simmons, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", University of California Berkeley, Aug. 24-25, 2009.
- [C263] Gerhard Klimeck, Rajib Rahman, Seung Park, Hoon Ryu, Neerav Kharche, Gabriel Lansbergen, Jan Verduijn, Bent Weber, Lloyd Hollenberg, Sven Rogge, Michelle Simmons, Richard Muller, "Million-Atom Electronic Structure Simulations for Realistically Large Si-Based Quantum Devices", University of California Berkeley, Aug. 24-25, 2009.
- [C262] Mincheol Shin, Sunhee Lee, Gerhard Klimeck, "k·p-based Quantum Transport Simulation of Silicon Nanowire pMOSFETs", Proceedings of the IEEE NANO 2009 Conference, Genoa July 26-30 2009.
- [C261] Mathieu Luisier, Gerhard Klimeck, "Performance limitations of graphene nano ribbon tunneling FETS due to line edge roughness", IEEE Device Research Conference, June 22-24, 2009;doi:10.1109/DRC.2009.5354951
- [C260] Kyle Montgomery, Samarth Agarwal, Gerhard Klimeck, Jerry Woodall, "Proposal of ZnSe/GaAs Digital Alloys for High Band Gap Solar Cells and True Green LEDs", 2009 IEEE Nanotechnology Materials and Devices Conference (NMDC 2009), June 2-5, 2009, Traverse City, Michigan, USA;doi:10.1109/NMDC.2009.5167542
- [C259] Kristof Tahy, Mathieu Luisier, Gerhard Klimeck, Siyu Koswatta, Huili Zing, Alan Seabaugh, Debdeep Jena, "Graphene Nanoribbon (GNR) Tunnel Transistor for Ultra-Low Power Applications", The Fifth International Nanotechnology Conference on Communication and Cooperation, Los Angeles, May 18-2, 2009.
- [C258] Amritanshu Palaria, Ya Zhou, Gerhard Klimeck, Alejandro Strachan, "Electronic properties of Si/Ge nanostructures and atomistic simulations in nanoHUB6", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 7, 2009.
- [C257] Neerav Kharche, Mathieu Luisier, Gerhard Klimeck, "Simulation study and tool development for ultra-scaled InAs HEMTs 6", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 7, 2009.
- [C256] SungGeun Kim, Mathieu Luisier, Gerhard Klimeck, "OMEN Nanowire : Full-band 3D quantum transport simulation in nanowire structure", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 7, 2009.
- [C255] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Bandstructure Lab: Scientific Impact and Tool Development", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 7, 2009.
- [C254] Gerhard Klimeck, Dragica Vasileska, "Semiconductor Device and Quantum Mechanics Education on nanoHUB.org", 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009;doi:10.1109/IWCE.2009.5091083
- [C253] Sunhee Lee, Hoon Ryu, Zhengping Jiang, Gerhard Klimeck, "Million Atom Electronic Structure and Device Calculations on Peta-Scale Computers", 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009; doi:10.1109/IWCE.2009.5091117
- [C252] Hoon Ryu, Sunhee Lee, Gerhard Klimeck, "A Study of Temperature-dependent Properties of n-type delta-doped Si Band-structures in Equilibrium", 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009;doi:10.1109/IWCE.2009.5091082
- [C251] Muhammad Usman, Hoon Ryu, Gerhard Klimeck, "Quantum Confined Stark Effect in Biased InAs/GaAs Quantum Dots", 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009.
- [C250] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "On the validity of the top of the barrier quantum transport model for ballistic nanowire MOSFETs", 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009;doi: 10.1109/IWCE.2009.5091134

- [C249] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Gerhard Klimeck, "Surface and Orientation dependence on performance of Trigated Silicon Nanowire pMOSFETs", 7th IEEE Workshop on Microelectronics and Electron Devices (WMED 2009), Apr 03, 2009, Boise Center on the Grove Boise, Idaho United States
- [C248] Rajib Rahman, Gerhard Klimeck, Lloyd Hollenberg, "Electric field control of single donors in silicon", American Physical Society, March Meeting, March 16-20, Pittsburgh, PA, 2009.
- [C247] Muhammad Usman, Gerhard Klimeck, "Quantum confined stark effect in non-identical InAs/GaAs coupled quantum dots: Dependence on vertical electrical field", American Physical Society, March Meeting, March 16-20, Pittsburgh, PA, 2009.
- [C246] Abhijeet Paul, Saumitra Mehrotra, "Study of Electronic Charge Distribution in Silicon Nanowire Transistors: An Atomistic Approach", American Physical Society, March Meeting, March 16-20, Pittsburgh, PA, 2009.
- [C245] Gerhard Klimeck, Mathieu Luisier, Muhammad Usman, Neerav Kharche, Hoon Ryu, Sunhee Lee, Dragica Vasileska, "Nano-Scale Carrier Transport on an atomistic basis using NEMO 3-D and OMEN", Aspen Winter Conference on Unifying Themes in Condensed Matter, Jan. 12-16, 2009.
- [C244] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, P.E. Rutten, J. Caro, Jerry Woodall, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Determination of the eigenstates and wavefunctions of a single gated As donor", International Conference on Nanoscience and Nanotechnology, ICONN 2008, Feb. 25-29, 2008;doi:10.1109/ICONN.2008.4639272
- [C243] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, J. Caro, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Transport-based dopant mapping in advanced FinFETs", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008; approx. 10% acceptance rate;doi:10.1109/IEDM.2008.4796794
- [C242] Mathieu Luisier, Neophytos Neophytou, Neerav Kharche, Gerhard Klimeck, "Full-Band and Atomistic Simulation of Realistic 40 nm InAs HEMT", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008; approx. 10% acceptance rate;doi:10.1109/IEDM.2008.4796842
- [C241] Gerhard Klimeck, Mathieu Luisier, Muhammad Usman, Neerav Kharche, Hoon Ryu, Sunhee Lee, Dragica Vasileska, "Nanoelectronic Modeling using NEMO 3-D and OMEN and their Deployment on nanoHUB.org", 13th Advanced Heterostructures nad Nanostructures Workshop, Hapuna Beach, Hawaii, Dec. 7-12, 2008.
- [C240] Hoon Ryu, Muhammad Usman, Shaikh Ahmed, Gerhard Klimeck, "Atomistic Tight Binding Study of Interband Light Transitions in Self-assembled InAs/GaAs Quantum Dots", MRS Fall Meeting, Boston, Dec. 1-4, 2008.
- [C239] Mathieu Luisier, Gerhard Klimeck, "A multi-level parallel simulation approach to electron transport in nano-scale transistors", Supercomputing 2008, Austin TX, Nov. 15-21 2008. Regular paper - 59 accepted papers, 277 submissions (21%);doi:10.1109/SC.2008.5215912
- [C238] Gerhard Klimeck, Mathieu Luisier, Saumitra Mehrotra, Neophytos Neophytou, Abhijeet Paul, Benjamin Haley, "Nanowire Simulations from atomistic tool development to deployed tools on nanoHUB.org", 3rd nanowire growth workshop, Duisburg, Germany, Sept. 14-16, 2008.
- [C237] Abhijeet Paul, Neophytos Neophytou, Gerhard Klimeck, "Silicon Nanowire Electrostatics using Self Consistent Dispersion Calculation", TECHCON 2008, Austin, TX, September 15 - 16, 2008, 50% acceptance rate.
- [C236] Amritanshu Palaria, Alejandro Strachan, Gerhard Klimeck, "Electronic Structure and Transport in Silicon Nano-Structures with Non-Ideal Bonding Environments", TECHCON 2008, Austin, TX, September 15 - 16, 2008, 50% acceptance rate.
- [C235] Samarth Agarwal, Gerhard Klimeck, "1D Hetero-Structure Tool for Atomistic Simulation of Nano-Devices", TECHCON 2008, Austin, TX, September 15 - 16, 2008, 50% acceptance rate.
- [C234] Mathieu Luisier, Gerhard Klimeck, "Full-band and atomistic simulation of n- and p-doped double-gate MOSFETs for the 22nm technology node", 2008 International Conference on Simulation of Semiconductor Processes and Devices, SISPAD 2008, September 9-11, 2008, Yumoto Fujiya Hotel, Hakone, Japan.
- [C233] Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, Timothy Boykin, Gerhard Klimeck, "A parallel sparse linear solver for nearest-neighbor tight-binding problems", 14th International Conference on Parallel and Distributed Computing. August 26-29, Las Palmas de Gran Canaria, Spain, 89 accepted papers out of 264 submissions;doi:10.1007/978-3-540-85451-7_84
- [C232] Gerhard Klimeck, "nanoHUB.org tutorial", IEEE nano 2008, Arlington, TX, August 18-21, 2008.
- [C231] Muhammad Usman, Shaikh Ahmed, Gerhard Klimeck, "Atomistic tight binding study of strain-reduced confinement potentials in identical and non-identical InAs/GaAs vertically stacked quantum dots", IEEE nano 2008, Arlington, TX, August 18-21, 2008;doi:10.1109/NANO.2008.161
- [C230] Mathieu Luisier, Gerhard Klimeck, "OMEN an atomistic and full-band quantum transport simulator for post-CMOS nanodevices", IEEE nano 2008, Arlington, TX, August 18-21, 2008;doi:10.1109/NANO.2008.110
- [C229] Muhammad Usman, Dragica Vasileska, Gerhard Klimeck, "Strain-Engineered Self Organized InAs/GaAs Quantum Dots for Long Wavelength (1.3-1.5um) Optical Applications", Proceedings of ICPS 2008 (International Conference on the Physics of Semiconductors), Rio de Janeiro, Brazil, July 27-Aug 1, 2008 (poster presentation).

- [C228] Gabriel Lansbergen, Rajib Rahman, Cameron. Wellard, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Lloyd Hollenberg, Sven Rogge, "Kondo Effects and Transport through a single gated donor atom", Proceedings of ICPS 2008 (International Conference on the Physics of Semiconductors), Rio de Janeiro, Brazil, July 27-Aug 1, 2008 (Oral presentation).
- [C227] Gerhard Klimeck, "nanoHUB.org in Science Gateways on Parade", Tutorial Session, TeraGrid 2008, June 9-13, 2008, Las Vegas.
- [C226] Hansang Bae, Steven Clark, Benjamin Haley, Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Mathieu Luisier, "A Nano-electronics Simulator for Petascale Computing: From NEMO to OMEN", TeraGrid 2008, June 9-13, 2008, Las Vegas.
- [C225] Gerhard Klimeck, Neerav Kharche, Muhammad Usman, Mathieu Luisier, "Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D and OMEN", Nanoelectronics Days, Aachen, Germany, May 13-16, 2008.
- [C224] Gerhard Klimeck, Michael McLennan, Mark Lundstrom, George Adams III., "nanoHUB.org - online simulation and more serving annually over 60,000 users", Nanoelectronics Days, Aachen, Germany, May 13-16, 2008.
- [C223] Abhijeet Paul, Neophytos Neophytou, Gerhard Klimeck, "Effects of Bandstructure in Nanostructures: Physics and Tool Development", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.
- [C222] Kaushik Balamukundhan, Gerhard Klimeck, "Development of a 1D hetero-structure tool", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.
- [C221] Saumitra Mehrotra, Benjamin Haley, Gerhard Klimeck, "Development and Enhancement of Nanowire on nanoHUB.org", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.
- [C220] SungGeun Kim, Sriraman Damodaran, Benjamin Haley, Gerhard Klimeck, "MuGFET: MultigateFETssimulated with drift-diffusion models at the nano-scale", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.
- [C219] Hansang Bae, Steven Clark, Benjamin Haley, Gerhard Klimeck, Sunhee Lee, Maxim Naumov, Faisal Saied, "A Massively Parallel Simulator for Nano-Electronics", Poster at Purdue HPC-Industry Workshop, April 7-8, 2008.
- [C218] Faisal Saied, Hansang Bae, Steven Clark, Benjamin Haley, Gerhard Klimeck, Sunhee Lee, Maxim Naumov, "A Massively Parallel Schroedinger Solver for Nano-Electronics", SIAM Conference on Parallel Processing for Scientific Computing, Atlanta, March 12-14 2008
- [C217] Neerav Kharche, Seongmin Kim, Timothy Boykin, Gerhard Klimeck, "Substrate orientation dependence of valley-splitting in Silicon nanostructures", American Physical Society, March Meeting 2008, March 10-14, 2008.
- [C216] Muhammad Usman, Shaikh Ahmed, Gerhard Klimeck, "Strain and Piezoelectric Effects on the Electronic Structure of Coupled $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ Self-Assembled Quantum Dots", American Physical Society, March Meeting 2008, March 10-14, 2008.
- [C215] Neophytos Neophytou, Abhijeet Paul, Gerhard Klimeck, "Atomistic Treatment of Electronic Transport: The Effect of Bandstructure", American Physical Society, March Meeting 2008, March 10-14, 2008.
- [C214] Timothy Boykin, Neerav Kharche, Mathieu Luisier, Gerhard Klimeck, "Zone Unfolding and Approximate Bandstructure Calculations in Tight-Binding", American Physical Society, March Meeting 2008, March 10-14, 2008.
- [C213] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Atomistic Treatment of Electronic Transport: The Effect of Bandstructure", Physics-Based Mathematical Models of Low-Dimensional Semiconductor Nanostructures: Analysis and Computation, Banff, Canada, Banff International Research Station (BIRS), Nov. 18-23, 2007.
- [C212] Gerhard Klimeck, "Rappture Tool Development: s/w Environment That Enabled 50+ Applications in Two Years", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [C211] Gerhard Klimeck, "generation-nano.org: Engagement K-12", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [C210] Gerhard Klimeck, "From nanoHUB to HUBzero: Roadmap to New HUBs", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [C209] Gerhard Klimeck, "nanoHPC: Multimillion Atom Simulations Using NEMO 3D", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [C208] Maxim Naumov, Sunhee Lee, Benjamin Haley, Hansang Bae, Steven Clark, Rajib Rahman, Hoon Ryu, Faisal Saied, Gerhard Klimeck, "Interior Spectrum Eigenvalue Solvers for NEMO 3-Ds", Supercomputing 2007, Reno, NV, electronic poster at Purdue University Exposition Booth, Nov. 13-16, 2007.
- [C207] Gerhard Klimeck, Faisal Saied, Steven Clark, Benjamin Haley, Hansang Bae, Sunhee Lee, "Preparing for the Peta-Scale: Scaling of NEMO 3D", Supercomputing 2007, Reno, NV, electronic poster at Purdue University Exposition Booth, Nov. 13-16, 2007.

- [C206] Hoon Ryu, Rajib Rahman, Gerhard Klimeck, "Efficient Calculation of Long-Range Coulomb interactions", Supercomputing 2007, Reno, NV, electronic poster at Purdue University Exposition Booth, Nov. 13-16, 2007.
- [C205] Hansang Bae, Steven Clark, Benjamin Haley, Gerhard Klimeck, Sunhee Lee, Maxim Naumov, Faisal Saied, "A Massively Parallel Simulator for Nano-Electronics", Supercomputing 2007, Reno, NV, late-news poster reception finalist for best poster award, Nov. 13, 2007.
- [C204] Maxim Naumov, Sunhee Lee, Benjamin Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Steven Clark, Gerhard Klimeck, "Alternative Sparse Eigensolvers and Performance Optimization for Electronic Structure Simulations with NEMO-3D", Purdue Computing Research Institute (CRI), High Performance Computing Research Poster Session, October 25 2007, LWSN Building.
- [C203] Bhaskaran Muralidharan, Hoon Ryu, Zhen Huang, Gerhard Klimeck, "NEMO-3D based Atomistic Simulation of a Double Quantum Dot Structure for Spin-Blockaded Transport", The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007;doi:10.1007/s10825-008-0203-9
- [C202] Roksana Golizadeh-Mojarad, A.N.M. Zainuddin, Shaikh Ahmed, Gerhard Klimeck, Supriyo Datta, "Atomistic NEGF Simulations of Carbon Nano-Ribbons in Magnetic Fields", The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007
- [C201] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Simulation of nanowire transistors: Atomistic vs. Effective Mass Models", The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007;doi:10.1007/s10825-008-0188-4
- [C200] Neerav Kharche, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Electronic Structure and Transmission Characteristics of SiGe Nanowires", The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007;doi:10.1007/s10825-008-0191-9
- [C199] Maxim Naumov, Sunhee Lee, Benjamin Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Steven Clark, Gerhard Klimeck, "Alternative Sparse Eigensolvers and Performance Optimization for Electronic Structure Simulations with NEMO-3D", The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007
- [C198] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Self-consistent simulations of nanowire transistors using atomistic basis sets", The 12th International Conference on Simulation of Semiconductor Devices and Processes (SISPAD), Vienna Austria, September 25-27, 2007;doi:10.1007/978-3-211-72861-1_51
- [C197] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, Gerhard Klimeck, "Self-consistent simulations of nanowire transistors using atomistic basis sets", SRC TECHCON 2007, September 10-12, 2007
- [C196] Tuna Toksoz, Gerhard Klimeck, Samarth Agarwal, "Implementation of a GUI for a Resonant Tunneling Diode Simulator", (Summer Undergraduate Research Fellowship), July 31, 2007.
- [C195] Raseong Kim, Mathieu Luisier, Neophytos Neophytou, Michael McLennan, Jing Wang, Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, "Bandstructure Calculation of Semiconductor Devices and Characteristic Features of 1D Transport in Nanowire MOSFETS", Network for Computational Nanotechnology annual site visit, June 18-20, 2007, Purdue University.
- [C194] Sunhee Lee, Hansang Bae, Steven Clark, Benjamin Haley, Gerhard Klimeck, Maxim Naumov, Hoon Rye, Faisal Saied, "Multi-Million Atom Electronic Structure simulations Towards Petaflop Operation", Network for Computational Nanotechnology annual site visit, June 18-20, 2007, Purdue University.
- [C193] Hansang Bae, Steven Clark, Gerhard Klimeck, Sunhee Lee, Maxim Naumov, Faisal Saied, "Large Scale Simulations of Nanoelectronic devices with NEMO3-D on the Teragrid", Teragrid 2007 Conference, Madison WI, June 2007
- [C192] Gerhard Klimeck, Michael McLennan, "Science Gateway Building Blocks: nanoHUB", Teragrid 2007 Conference, Madison WI, June 2007.
- [C191] Michael McLennan, Rick Kennel, Paul Ruth, Gerhard Klimeck, Alain Roy, Renato Figueiredo, "nanoHUB Tutorial: Using nanoHUB.org as a Science Gateway", Teragrid 2007 Conference, Madison WI, June 2007.
- [C190] Sriraman Damodaran, Selvakumaran Vadivelmurugan, Quoc Do, Clemens Heitzinger, Gerhard Klimeck, "Investigation of the Conductance of Silicon Nanowire Biosensors Using the 2D Drift-diffusion Model", NSTI Nanotech 2007, Santa Clara, CA, May 20-24 2007
- [C189] Martha Prada, Neerav Kharche, Gerhard Klimeck, "Electronic Structure of Si/ InAs Composite Channels", MRS Spring conference April 10, 2007, Symposium G: Extending Moore's Law with Advanced Channel Materials.
- [C188] Michael McLennan, Mark Lundstrom, Gerhard Klimeck, "GOMACTech Tutorial: Using nanoHUB for Scientific Computing, Education, and Outreach", GOMACTech Conference, Orlado, FL, March 19, 2007
- [C187] Hansang Bae, Steven Clark, Benjamin Haley, Gerhard Klimeck, Sunhee Lee, Maxim Naumov, Hoon Ryu, Faisal Saied, "Large Scale Simulations of Nanoelectronic devices with NEMO3-D on HPC platforms", Computing Research Institute (CRI) Poster session on HPC Research and Education, April 5 (2007), MSEE Building, Purdue University.

- [C186] Neerav Kharche, Martha Prada, Timothy Boykin, Gerhard Klimeck, "Valley-splitting in strained Silicon quantum wells on a miscut substrate using tight-binding model", American Physical Society, March Meeting 2007
- [C185] Shaikh Ahmed, Muhammad Usman, Neerav Kharche, Andrei Schliwa, Gerhard Klimeck, "Atomistic Simulation of Non-Degeneracy and Optical Polarization Anisotropy in Pyramidal Quantum Dots", IEEE International Conference on Nano/Micro Engineered and Molecular Systems (IEEE-NEMS), Jan 16-19, 2007, Bangkok Thailand. oral presentation, 340 submission, 90% acceptance, 55% oral presentations;doi:10.1109/NEMS.2007.352172
- [C184] Michael McLennan, Wei Qiao, Rick Kennel, Gerhard Klimeck, "Visualizing Current Flow in Quantum Wires and other Devices on nanoHUB.org", Advanced Heterostructure Workshop, Hawaii, Dec. 3 - 8, 2006.
- [C183] Gerhard Klimeck, Timothy Boykin, Mathieu Luisier, Neerav Kharche, Andreas Schenk, "Electronic structure and transport in random alloy AlGaAs nanowires", Advanced Heterostructure Workshop, Hawaii, Dec. 3 - 8, 2006.
- [C182] Wei Qiao, Michael McLennan, Rick Kennel, David Ebert, Gerhard Klimeck, "Hub-based Simulation and Graphics Hardware Accelerated Visualization for Nanoelectronics Applications", IEEE Visualization 2006, Baltimore, MD, October 29 - Nov 3, 2006. Accepted as one of 63 in 228 submissions;doi:10.1109/TVCG.2006.150
- [C181] Eddie Howell, Clemens Heitzinger, Gerhard Klimeck, "Investigation of Device Parameters for Field-Effect DNA-Sensors by Three-Dimensional Simulation", IEEE Nanotechnology Materials and Devices Conference, October 22-25, 2006, about 67% acceptance rate, www.ieee-nmdc.org;doi:10.1109/NMDC.2006.4388725
- [C180] Krishna Madhavan, Sebastien Goasguen, Gerhard Klimeck, "The impact of the nanoscale vision on the future of learning and teaching", Nanomodeling 2006 Conference, International Society for Optical Engineering, San Diego, CA.
- [C179] Clemens Heitzinger, Gerhard Klimeck, "Investigation of Conventional DNAFETs for Genome-wide Detection of Polymorphisms", Eurosensor Conference, Goteborg, Sweden, September 21, 2006.
- [C178] Shaikh Ahmed, M. Anantram, Neophytos Neophytou, Marek Korkusinski, Gerhard Klimeck, "Quantum Simulations of Electronic Structure and Transport Properties in Conventional and Novel Nanoscale Devices", 7th World Congress on Computational Mechanics, Minisymposium on Transport and Coupled Processes in Micro- and Nanotechnology Los Angeles, July 16-22, 2006
- [C177] Gerhard Klimeck, Timothy Boykin, Mathieu Luisier, Neerav Kharche, Andreas Schenk, "A Study of alloyed nanowires from two perspectives: approximate dispersion diagrams and transmission coefficients", 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006.
- [C176] Muhammad Usman, Shaikh Ahmed, Gerhard Klimeck, "Symmetry Breaking and Fine Structure Splitting in Self-Assembled Zincblende Quantum Dots: Atomistic Simulations of Long-Range Strain and Piezoelectric Field", 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006.
- [C175] Clemens Heitzinger, Muhammad Usman, Shaikh Ahmed, Gerhard Klimeck, Marek Korkusinski, "Strain and electronic structure interactions in realistically scaled quantum dot stacks", 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006.
- [C174] Gerhard Klimeck, Mathieu Luisier, Timothy Boykin, Neerav Kharche, Andreas Schenk, "A Study of alloyed nanowires from two perspectives: approximate dispersion diagrams and transmission coefficient", 28th International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006.
- [C173] Mathieu Luisier, Raseong Kim, Neophytos Neophytou, Michael McLennan, Jing Wang, Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, "Bandstructure Lab", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C172] Ahmet Yanik, Gerhard Klimeck, Supriyo Datta, "Impurity Effects in Magnetic Tunnel Junctions", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C171] Neerav Kharche, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Is it a Device or a Material? Atomistic Modeling of AlGaAs Nanowires", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C170] Neophytos Neophytou, Shaikh Ahmed, Gerhard Klimeck, "Non-Equilibrium Green's function (NEGF) Simulation of Metallic CNTs Including Vacancy Defects", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C169] Rajib Rahman, Martha Prada, Gerhard Klimeck, "Si:P Quantum Computer Architecture", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C168] Neerav Kharche, Martha Prada, Gerhard Klimeck, "Valley Splitting in Strained Si/SiGe Quantum Wells: Grown on (100) and Miscut Substrates", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.

- [C167] Amritanshu Palaria, Arvind Arumbakkam, Gerhard Klimeck, Alejandro Strachan, "nanoMaterials simulations toolkit and sample learning module", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C166] Clemens Heitzinger, Gerhard Klimeck, "Theory of DNAFETs and BioFETs", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C165] Wei Qiao, Michael McLennan, Rick Kennel, David Ebert, Gerhard Klimeck, "nanoHUB Visualization Tools", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C164] Clemens Heitzinger, Gerhard Klimeck, "Simulation study of silicon-nanowire field-effect DNA-sensors", International Congress on Nanobiotechnology and Nanomedicine (NanoBio 2006), San Francisco, CA, USA, June 2006.
- [C163] Sebastien Goasguen, Jon Camden, Muhammad Usman, Steven Clark, Jaime Frey, Clemens Heitzinger, Gerhard Klimeck, "nanoHUB - nanoscience gateway to the TeraGrid", Teragrid 2006, Indianapolis, IN June 12-15, 2006.
- [C162] Michael McLennan, Sebastien Goasguen, Krishna Madhavan, Derrick Kearney, Joe Cychosz, Alicia Goodman, Shaikh Ahmed, Swaroop Shivarajapura, Shawn Rice, Carol Song, Steven Clark, Rick Kennel, Clemens Heitzinger, Mark Lundstrom, Gerhard Klimeck, "The nanoHUB -- Online simulations and a community for nano-science and nano-technology", Teragrid 2006, Indianapolis, IN June 12-15, 2006.
- [C161] Srikant Srinivasan, Gerhard Klimeck, Leonid Rokhinson, "Modeling of a strained-Silicon quantum dot embedded in strain-relaxed Silicon-Germanium", Synergy Between Experiment and Computation in Nanoscale Science, Harvard University, May 31-June 3.
- [C160] Clemens Heitzinger, Gerhard Klimeck, "Numerical aspects of the three-dimensional feature-scale simulation of silicon-nanowire field-effect sensors for DNA detection", 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [C159] Mathieu Luisier, Gerhard Klimeck, Andreas Schenk, Wolfgang Fichtner, "Transport Calculation of Semiconductor Nanowires Coupled to Quantum Well Reservoirs", 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [C158] Gianluca Fiori, Giuseppe Iannaccone, Gerhard Klimeck, "Coupled mode space vs Real space approach for the simulation of CNT-FETs", 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [C157] Neophytos Neophytou, Shaikh Ahmed, M. Anantram, Gerhard Klimeck, "Non-Equilibrium Green's Function (NEGF) Simulation of Metallic Carbon Nanotube Transistors: Impact of Vacancy Defect ", 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [C156] Vladimir Mitin, Nizami Vagidov, Mathieu Luisier, Gerhard Klimeck, "Energy dispersion relations for holes in silicon quantum wells and quantum wires", 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.
- [C155] Neerav Kharche, Mathieu Luisier, Timothy Boykin, Gerhard Klimeck, "Is it a Device or a Material? Atomistic Modeling of AlGaAs Nanowires", Purdue University, Electrical Engineering Graduate Student Conference, April 7, 2006
- [C154] Elizabeth Gardner, Mark Lundstrom, Gerhard Klimeck, "NCN NanoHUB: a resource for nanotechnology education", Presentation at 2006 Materials Research Society Spring Meeting, April 17-21, 2006.
- [C153] Elizabeth Gardner, Mark Lundstrom, Gerhard Klimeck, "NCN NanoHUB: a resource for nanotechnology education", Poster at American Chemical Society Meeting and Exposition, March 26 - 30, 2006, Atlanta, GA USA.
- [C152] Neophytos Neophytou, Shaikh Ahmed, Diego Kienle, Mark Lundstrom, Gerhard Klimeck, "Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org -- Non-Equilibrium Green's Function Simulations of the Impact of Atomic Defects on the Performance of Carbon Nanotube Transistors", March Meeting of the American Physical Society, March 13-17, 2006, Baltimore, MD.
- [C151] Gerhard Klimeck, Shaikh Ahmed, Marek Korkusinski, Seungwon Lee, Faisal Saied, "Atomistic Simulations of Long-Range Strain and Close-Range Electronic Structure in Self-Assembled Quantum Dot Systems", March Meeting of the American Physical Society, March 13-17, 2006, Baltimore, MD.
- [C150] Neerav Kharche, Clemens Heitzinger, Gerhard Klimeck, Mathieu Luisier, Timothy Boykin, "Bandstructure Effects in Unstructured AlGaAs Nanowires", March Meeting of the American Physical Society, March 13-17, 2006, Baltimore, MD.
- [C149] Shaikh Ahmed, Dragica Vasileska, Gerhard Klimeck, Christian Ringhofer, "Efficiency of the Thermalized Quantum Potential Approach for Modeling Nanoscale Semiconductor Devices", March Meeting of the American Physical Society, March 13-17, 2006, Baltimore, MD.
- [C148] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Atomistic simulations of long-range strain and spatial asymmetry effects in single and coupled quantum dots", Joint International Conference on New Phenomena in Mesoscopic Systems and Surfaces and Interfaces of Mesoscopic Devices (NPMS-7/SIMD-5), Kapalua, Hawaii, Nov. 27-Dec2, 2005

- [C147] Jing Wang, Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, "Bandstructure and Orientation Effects in Si and Ge Nanowire FETs", 2005 IEEE International Electron Devices Meeting, Washington, DC, December 5 - 7, 2005. (One of 27 accepted out 120 submitted Modeling and Simulation abstracts).
- [C146] Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, "Novel channel materials for ballistic nanoscale MOSFETs bandstructure effects", 2005 IEEE International Electron Devices Meeting, Washington, DC, December 5 - 7, 2005. (One of 27 accepted out 120 submitted Modeling and Simulation abstracts).
- [C145] Gianluca Fiori, Giuseppe Iannaccone, Gerhard Klimeck, "Performance of Carbon Nanotube Field Effect Transistors with doped source and drain extensions and arbitrary geometry", 2005 IEEE International Electron Devices Meeting, Washington, DC, December 5 - 7, 2005. (One of 27 accepted out 120 submitted Modeling and Simulation abstracts).
- [C144] Wei Qiao, David Ebert, Alireza Entezari, Marek Korkusinski, Gerhard Klimeck, "VolQD: Direct Volume Rendering of Multi-million Atom Quantum Dot Simulations", IEEE Visualization 2005, October 23-28, Minneapolis, Minnesota, USA, one of 88 accepted from 268 submissions.
- [C143] Jing Wang, Neophytos Neophytou, Avik Ghosh, Gerhard Klimeck, Mark Lundstrom, "Full Band Simulation of Silicon Nanowire Transistors", SRC TECHCON, September, 2005.
- [C142] Gianluca Fiori, Giuseppe Iannaccone, Mark Lundstrom, Gerhard Klimeck, "Three-dimensional atomistic simulation of Carbon Nanotube FETs with realistic geometry", European Solid-State Device Research Conference, ESSDERC, Grenoble, France, 12 - 16 September 2005
- [C141] Neerav Kharche, Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Atomistic Simulation of Multimillion-Atom Nanostructures using the Nanoelectronic Modeling Tool NEMO-3D", Poster Session on Computational Science and Engineering Research, joint CRI/RCAC HPC Training Workshop, Purdue University, September 7-8, 2005.
- [C140] Sebastien Goasguen, Gerhard Klimeck, Suma Adabala, Rick Kennel, Renato Figueiredo, Alain Roy, Steven Clark, Wendy Lin, Jose Fortes, Jaime Frey, Paul Ruth, "The Cyberinfrastructure supporting the nanoHUB", Poster Session on Computational Science and Engineering Research, joint CRI/RCAC HPC Training Workshop, Purdue University, September 7-8, 2005.
- [C139] Gerhard Klimeck, "Parallel Applications in Nanoelectronics", joint CRI/RCAC HPC Training Workshop, Purdue University, September 7-8, 2005.
- [C138] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Atomistic simulations of long-range strain effects in multimillion-atom quantum dot nanostructures", IEEE SISPAD 2005, International Conference on Simulation of Semiconductor Processes and Devices, Komaba Eminence, Tokyo, Japan, September 1-3, 2005.
- [C137] Sebastien Goasguen, Krishna Madhavan, Michael McLennan, Mark Lundstrom, Gerhard Klimeck, "The nanoHUB: A Science Gateway for nanotechnology", GGF14 - The Fourteenth Global Grid Forum, Science Gateways workshop, June 27-30, 2005 Chicago, IL, USA
- [C136] Marek Korkusinski, Gerhard Klimeck, Haiying Xu, S. Lee, Sebastien Goasguen, Faisal Saied, "Atomistic simulations in nanostructures composed of tens of millions of atoms", 2005 NSTI Nanotechnology Conference and Trade Show, Anaheim, CA, May 8-12, 2005.
- [C135] Sebastien Goasguen, Michael McLennan, Gerhard Klimeck, Mark Lundstrom, "What do Mambo, VNC, UML and Grid computing have in common?", 2005 Linux Cluster Institute Conference, Raleigh, NC, April, 2005
- [C134] Marek Korkusinski, Faisal Saied, Haiying Xu, Seungwon Lee, Mohammed Sayeed, Sebastien Goasguen, Gerhard Klimeck, "Large Scale Simulations in Nanostructures with NEMO3-D on Linux Clusters", 2005 Linux Cluster Institute Conference, Raleigh, NC, April, 2005
- [C133] Olga Lazarenkova, S. Lee, Paul Allmen, Fabiano Oyafuso, Gerhard Klimeck, Marek Korkusinski, R. Timm, H. Eisele, M. Dahne, "Effect of anharmonicity of the inter-atomic potential on the built-in strain in epitaxial quantum dot structures", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C132] Fabiano Oyafuso, Paul Allmen, Seungwon Lee, Gerhard Klimeck, "Modeling transport through Si nanowires using a nonequilibrium Green function approach", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C131] Marek Korkusinski, Gerhard Klimeck, Haiying Xu, S. Lee, Sebastien Goasguen, Faisal Saied, "Atomistic simulations in nanostructures composed of tens of millions of atoms", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C130] Arkady Satanin, Y. Joe, Gerhard Klimeck, "Fano quadrupole in a nanoscale ring", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C129] Timothy Boykin, Gerhard Klimeck, Susan Coppersmith, Mark Friesen, Paul Allmen, Seungwon Lee, Fabiano Oyafuso, "Valley splitting in low-density quantum-confined heterostructures: Superposition, not Spin!", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C128] "Bandstructure Effects in Nanoscale MOSFETs", IEEE IEDM, San Francisco, CA, Dec. 6-8 2004.
- [C127] Fabiano Oyafuso, Paul Allmen, Seungwon Lee, Gerhard Klimeck, "Nonequilibrium Transport in Silicon Nanowires", 2004 MRS Fall Meeting, Boston, MA, Nov. 29 - Dec. 3, 2004.

- [C126] E. Khorenko, W. Prost, F.-J. Tegude, M. Stoffel, R. Duschl, M. Dashiell, O.G. Schmidt, Gerhard Klimeck, "Manufacturability and Electrical Characteristics of Si/SiGe Interband Tunnelling Diodes", ASDAM '04, The Fifth International Conference on Advanced Semiconductor Devices and Microsystems, Smolenice, Slovakia, Oct. 17-21, 2004.
- [C125] Seungwon Lee, Paul Allmen, Fabiano Oyafuso, Gerhard Klimeck, Timothy Boykin, Susan Coppersmith, Mark Friesen, Mark Eriksson, "Electron Exchange Interaction in Electronically Confined Si Quantum Dots", 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, 2004.
- [C124] Yun Zheng, Christian Rivas, Roger Lake, Khairul Alam, Timothy Boykin, Gerhard Klimeck, "Electronic Properties of Silicon Nanowires", 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, 2004.
- [C123] Faisal Saied, Haiying Xu, Mohammed Sayeed, Sebastien Goasguen, Gerhard Klimeck, "Tuning a Nanotechnology Simulator for High Performance: Performance Improvement of the NEMO 3-D Eigenvalue solver", NSF Network for Computational Nanotechnology (NCN), Annual site visit, Student Poster Presentation, Purdue University, West Lafayette, June 24, 2004.
- [C122] Olga Lazarenkova, Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "The effect of the strain relaxation in InAs/GaAs stacked quantum dots and multiple quantum wells on the Raman spectrum", 12th International Symposium "Nanostructures: Physics and Technology", June 21-25, 2004 in St Petersburg, Russia.
- [C121] Olga Lazarenkova, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, Gerhard Klimeck, "Effect of Anharmonicity of Interatomic Potential on Strain Distribution in Semiconductor Nanostructures", MRS Spring Meeting, April 12-16, San Francisco, CA, April 12-16, 2004.
- [C120] Sebastien Goasguen, Mark Lundstrom, Gerhard Klimeck, "Using I-Light and the Purdue Nanohub Computing Resources to Run Computationally Intensive Codes in Nanotechnologies", I-Light Symposium, IUPUI University Place Conference Center, Indianapolis, March 9, 2004.

Work Performed at JPL (79 Total)

- [C119] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, Olga Lazarenkova, "Coupled electron and nuclear spin dynamics in InAs quantum dots: impact on single and two-qubit operations", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C118] Seungwon Lee, Olga Lazarenkova, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Effect of Wetting Layers on Strain and Electronic Structures of Self-Assembled Quantum Dots", Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C117] Olga Lazarenkova, Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "Atomistic-Level Simulation of the Vibration Spectrum of Quantum Dot Crystals", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C116] Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Paul Allmen, Fabiano Oyafuso, S. Lee, "Conduction band valley splitting in Si", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C115] Seungwon Lee, Paul Allmen, Fabiano Oyafuso, Gerhard Klimeck, K. Whaley, "Effect of electron-nuclear spin interactions on electron-spin qubits localized in self-assembled quantum dots", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C114] Seungwon Lee, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Efficient boundary condition for the electronic structure of embedded semiconductor nanostructures", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C113] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "Effect of nuclear spin dynamics on quantum computing operations in spin based qubits", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C112] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "Sensitivity and response time of palladium nanowire hydrogen sensors", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C111] Olga Lazarenkova, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, Gerhard Klimeck, "Effect of strain on the phonon dispersion in Ge/Si quantum dot superlattices with an atomistic level model", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C110] Mark Kordon, Gerhard Klimeck, Dave Hanks, Hook Hua, "Evolutionary Computing for the Design Search and Optimization of Space Vehicle Power Subsystems", IEEE Aerospace Conference, Big Sky, Montana, March 2004. Proceedings
- [C109] Gerhard Klimeck, Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Timothy Boykin, "Nanoelectronic Modeling (NEMO) for Realistic Simulations of Solid-State Quantum Computing Gates", DARPA Focused Quantum Systems (FoQuS) Workshop, Falls Church, VA, Jan 28-29 (2004).

- [C108] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "Simulation of Hydrogen Sensors using Pd Nanowires", JPL conference on internal research and development, December 4, 2003, Pasadena, CA.
- [C107] Richard Terrile, Christoph Adami, Michael Ferguson, Wolfgang Fichtner, Terrance Huntsberger, Gerhard Klimeck, Mark Kordon, Erick Mjolsness, Savio Chau, "Evolutionary Computing Technologies for Space Systems", JPL conference on internal research and development, December 4, 2003, Pasadena, CA.
- [C106] Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Paul Allmen, Fabiano Oyafuso, Seungwon Lee, "Conduction band valley splitting in silicon nano-structures", Sixth International Conference on New Phenomena in Mesoscopic Structures, Fourth International Conference on Surfaces and Interfaces of Mesoscopic Devices, December 1-5, 2003, Maui, Hawaii.
- [C105] Seungwon Lee, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Numerical surface treatment for finite-extent semiconductor nanostructures", 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona, Spain. October 16-17 2003.
- [C104] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, Paul Allmen, Seungwon Lee, Olga Lazarenkova, "Development of a 3-D Nanoelectronic Modeling Tool (NEMO 3-D)", accepted in 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona (Casa Convalescencia) 16, 17 October 2003
- [C103] Hans Kosina, Gerhard Klimeck, Michail Nedjalkov, Siegfried Selberherr, "Comparison of Numerical Quantum Device Models", International Conference on Simulation of Semiconductor Processes and Devices (SISPAD 2003), September 3-5, 2003, Boston, MA.
- [C102] Seungwon Lee, Gerhard Klimeck, K. Whaley, "Electron-spin g-factor engineering with SiGe heterostructures", Spintech II International Conference and School, Semiconductor Spintronics and Quantum Information Technology. It is held on August 4-8, 2003 at Brugge, Belgium.
- [C101] Gerhard Klimeck, Gary Yagi, Robert Deen, Michael McAuley, Eric DeJong, Fabiano Oyafuso, "Near Real-Time Parallel Image Processing using Cluster Computers", International Conference on Space Mission Challenges for Information Technology (SMC-IT), Pasadena, CA July 13-16, 2003.
- [C100] Fabiano Oyafuso, Gerhard Klimeck, Timothy Boykin, R. Bowen, Paul Allmen, "Study of Strain Boundary Conditions and GaAs Buffer Sizes in InGaAs Quantum Dots", International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [C99] Gerhard Klimeck, Phillip Stout, R. Bowen, "Quantum and semi-classical transport in RTDs using NEMO 1-D", International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [C98] Jeremy Green, Corrie Farmer, Michel Garcia, Hock Lee, Colin Stanley, Charles Ironside, Gerhard Klimeck, Roger Lake, "Quantum cascade laser simulation using sp3s* full Brillouin zone tight-binding model", CLEO/Europe 2003, Munich 22-27 June 2003;doi:10.1109/CLEOE.2003.1312243
- [C97] Titus Sandu, Gerhard Klimeck, Wiley Kirk, "Structure of Transverse Electron Current in Resonant Tunneling Diodes and Breakdown of Tsu-Esaki Formula", March Meeting of American Physical Society, March 16-21, Austin, TX (2003)
- [C96] Fabiano Oyafuso, Gerhard Klimeck, Timothy Boykin, R. Bowen, Paul Allmen, "Effects of Electronic and Strain Boundary Conditions in Multi-million Atom Electronic Structure Simulations", March Meeting of American Physical Society, March 16-21, Austin, TX (2003)
- [C95] Timothy Boykin, Gerhard Klimeck, R. Bowen, Fabiano Oyafuso, "Diagonal parameter shifts in strained semiconductors in the empirical tight-binding theory", March Meeting of American Physical Society, March 16-21, Austin, TX (2003)
- [C94] Gerhard Klimeck, Fabiano Oyafuso, R. Bowen, Timothy Boykin, Paul Allmen, "NEMO 3-D: Multi-Million Atom Electronic Structure Calculation, Simulation of Alloy Disorder in Quantum Dots", The NASA University Research, Engineering, and Technology Institute for Nanoelectronics and Computing (INAC) and The NSF Network for Computational Nanotechnology (NCN), Official Kickoffs and Workshop, Purdue University, West Lafayette, IN, Jan. 15-17, 2003.
- [C93] Gerhard Klimeck, "Transport simulation of precessing spin distribution across semiconductor heterojunctions", Twenty-Five Years Ultra-Small Electronics Research, Larry Cooper Symposium, November 29, 2002, Hapuna Beach, Hawaii.
- [C92] Paul Allmen, Gerhard Klimeck, "NEMO: A User-friendly Quantum Device Design Tool", Materials Research Society Meeting, Boston, MA, Dec 1-6, 2002.
- [C91] Gerhard Klimeck, Fabiano Oyafuso, R. Bowen, Paul Allmen, Tom Cwik, Edward Vinyard, Edith Huang, Timothy Boykin, "Quantum Dot Modeling using NEMO 3-D: IT Challenges in the development of quantum device simulator", JPL representation in the NASA booth of Supercomputing 2002, Baltimore, MD, Nov 17-22, 2002.
- [C90] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, Paul Allmen, "Study of Alloy Induced Disorder in Quantum Dots using Tight-binding", 4th Motorola Workshop on Computational Materials and Electronics, Tempe, AZ, Nov 14-15, 2002.

- [C89] Gerhard Klimeck, Fabiano Oyafuso, Paul Allmen, "Development of a 3-D tight-binding-based electronic structure simulator for multi-million atom systems NEMO 3-D", SOCAL - Southern California Workshop on Parallel Computing, Santa Barba, CA, Oct. 28, 2002.
- [C88] Akos Czikmantory, Tom Cwik, Edward Vinyard, Hook Hua, Fabiano Oyafuso, Gerhard Klimeck, "WIGLAF - A Web Interface Generator and Legacy Application Facade", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C87] Paul Allmen, Gerhard Klimeck, Fabiano Oyafuso, "Simulation of the electric field dependent spin dynamics in semiconductor thin films", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C86] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, Paul Allmen, "Modeling of Disordered Multimillion Atom Quantum Dot Systems", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C85] Gerhard Klimeck, Gary Yagi, Robert Deen, Michael McAuley, Eric DeJong, Fabiano Oyafuso, "Image Correlation Quality Control enabled by Cluster Computing", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C84] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, Paul Allmen, "Boundary Conditions in Disordered Multimillion Atom Quantum Dot Systems", 2nd International Conference on Semiconductor Quantum Dots - QD2002-, September 30 - October 3, 2002 Komaba Campus, University of Tokyo.
- [C83] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, "Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems", SISPAD 2002, Kobe, Japan, Sept. 3-6, 2002.
- [C82] Gerhard Klimeck, Fabiano Oyafuso, E. Tisdale, Akos Czikmantory, "Eigensolver and Cluster Middleware Development", Computational Technology Project Meeting, NASA Goddard Space flight center, MD, July 10, 2002.
- [C81] Gerhard Klimeck, Thomas Cwik, "GENES: Genetically Engineered Nanostructures", Nanospace 2002, Galveston, TX, June 24-28, 2002.
- [C80] Paul Allmen, Gerhard Klimeck, "Transport Simulation of Precessing Spin Distribution across Semiconductor Heterojunctions", Nanospace 2002, Galveston, TX, June 24-28, 2002.
- [C79] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, "Quantum Dot Simulation", AFRL-JPL workshop on Nanotechnology, Pasadena, CA, May 8-10, 2002.
- [C78] Michael McAuley, Gerhard Klimeck, Bob Deen, Tom Cwik, Eric DeJong, "Mars Image Processing on Commodity Cluster Computers", Science Data Processing Session, 4th Quality Mission Software Workshop, Dana Point, CA, May 7-8 2002.
- [C77] Gerhard Klimeck, "JPL interaction with the proposed NSF funded Network for Computational Nanotechnology", Workshop on a National Network for Nanoscale Modeling and Simulation, Sponsored by the National Science Foundation, Purdue University, April 11, 2002.
- [C76] Gerhard Klimeck, Fabiano Oyafuso, Timothy Boykin, R. Bowen, "Multi-million Atom Electronic Structure Simulations using NEMO 3-D", March Meeting of American Physical Society, March 17-22, Indianapolis, IN (2002)
- [C75] Seungwon Lee, Lars Jönsson, Jeongnim Kim, John Wilkins, Garnett Bryant, Gerhard Klimeck, "Many-body interactions in multiply-charged quantum dots modeled by empirical tight-binding", March Meeting of American Physical Society, March 17-22, Indianapolis, IN (2002)
- [C74] Gerhard Klimeck, "A GA practitioner's view on what is needed for efficient use of a 1000 CPU cluster", JPL workshop on Evolvable Systems, Feb 25, 2002.
- [C73] Gerhard Klimeck, "Full Brillouin-Zone, Charge Self-consistent Quantum Transport Simulations Enabled by Parallelization of the Nanoelectronic Modeling Tool (NEMO 1-D) on a Beowulf Cluster", 8th International Workshop on Computational Electronics, October 15-18, Univ. of Illinois
- [C72] Fabiano Oyafuso, Gerhard Klimeck, R. Bowen, Timothy Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", 8th International Workshop on Computational Electronics, October 15-18, Univ. of Illinois
- [C71] Tom Cwik, Gerhard Klimeck, Michael McAuley, Bob Deen, Eric DeJong, "Applications on High Performance Cluster Computers Production of Mars Panoramic Mosaic Images", 2001, AMOS Technical Conference, September 10-14, Maui
- [C70] Tom Cwik, Gerhard Klimeck, Charles Norton, Thomas Sterling, Frank Villegas, Ping Wang, "The Use of Cluster Computers Systems for NASA/JPL Applications", AIAA Space 2001 Conference and Exposition Albuquerque, New Mexico 28-30 August 2001.
- [C69] Tom Cwik, Gerhard Klimeck, Frank Villegas, "Large-Scale Design and Optimization Using Cluster Computers", IEEE AP-S International Symposium and USNC/URSI National Radio Science Symposium, Boston, MA, July 8-13 (2001).
- [C68] Gerhard Klimeck, Fabiano Oyafuso, R. Bowen, Timothy Boykin, Thomas Cwik, Edith Huang, Edward Vinyard, "Quantum Dot Modeling using NEMO 3-D, or Development of a Bottom-Up Nanoelectronic Simulator", Sackler Colloquium, National Academy of Sciences, Washington DC, May 18-20 (2001)

- [C67] Gerhard Klimeck, R. Bowen, Fabiano Oyafuso, Tom Cwik, Edith Huang, "IT Challenges in Nanoscale Electronic Devices Modeling", JPL IT Symposium, Pasadena, CA, May 9 (2001)
- [C66] Gerhard Klimeck, Michael McAuley, Tom Cwik, Bob Deen, Eric DeJong, "Beowulf Processing for Real-time Mission Science and Operations Products", JPL IT Symposium, Pasadena, CA, May 9 (2001)
- [C65] Tom Cwik, Viktor Decyk, Daniel Katz, Gerhard Klimeck, Nooshin Meshkaty, Charles Norton, Fabiano Oyafuso, Paul Springer, Thomas Sterling, E. Tisdale, Frank Villegas, Edward Vinyard, Ping Wang, "The Use of Cluster Computer Systems for NASA/JPL Applications", High Performance Computing Group, Section 385, JPL IT Symposium, Pasadena, CA, May 9 (2001).
- [C64] Gerhard Klimeck, R. Bowen, Timothy Boykin, Fabiano Oyafuso, "Atomistic Quantum Dot Simulation using NEMO-3D", Nanospace 2001, Galveston, Texas, March 13-16 (2001)
- [C63] Lars Jönsson, Seungwon Lee, John Wilkins, Garnett Bryant, Gerhard Klimeck, "Sensitivity of electron-hole integrals to choice of atomic orbitals in tight-binding models for nanocrystals.", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001)
- [C62] Gerhard Klimeck, R. Bowen, Timothy Boykin, "A tiger by the tail: the momentum operator in tight-binding", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001)
- [C61] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Quantum Dot Modeling using NEMO 3-D", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001)
- [C60] Seungwon Lee, Lars Jönsson, John Wilkins, Garnett Bryant, Gerhard Klimeck, "Long-range electron-hole exchange in semiconductor quantum dots", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001)
- [C59] Didier Keymeulen, Gerhard Klimeck, Ricardo Zebulum, Adrian Stoica, Yili Jin, Carlos Salazar-Lazaro, "EHWPack: an Evolvable Hardware Environment using the Spice Simulator and the Field Programmable Transistor Array", ANNIE 2000 (Smart Engineering System Design), St. Louis, MO, November 5-8, 2000.
- [C58] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Full Band Simulation of Hole Transport in 1-D Heterostructures", 27th international Symposium on Compound Semiconductors (ISCS), IEEE, (2000), Monterey, CA, Oct 2-5 (2000)
- [C57] Didier Keymeulen, Gerhard Klimeck, Ricardo Zebulum, Adrian Stoica, Carlos Salazar-Lazaro, "EHWPack: A Parallel Software/Hardware Environment for Evolvable Hardware", Genetic and Evolutionary Computation Conference (GECCO-2000), July 8-12, 2000, Las Vegas, Nevada USA.
- [C56] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Atomistic Simulation of Quantum Dots Including Strain and Bandstructure", Electronic Materials Conference, Denver, CO, June 21-23, 2000
- [C55] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Atomistic Simulation of Quantum Dots Including Strain and Bandstructure and Full Band Simulation of Hole Transport in 1-D Heterostructures", International Workshop on Computational Electronics, Glasgow, Scotland, UK, May 22-25, 2000
- [C54] Gerhard Klimeck, R. Bowen, Timothy Boykin, Tom Cwik, "sp3s* and sp3d5s* Tight-Binding Parameter Sets for GaAs, AlAs, InAs, GaSb, AlSb, InSb, GaP, AlP, and InP for quantum dot simulations", March Meeting of the American Physical Society, Minneapolis, MN, March 20-24, 2000
- [C53] Gerhard Klimeck, R. Bowen, Timothy Boykin, Tom Cwik, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Nanospace 2000, Houston, TX Jan. 23-28, 2000
- [C52] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Nanoelectronic Device Calculation from an atomistic point of view: Empirical Tight-Binding Models for Semiconductor Heterostructures", Nanospace 2000, Houston, TX Jan. 23-28, 2000
- [C51] Gerhard Klimeck, R. Bowen, Timothy Boykin, "Development of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Surfaces and Interfaces in Mesoscopic Devices, Maui, Hawaii, Dec. 5-10, 1999.
- [C50] Gerhard Klimeck, R. Bowen, "Nanoelectronic Modeling (NEMO 1-D and NEMO 3-D)", Supercomputing 99, Portland Oregon, Nov. 13-19, 1999, demo exhibit in NASA booth.
- [C49] Tom Cwik, Gerhard Klimeck, "Genetically Engineered Microelectronic Infrared Filters", First NASA/DoD Workshop on Evolvable Hardware, July 19-21, 1999, Pasadena, CA.
- [C48] Gerhard Klimeck, Carlos Salazar-Lazaro, Adrian Stoica, Tom Cwik, "Genetically Engineered Nanoelectronics", First NASA/DoD Workshop on Evolvable Hardware, July 19-21, 1999, Pasadena, CA.
- [C47] Adrian Stoica, Gerhard Klimeck, Carlos Salazar-Lazaro, Didier Keymeulen, Anil Thakor, "Evolutionary design of electronic devices and circuits", Congress on Evolutionary Computation, Washington, D.C. July 6-9, 1999.
- [C46] Tom Cwik, Gerhard Klimeck, "Optimization of Microelectronic Devices for Sensor Applications", Micro and NanoTechnology 99, Pasadena, CA, April 12, 1999.
- [C45] Timothy Boykin, Lisa Gamble, Gerhard Klimeck, R. Bowen, "Valence-band warping in tight-binding models and its effect on heterostructure electronic states", American Physical Society Centennial Meeting, March 22-26, 1999, Atlanta, GA.
- [C44] Gerhard Klimeck, R. Bowen, Tom Cwik, Timothy Boykin, "Tight Binding sp3s* Material Parameters from Genetic Algorithms", American Physical Society Centennial Meeting, March 22-26, 1999, Atlanta, GA.

- [C43] Tom Cwik, Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", IEEE Aerospace Conference, March 15-19, 1999, Aspen CO.
- [C42] Gerhard Klimeck, Carlos Salazar-Lazaro, Adrian Stoica, Tom Cwik, Timothy Boykin, "Material Parameter Analysis using quantum mechanical electron transport simulations and genetic algorithms.", Material Research Society Meeting, Materials in Space - Science, Technology, and Exploration November 29 - December 2, 1998, Boston MA.
- [C41] Gerhard Klimeck, Carlos Salazar-Lazaro, Adrian Stoica, Tom Cwik, "Genetically Engineered Nanostructure Device", NanoSpace98, International Conference on Integrated Nano/Microtechnology for Space Applications. Nov. 1-6, 1998, Houston, TX.

Work Performed at UTD/TI (26 Total)

- [C40] Gerhard Klimeck, Daniel Blanks, Roger Lake, Timothy Boykin, R. Bowen, "NEMO: A 1-D Heterostructure Design Tool", March Meeting of the American Physical Society, March 16-20, Los Angeles, CA (1998).
- [C39] Timothy Boykin, Gerhard Klimeck, Roger Lake, R. Bowen, "The Well-Tempered Tight-Binding Model: Many Parameters Do Not Necessarily Imply Flexibility", March Meeting of the American Physical Society, March 16-20, Los Angeles, CA (1998).
- [C38] Harold Grubin, Gerhard Klimeck, Daniel Blanks, "NEMO-PC", 1997 DARPA ULTRA Electronics and Advanced MicroElectronics Program Review, October 26-31, Santa Fe, NM (1998).
- [C37] Gerhard Klimeck, Roger Lake, Daniel Blanks, "Numerical Approximations to the Treatment of Interface Roughness Scattering in Resonant Tunneling Diodes", Surfaces and Interfaces of Mesoscopic Devices, December 7-12, 1997, Kaanapali, Maui, Hawaii.
- [C36] Roger Lake, Gerhard Klimeck, Daniel Blanks, "Interface Roughness and Polar Optical Phonon Scattering in InGaAs/AlAs/InAs RTDs", Surfaces and Interfaces of Mesoscopic Devices, December 7-12, 1997, Kaanapali, Maui, Hawaii.
- [C35] R. Bowen, Chenjing Fernando, Gerhard Klimeck, Amitava Chatterjee, Daniel Blanks, Roger Lake, Jerry Woodall, Joseph Davis, Mak Kulkarni, Sunil Hattangady, Cheng-Kok Koh, "Physical Oxide Thickness extraction and Verification using Quantum Mechanical Simulation", IEEE IEDM, Washington, DC, Dec. 8-10 1997.
- [C34] J. Wagt, Alan Seabaugh, Gerhard Klimeck, Shaikh Ahmed, Timothy Boykin, R. Bowen, R. Lake, "Ultralow current density RTDs for tunneling-based SRAM", IEEE International Symposium on Compound Semiconductors, San Diego, CA, Sept. 8-11 1997.
- [C33] Roger Lake, Berinder Brar, Glen Wilks, Alan Seabaugh, Gerhard Klimeck, "Resonant Tunneling in Disordered Systems such as SiO₂/Si/SiO₂", IEEE International Symposium on Compound Semiconductors, San Diego, CA, Sept. 8-11 1997.
- [C32] Daniel Blanks, Gerhard Klimeck, Roger Lake, R. Bowen, Manhua Leng, Chenjing Fernando, William Frensley, Dejan Jovanovic, "NEMO: General Release of a New Comprehensive Quantum Device Simulator", IEEE International Symposium on Compound Semiconductors, San Diego, CA, Sept. 8-11 1997.
- [C31] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, Timothy Boykin, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, William Frensley, Ted Moise, Y. Kao, "The effects of self-consistent charging, incoherent scattering and realistic bandstructure on the non-equilibrium transport of electrons in resonant tunneling diodes.", Nonequilibrium Carrier Dynamics in Semiconductors (HCIS-10), Berlin, Germany, July 28 - August 1 1997.
- [C30] Roger Lake, Gerhard Klimeck, R. Bowen, Dejan Jovanovic, "Numerical Modeling of Non-Equilibrium Incoherent Scattering in Quantum Devices", Nonequilibrium Carrier Dynamics in Semiconductors (HCIS-10), Berlin, Germany, July 28 - August 1 1997.
- [C29] Gerhard Klimeck, Timothy Boykin, R. Bowen, Roger Lake, Daniel Blanks, Ted Moise, Y. Kao, William Frensley, "Quantitative Simulation of Strained InP-Based Resonant Tunneling Diodes", The 1997 55th IEEE Device Research Conference Digest, IEEE, NJ (1997).
- [C28] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, Manhua Leng, Chenjing Fernando, William Frensley, Dejan Jovanovic, "NEMO: A General Purpose 1-D Quantum Device Simulator", Texas Instruments Corporate Research and Development Conference Aug. 19-20, 1996.
- [C27] Roger Lake, Gerhard Klimeck, "Experimentally Verified Quantum Device Simulations Based on Multiband Models, Hartree Selfconsistency, and Scattering Assisted Charging", 1996 54th IEEE Device Research Conference, Santa Barbara, CA, June 24-26, 1996.
- [C26] Gerhard Klimeck, R. Bowen, Roger Lake, Daniel Blanks, Manhua Leng, Dejan Jovanovic, Chenjing Fernando, William Frensley, Paul Sotirelis, "NEMO: A General Purpose 1-D Quantum Device Simulator", International Conference on Quantum Devices and Circuits, Alexandria, Egypt, June 4-8, 1996.
- [C25] Daniel Blanks, Gerhard Klimeck, Roger Lake, Manhua Leng, Dejan Jovanovic, Paul Sotirelis, "NanoElectronic Modeling (NEMO)", March Meeting of the American Physical Society, St. Louis, March 1996.

- [C24] Roger Lake, Gerhard Klimeck, Chenjing Fernando, R. Bowen, Ted Moise, Y. Kao, "Interface Roughness and Polar Optical Phonon Scattering in Resonant Tunneling Devices", Third International Symposium on new Phenomena in Mesoscopic Structures, Maui, HI, Dec. 4-8, 1995.
- [C23] Gerhard Klimeck, Roger Lake, R. Bowen, Chenjing Fernando, William Frensley, "Energy Grid Generation for Resolving and Integrating Ultra-Fine Resonances in Quantum Device Simulation", International Workshop on Computational Electronics, Tempe, AZ, Oct. 30 - Nov. 2, 1995.
- [C20] Roger Lake, Gerhard Klimeck, R. Bowen, Dejan Jovanovic, Paul Sotirelis, William Frensley, "A Generalized Tunneling Formula for Quantum Device Modeling", Tempe, AZ, International Workshop on Computational Electronics, Oct. 30 - Nov. 2, 1995.
- [C19] Dejan Jovanovic, Roger Lake, Gerhard Klimeck, Daniel Blanks, Paul Sotirelis, R. Bowen, Chenjing Fernando, Manhua Leng, "Quantum Mechanical Simulation Tools For Semiconductor Devices", Texas Instruments Corporate Research and Development Conference, Aug. 1995
- [C18] R. Bowen, William Frensley, Gerhard Klimeck, "Efficient Multiband I-V simulations for quantum devices nv", IEEE Cornell Device Conference, Ithaca, NY Aug. 7-9, 1995.
- [C17] Gerhard Klimeck, Roger Lake, R. Bowen, William Frensley, Daniel Blanks, "Nanoelectronic Modeling (NEMO)", 1995 53rd Device Research Conference, Charlottesville, VA, June 19-21, 1995.
- [C16] William Frensley, Chenjing Fernando, R. Bowen, Gerhard Klimeck, "Modeling Tools for the Development of Quantum and Conventional Semiconductor Heterostructure Devices", Government Microcircuit Application Conference, San Diego, CA, Nov. 1994.
- [C15] Gerhard Klimeck, Roger Lake, R. Bowen, William Frensley, "Treatment of Continuum and Discrete Quantum States in the Leads of Resonant Tunneling Diodes", March meeting of the American Physical Society, San Jose, March 19-24, 1994.

Work Performed in Graduate School (14 Total)

- [C14] Gerhard Klimeck, Roger Lake, Supriyo Datta, "The Phonon Peak in Resonant Tunneling Diodes", Second International Symposium on Quantum Confinement, Electrochemical Society, San Francisco, May 22-27, 1994.
- [C13] Gerhard Klimeck, Roger Lake, Supriyo Datta, Garnett Bryant, "High Bias Transport through Quantum Dots", Second International Symposium on Quantum Confinement, Electrochemical Society, San Francisco, May 22-27, 1994.
- [C12] Gerhard Klimeck, Roger Lake, Supriyo Datta, Garnett Bryant, "High Bias Transport through Quantum Dots", Workshop on Surfaces and Interfaces, Hawaii, April 24-29, 1994.
- [C11] Gerhard Klimeck, Roger Lake, Garnett Bryant, Supriyo Datta, "High Bias Transport through Quantum Dots", March meeting of the American Physical Society, Pittsburgh, March 20-25, 1994.
- [C10] Gerhard Klimeck, Guanlong Chen, Supriyo Datta, "Conductance Spectroscopy in Coupled Quantum Dots", March meeting of the American Physical Society, Pittsburgh, March 20-25, 1994.
- [C9] Gerhard Klimeck, Guanlong Chen, Roger Lake, Supriyo Datta, "Quantum Transport in Single and Coupled Quantum Dots", Texas Instruments Quantum Device Modeling Workshop, Dallas, Feb. 4-6, 1994.
- [C8] Supriyo Datta, Gerhard Klimeck, Roger Lake, "Two Approaches to Resonant-Tunneling with Inelastic Scattering: A Comparison", March meeting of the American Physical Society, Seattle, March 22-26, 1993.
- [C7] Roger Lake, Gerhard Klimeck, Supriyo Datta, "Rate Equations from the Keldysh Formalism Applied to the Phonon Peak in Resonant Tunneling Diodes", March meeting of the American Physical Society, Seattle, March 22-26, 1993.
- [C6] Roger Lake, Gerhard Klimeck, Supriyo Datta, "Elastic and Inelastic Scattering in the Coulomb Blockade Regime", March meeting of the American Physical Society, Seattle, March 22-26, 1993.
- [C5] Roger Lake, Gerhard Klimeck, Supriyo Datta, "Rate equations from the Keldysh Formalism Applied to the Phonon Peak in Resonant-Tunneling Diodes", Second International Symposium on New Phenomena in Mesoscopic Structures, Hawaii, Dec. 7-11, 1992.
- [C4] Roger Lake, Gerhard Klimeck, Supriyo Datta, "Quantum devices: Where Scattering May Enhance Transport", Purdue Electrical Engineering Industrial Institute Fall Workshop, LEDs, HBTs, MBEs, ETC.: What's New in Solid State, October 18-20, 1992.
- [C3] Roger Lake, Gerhard Klimeck, Supriyo Datta, "A Quantum Device Simulator Based on the Non-Equilibrium Green Function Equations of Keldysh, Kadanoff, and Baym", International Workshop on Computational Electronics, Beckman Institute of the University of Illinois; May 28-29, 1992.
- [C2] Gerhard Klimeck, Ce Chen, Daniel Elliott, "Nonlinear Interactions Involving The Real Gaussian Field", Twelfth International Conference on Atomic Physics, University of Michigan, Ann Arbor, July 1990.
- [C1] C. Xie, Gerhard Klimeck, Ce Chen, Daniel Elliott, "Nonlinear Interactions Involving The Real Gaussian Field", Optical Society of America Annual Meeting, 1990.

TECHNICAL REPORTS (36+, STOPPED TRACKING)**Work Performed at Purdue (16 total)**

The nanoHUB/NCN annual reports had typically taken **2 months of preparations** for me personally. These reports were typically distributed to funding agencies. I stopped tracking these reports in 2015

Some of the JPL reports resulted in NASA Space act awards

- [T36] Gerhard Klimeck, "ATOMISTIC MODELING OF FUTURE NANOSCALE ELECTRONIC DEVICES WITH NEMO5", Blue waters 2015 annual report
- [T35] Gerhard Klimeck, Michael McLennan, George Adams III., "Network for Computational Nanotechnology", Annual Report, April 2011
- [T34] Gerhard Klimeck, Michael McLennan, George Adams III., "Network for Computational Nanotechnology", Annual Report, May 2010
- [T33] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, George Adams III., "Network for Computational Nanotechnology", Annual Report, May 2009
- [T32] Gerhard Klimeck, Mark Lundstrom, Cheng-Kok Koh, Timothy Boykin, Venkataramanan Balakrishnan, "Device Simulation at the Scaling Limit and Beyond", Semiconductor Research Corporation - Deliverables Report: Research ID 1374 - Task IDs: 1374.001, 1374.002, 1374.003, December 2008.
- [T31] Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "Network for Computational Nanotechnology", Annual Report, May 2008.
- [T30] Hoon Ryu, Gerhard Klimeck, "Contact Block Reduction Method for transport in Multimillion Atom Systems", Annual Research report to NSF, April 1, 2008.
- [T29] Gerhard Klimeck, Mark Lundstrom, Cheng-Kok Koh, Timothy Boykin, "Device Simulation at the Scaling Limit and Beyond", Semiconductor Research Corporation - Deliverables Report: Research ID 1374 - Task IDs: 1374.001, 1374.002, 1374.003, December 2007.
- [T28] Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "Network for Computational Nanotechnology", Annual Report, May 2007.
- [T27] Jonathan Dowling, Gerhard Klimeck, "Final Report on ECCS/NSF Workshop on Quantum, Molecular and High Performance Modeling and Simulation for Devices and Systems", Community Report on NSF workshop
- [T26] Gerhard Klimeck, Mark Lundstrom, Cheng-Kok Koh, Timothy Boykin, "Device Simulation at the Scaling Limit and Beyond", Semiconductor Research Corporation - Deliverables Report: Research ID 1374 - Task IDs: 1374.001, 1374.002, 1374.003, December 2006.
- [T25] Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "Network for Computational Nanotechnology", Annual Report, May 2006.
- [T24] Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "Network for Computational Nanotechnology", Annual Report, May 2005.
- [T23] Mark Lundstrom, Gerhard Klimeck, Sebastien Goasguen, Michael McLennan, Renato Figueiredo, Jose Fortes, "The Network for Computational Nanotechnology: A Global Infrastructure for Researchers, Educators, and Students", JIUMRS Facets, Vol. 4, Num. 2, pp. 1-7, April 2005.
- [T22] Seungwon Lee, Fabiano Oyafuso, Paul Allmen, Gerhard Klimeck, "Efficient boundary condition for embedded semiconductor nanostructure modeling", Jan. 4, 2005, NTR-41155, JPL New Technology Report.
- [T21] Mark Lundstrom, Gerhard Klimeck, "Network for Computational Nanotechnology", Annual Report, May 2004.

Work Performed at JPL (15 Total)**Some of the JPL reports resulted in NASA Space act awards**

- [T20] Gerhard Klimeck, Fabiano Oyafuso, Hook Hua, "XML-based C++ Code Generation for User Interface Integration", Oct. 8, 2002, NTR 30844, JPL New Technology Report.
- [T19] Gerhard Klimeck, E. Tisdale, Fabiano Oyafuso, Hook Hua, "Nanoelectronic Modeling (NEMO 3-D) upgrade to no license restrictions", Oct. 8, 2002, NTR 30843, JPL New Technology Report.
- [T18] Thomas Cwik, Akos Czikmantory, Fabiano Oyafuso, Gerhard Klimeck, Hook Hua, Edward Vinyard, "WIGLAF (A Web Interface Generator and Legacy Application Façade)", Oct. 8, 2002, NTR 30842, JPL New Technology Report.
- [T17] Gerhard Klimeck, "Structure Based simulator Input using tcl/tk", Oct. 3, 2002, NTR 30835, JPL New Technology Report.
- [T16] Gerhard Klimeck, E. Tisdale, Fabiano Oyafuso, R. Bowen, "Parallel Complex Hermitian Sparse Matrix Eigensolvers", Oct. 3, 2002, NTR 30834, JPL New Technology Report.
- [T15] Gerhard Klimeck, Gary Yagi, "Quality Control of Tiepoints Computed from Image Correlation", April 1, 2002, NTR 30632, JPL New Technology Report.
- [T14] Gerhard Klimeck, Robert Deen, Michael McAuley, Eric DeJong, "Parallel Algorithms for Near-Realtime Image Correlation", April 1, 2002, NTR 30631, JPL New Technology Report.

- [T13] Gerhard Klimeck, Robert Deen, Michael McAuley, "Parallel Algorithms for Near-Realtime Mosaic Generation", April 1, 2002, NTR 30630, JPL New Technology Report.
- [T12] Gerhard Klimeck, Fabiano Oyafo, R. Bowen, Timothy Boykin, "Nanoelectronic Modeling 3-D (NEMO 3-D) upgrade", Jan. 6, 2002, NTR 30520, JPL New Technology Report.
- [T11] Gerhard Klimeck, "Tighgen - genetic algorithm-based tight binding parameter generation", Oct. 3, 1999, NTR 20877, JPL New Technology Report.
- [T10] Gerhard Klimeck, "Nanotechnology", Annual report of the Center for Integrated Space Microsystems (CISM) 1999.
- [T9] Thomas Cwik, Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", Dec. 16, 1998, NTR 20625, JPL New Technology Report.
- [T8] Gerhard Klimeck, "JPL NEMO, Benchmarks including Compiler-Based Parallelization", Sept. 23, 1998, NTR 20552, JPL New Technology Report.
- [T7] Gerhard Klimeck, "JPL NEMO extension for Hole transport", Aug. 1998, JPL New Technology Report.
- [T6] Gerhard Klimeck, "NEMO Benchmarks on SUN, HP, SGI, and Intel Pentium II",

Work Performed at UTD/TI (2 Total)

These 2 technical reports deliver the full 3,000+ page NEMO documentation.

- [T5] Gerhard Klimeck, Roger Lake, Daniel Blanks, "NEMO 3.0 User's, Theory and Technical Guide", Raytheon Corporation (1997)
- [T4] Gerhard Klimeck, Roger Lake, Daniel Blanks, "NEMO 2.0 User's and Theory Guide", Texas Instruments Incorporated, 1995.

Work Performed in Graduate School (3 Total)

- [T3] Gerhard Klimeck, "Electron-Phonon and Electron-Electron Interactions in Quantum Transport", Technical Report TR-EE 94-7, Purdue University, May 1994.
- [T2] Gerhard Klimeck, Roger Lake, Michael McLennan, Supriyo Datta, "QUEST User's Manual", Technical Report TR-EE 93-17, Purdue University, April 1993.
- [T1] Michael McLennan, Gerhard Klimeck, Supriyo Datta, "SQUALID-2D: Version 1.0 and 1.1, A Guide for the User", Technical Report TR-EE 91-15, Purdue University, April 1991.

INVITED SEMINARS (182 +9 TOTAL)**Work Performed at Purdue (145 +9 total)**

- [S191] Jinying Jessica Wang, Hong-Yang Lin, Dain Kang, Dmitri Nikonov*, Gerhard Klimeck, "Impact of Intel's Industrial Membership at the Network for Computational Nanotechnology (NCN/nanoHUB): 1) Adoption of NEMO (full atomistic quantum transport) into the TCAD pipeline, 2) global user impact, and 3) recent explorations of Spin-Orbit-Torque Materials", Intel Corporation Seminar, Nov. 30, 2022
- [S190] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", Presentation in Purdue Supercomputing Booth, Supercomputing Conference SC22, Dallas TX, Nov. 14, 2022
- [S189] Gerhard Klimeck, "Semiconductor workforce development through immersive simulations on nanoHUB.org", University of Texas At Dallas, TX, Nov. 13, 2022, Host. Prof. VanDerBerghe
- [S188] Gerhard Klimeck, "Semiconductor workforce development through immersive simulations on nanoHUB.org", University of Texas Austin, Host Prof. Sanjay Bannerjee, Oct. 28, 2022
- [S187] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", SLAC Colloquium, Host Steve Eglash, Oct. 25, 2022
- [S186] Gerhard Klimeck, "nanoHUB.org – always "on" New Paradigms in Global Scientific Knowledge Transfer, Publishing, and Assessment", Purdue-Taiwan Student Exchange workshop, June 29, 2022.
- [S185] Gerhard Klimeck, Tanya Faltens, Daniel Mejia, Alejandro Strachan, Lynn Zentner, Michael Zentner "Semiconductor workforce development through immersive simulations on nanoHUB.org", Departmental Seminar series at the Advanced Materials Division in Instituto Potosino de Investigación Científica y Tecnológica (IPICYT), San Luis Potosí, Mexico, May 5, 2022, Host. Prof. Braulio Gutierrez Medina
- [S184] Gerhard Klimeck, Tanya Faltens, Daniel Mejia, Alejandro Strachan, Lynn Zentner, Michael Zentner, "Semiconductor workforce development through immersive simulations on nanoHUB.org", National Nanotechnology Coordination Office (NNCO) Seminar, April 27, 2023,
- [S183] Gerhard Klimeck, "nanoHUB overview", Ohio State University ECE/MSE Seminar, April 5, 2023, Host Prof. Wolfgang Windl
- [S182] Gerhard Klimeck, "nanoHUB Integration into Semiconductor Education", Air Force Institute of Technology (AFIT), Nov. 3, 2021, Host Prof. Timothy Wolfe
- [S181] Gerhard Klimeck, "Challenges at the Frontier of Modeling", Microsystems Exploratory Council, Spring Meeting, April 7-8. Host Dr. George Thompson,
- [S180] Muhammad Alam, Joerg Appenzeller, Zhihong Chen, Supriyo Datta, Sumeet Gupta, David Janes, Gerhard Klimeck, Dana Weinstein, Pramey Upadhyaya, Peter Ye, "Purdue Microelectronics/Nanotechnology Webinar", DOE Crane Webinar, Purdue Westgate, May 12, 2021.
- [S179] Gerhard Klimeck, "Cohesion & Story Telling - My Recipe", Purdue University, EVPR's FLAIR Program (Faculty Leadership Academy for Interdisciplinary Research), Feb 10, 2020, Host: Prof. Carrie Berger
- [S178] Gerhard Klimeck, "The single-atom transistor: How it was created and what it may mean for the future", Ohio State University, Nov. 1, 2019, Host. Prof. Wolfgang Windl
- [S177] Gerhard Klimeck, "A Single Atom Transistor and Global Impact on Research and Education through nanoHUB.org", Serbian Academy of Science, Host: Veljiko Milutinovic, Member of Academy, June 17, 2019
- [S176] Gerhard Klimeck, "Cohesion & Story Telling - My Recipe", Purdue University, EVPR's FLAIR Program (Faculty Leadership Academy for Interdisciplinary Research), January 28, 2019, Host: Prof. Carrie Berger
- [S175] Gerhard Klimeck, "Cohesion & Story Telling - My Recipe", University of Hamburg, Jan. 24, 2019, Host. Prof. Robert Blick
- [S174] Gerhard Klimeck, "Bandstructure effects in nano devices – Examples using NEMO5", Silvaco Seminar, promoted and broadcast globally by Silvaco Inc., Dec. 12, 2018
- [S173] Gerhard Klimeck, "A Single Atom Transistor - The Ultimate Scaling Limit", Hamburg University, Nov. 27, 2018, Host: Prof. Dr. Robert Blick
- [S172] Gerhard Klimeck, Tillmann Kubis, Michael Povolotskyi, James Fonseca, Bozidar Novakovic, Tarek Ameen, James Charles, ChiYi Chen, Yanchen Chu, Junzhe Geng, Xinchun Guo, Kaspar Haume, Yu He, Ganesh Hegde, Hesam Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Lemus, Daniel Mejia, Kai Miao, Samik Mukherjee, Seung Park, Ahmed Reza, Mehdi Salmani, Prasad Sarangapani, Parijat Sengupta, Saima Sharmin, Yaohua Tan, Archana Tankasala, Daniel Valencia, KuangChung Wang, Evan Wilson, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Korea Institute of Science and Technology (KIST), Seoul, July 9 2018, Host. Dr. Kwang-Reol Lee
- [S171] Tillmann Kubis, Michael Povolotskyi, James Fonseca, Bozidar Novakovic, Tarek Ameen, James Charles, ChiYi Chen, Yanchen Chu, Junzhe Geng, Xinchun Guo, Kaspar Haume, Yu He, Ganesh Hegde, Hesameddin Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Lemus, Daniel Mejia, Kai Miao, Samik Mukherjee, Seung Park, Ahmed Reza, Mehdi Salmani, Prasad Sarangapani, Parijat Sengupta, Saima Sharmin, Yaohua Tan, Archana Tankasala, Daniel Valencia, KuangChung Wang, Evan Wilson, "NEMO5, a Parallel, Multiscale,

- Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Korea Advanced Institute of Science and Technology (KAIST), Daejeon, July 6 2018, Host Prof. Mincheol Shin
- [S170] Gerhard Klimeck, "Your Career Choices: A Perspective from 24 years in Industry, National Laboratory, and Academia", Summer Undergraduate Research Fellowship Seminar, June 20, 2018. Host: Dr. Tanya Faltens
- [S169] Gerhard Klimeck, "nanoHUB in a Nutshell: Delivering New Paradigms in Education and Research", Undergraduate Research Fellowship Seminar, May 22, 2018. Host: Dr. Tanya Faltens
- [S168] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Fudan University, July 6 2016, Host: Prof. Prof. Jian Shen and Prof. Jiang Xiao
- [S167] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Fudan University, Shanghai, China, July 1, 2016
- [S166] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Behang University, July 1, 2016, Host: Prof. Lang Zang
- [S165] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Peking University, June 27, 2016, Host: Prof. Xiaoyan Liu
- [S164] Gerhard Klimeck, "nanoHUB: always ON 24/7", USC/ISI Lectures on Cyberinfrastructure, The USC Information Sciences Institute, Marina Del Rey, CA, Host: Ewa Deelman, June 7, 2016
- [S163] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Lund University Lecture Series, Lund, Sweden, May 12, 2016
- [S162] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", UCSB Distinguished Lectures 2015-2016, Host: Prof. Mark Rodwell, June 6th, 2016
- [S161] Gerhard Klimeck, "NEMO5, a Parallel Multiscale, Multiphysics Nanoelectronics Modeling Tool", STARnet ACCEL e-Workshop Series, Host: Prof. Alan Seabaugh, February 24, 2016
- [S160] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool", TSMC, Host: WilmanTsai, February 29, 2016
- [S159] Gerhard Klimeck, "The Single-Atom Transistor: How it was Created and What it May Mean for the Future", University of Udine, Host: Prof. David Esseni, July 23, 2015
- [S158] Gerhard Klimeck, "The Single-Atom Transistor: How it was Created and What it May Mean for the Future and Mythbusting Today's Nanotechnology", Hosts Prof. Gianluca Fiori and Giuseppe Iannacone, July 20, 2015
- [S157] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool", Technical University Vienna, Host Prof. Hans Kosina, June 19, 2015
- [S156] Gerhard Klimeck, "Development of the NEMO tool suite: from basic physics to real industrial devices and to global impact on nanoHUB.org", Technical University Munich, Host: Prof. Gerhard Wachutka, June 17, 2015
- [S155] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics", University of Duisburg-Essen, Host Dr. Werner Prost, June 12, 2015
- [S154] Gerhard Klimeck, "Mythbusting Today's Nanotechnology", Ruhr-University Bochum, Host Prof. Ulrich Kunze, June 8, 2015
- [S153] Gerhard Klimeck, "Talk-run-de mit Ken-nern der Fa-kul-tät", Ruhr-University Bochum, Germany, Host Dr. Robert Grosche, June 5, 2015
- [S152] Gerhard Klimeck, "Mythbusting : Today's Nanotechnology & Knowledge Transfer through nanoHUB.org", Purdue University, ECET 321, Host: Prof. Helen McNally. April 21, 2015
- [S151] Gerhard Klimeck, Mehdi Salmani-Jelodar, SungGeun Kim, Saumitra Mehrotra, Abhijeet Paul, Hoon Ryu, Sunhee Lee, Yu He, Daniel Lemus, Bozidar Novakovic, Tillmann Kubis, Michael Povolotskyi, "Development of the NEMO Tool Suite From Basic Physics to Real Devices and to Global Impact on nanoHUB.org", Arizona State, Electrical Engineering Advanced Semiconductor Device Class, Host: Prof. Dragica Vasileska, April 20, 2015
- [S150] Gerhard Klimeck, "The single-atom transistor: How it was created and what it may mean for the future", ECEGSA - Purdue ECE Graduate student association seminar, March 25, 2015
- [S149] Gerhard Klimeck, Michael McLennan, "Elevating nanoHUB to the Next Level: Vision and Status 2014", NSF seminar, Arlington Virginia, Oct 16, 2014
- [S148] Gerhard Klimeck, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool", Teleseminar to GLOBAL FOUNDRIES, Nov. 19, 2014, Host Dr. Sahu Bhagawan

- [S147] Gerhard Klimeck, "Elevating nanoHUB to the Next Level - Vision and Status 2014", eScience workshop, MURPA, Melbourne, Australia, Sept 4th 2014 (remote)
- [S146] Gerhard Klimeck, "Mythbusting Knowledge Transfer with nanoHUB.org", Yegor Gaidar Summer Leadership Program July 15, 2014, Burton D. Morgan Center for Entrepreneurship, West Lafayette, IN
- [S145] Gerhard Klimeck, "Purdue University: An overview, the home of nanoHUB, and the Klimeck research group", Ruhr University Bochum, Germany, June 27, 2014, Host: Prof. Aydin Sezgin
- [S144] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org ", Purdue Postdoc Association Keynote address, June 5, 2014, West Faculty Lounge, Purdue Memorial Union, West Lafayette, IN
- [S143] Gerhard Klimeck, Michael Povolotskyi, Tillmann Kubis, Jim Fonseca, Bozidar Novakovic, Yu He, Daniel Mejia, Zhengping Jiang, SungGeun Kim, Saumitra Mehrotra, "NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool", Synopsys, Oct 18, 2013, Host: Dr. Victor Moroz
- [S142] Gerhard Klimeck, "Atomistic Modeling of Realistic Nanoelectronic Devices and nanoHUB tools", Philips - Lumileds, Oct 17, 2013, Host: Dr. Paco Leon.
- [S141] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer on nanoHUB.org", Yegor Gaidar Summer Leadership Program, Purdue University, July 15, 2013, Host: Timothy Peoples, Purdue Research Foundation
- [S140] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development ", Purdue SURF Summer Seminar, July 2, 2013, Host: Vicki Leavitt
- [S139] Gerhard Klimeck, "Career Advice Panel", Purdue SURF Summer Seminar, June 17, 2013, Host Vicki Leavitt
- [S138] Gerhard Klimeck, "The Ultimate Scaling Limit – A Deterministic Single Atom Transistor", University of Michigan, NNIN-C presentation, Feb 26, 2013, Prof. Najafi
- [S137] Gerhard Klimeck, "Web Platforms for Collaborative Research and Education: The Quantifiably Positive nanoHUB Impacts", Washington Philosophical Society, Washington DC, Cosmos Club, Feb 22, 2013, Host. Dr. Larry Millstein.
- [S136] Gerhard Klimeck, "nanoHUB", Purdue Presidents Council Back to School Event, Naples , FL, Feb 16, 2013
- [S135] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", Ruhr University Bochum, July 22, 2012
- [S134] Gerhard Klimeck, "The Single Atom Transistor", Purdue PUGWASH Seminar, November 27 2012
- [S133] Gerhard Klimeck, "The single-atom transistor: How it was created and what it might mean for the future", Mentor Graphics, Sponsored Dinner Event, San Jose, CA, Oct. 17, 2012
- [S132] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", Ruhr University Bochum, July 23, 2012, Host Prof. Ulrich Kunze
- [S131] Gerhard Klimeck, "The single-atom transistor: How it was created and what it might mean for the future", Mentor Graphics, Technology Development Group, Freemont, CA, Oct. 17, 2012
- [S130] Gerhard Klimeck, "Band-to-Band Tunneling Transistors", NCN Summer School, Nanoelectronics from the Bottom-Up, July 17, 2012
- [S129] Gerhard Klimeck, "nanoHUB.org: Mythbusting Scientific Knowledge Transfer", Monash eScience and Grid Engineering Laboratory, Monash University, Australia, Oct. 5, 2012, (via teleconference)
- [S128] Gerhard Klimeck, " Impurities: Atomistic, Multi-Scale, Multi-Physics Modeling of Extended Si Quantum Devices", NCN Summer School, Nanoelectronics from the Bottom-Up, July 17, 2012
- [S127] Gerhard Klimeck, "Band to Band Tunneling", 2012 NCN Summer School, Electronics from the Bottom Up, July 16-20, 2012
- [S126] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org", NCN Summer School, Nanoelectronics from the Bottom-Up, July 16, 2012
- [S125] Gerhard Klimeck, "Single Impurities", 2012 NCN Summer School, Electronics from the Bottom Up, July 16-20, 2012
- [S124] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development", Purdue SURF Summer Seminar, June 25, 2012, Host: Vicki Leavitt
- [S123] Gerhard Klimeck, "Atomistic Modeling of Realistic Nanoelectronic Devices and nanoHUB tools", Philips Lumiled, June 19, 2012, Host Dr. Paco Leon
- [S122] Gerhard Klimeck, "nanoHUB.org powered by HUBzero® – A Platform for Collaborative Research with Quantifiable Impact on Research and Education", University of Michigan, April 27, 2012. Host Prof. Daniel Atkins
- [S121] Krishna Madhavan, Gerhard Klimeck, Mihaela Vorvoreanu, Xin Chen, "Interactive large scale data analyses and visualization for learning", Student Learning and Analytics at Michigan Seminar Series. University of Michigan Provost Initiative on Learning Analytics. Ann Arbor, IN., October 19, 2012
- [S120] Gerhard Klimeck, Michael Povolotskyi, Tillmann Kubis, Hong-Hyun Park, Sebastian Steiger, Jim Fonseca, Jean Sellier, Seung Park, Yu He, Ganesh Hegde, SungGeun Kim, Mark Rodwell, "The Nanoelectronic Modeling Tool NEMO 5: Capabilities, Validation, and Application to Advanced Transistor Structures", MSD/FENA Teleseminar Series, Dec. 15 2011.

- [S119] Gerhard Klimeck, "nanoHUB.org powered by HUBzero® - A Platform for Collaborative Research with Quantifiable Impact on Research and Education", Tuesday, November 22, 2011, Arizona State University, host: Prof. Dragica Vasileska
- [S118] Gerhard Klimeck, "Million-Atom Electronic Structure Simulations for Realistically Large Si-Based Quantum Devices", Monday, November 21, 2011, Arizona State University, Host: Prof. Dragica Vasileska
- [S117] Gerhard Klimeck, "Modeling of Thermal and Electron Transport in Nano-Scale Devices", University of Duisburg Essen, Oct. 13, 2011, Host: Dr. Werner Probst
- [S116] Gerhard Klimeck, "nanoHUB.org powered by HUBzero® – A Platform for Collaborative Research with Quantifiable Impact on Research and Education", Network Science Center, School of Library and Information Science, Indiana University, Host. Prof. Katy Borner, Sep 12, 2011
- [S115] Gerhard Klimeck, "nanoHUB.org powered by HUBzero®: A Platform for Collaborative Research - Mythbusting Scientific Knowledge Transfer", Wright Patterson Air Force Base, Directorate RX, July 15, 2011, Host Dr. Andrey Voevodin
- [S114] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development", Purdue SURF Summer Seminar, June 2, 2011, Host: Vicki Leavitt
- [S113] Gerhard Klimeck, "Success Examples and Challenges of Multi-Scale and Multi-Expertise Modeling and Simulations", Department of Energy, Germantown, April 20, 2011, Host: Dr. Harriett Kung, Office of Basic Energy Sciences.
- [S112] Gerhard Klimeck, "nanoHUB.org: Impact on Research and Education, Suggested Usage Examples for NSU", Norfolk State University, May 11, 2011, Host Prof. Mikhail Noginov.
- [S111] Gerhard Klimeck, "nanoHUB.org - Future Cyberinfrastructure serving over 170,000 users today", NASA JPL, April 1, 2011, Host. Dr. Thomas Cwik.
- [S110] Gerhard Klimeck, "Atomistic Modeling and Simulation Tools for Nanoelectronics and their Deployment on nanoHUB.org, serving thousands of users", Universidad Nacional, Department of Chemistry, March 19, 9am, Bogota, Colombia, Catedra lecture to 1,400 students in Bogota and over 200 students nationwide via telecom. Host Prof. Alvaro Duarte Ruiz aduarter[at]unal.edu.co
- [S109] Gerhard Klimeck, "nanoHUB tutorial", Universidad de los Andes, Department of Electrical Engineering, March 18, 11am, Bogota, Colombia, Host Prof. Alba Avila Bernal
- [S108] Gerhard Klimeck, "Atomistic Modeling and Simulation Tools for Nano Transistors", Universidad Nacional, Department of Chemistry, March 17, 11am, Bogota, Colombia, Host Prof. Eduardo Alvarez.
- [S107] Gerhard Klimeck, "nanoHUB.org Operation Model", Purdue University, Burton Morgan Entrepreneurial Leadership Academy, Dec. 2, 2010, Host: Candiss Vibbet
- [S106] Gerhard Klimeck, "Atomistic Modeling and Simulation Tools for Nanoelectronics and their Deployment on nanoHUB.org", Arizona State University, Nov. 22 2010, Host: Prof. Steven Goodnick
- [S105] Gerhard Klimeck, "nanoHUB.org - Future Cyberinfrastructure serving over 150,000 users today", Lawrence Livermore National Laboratory, Nov. 3 2010, Host: Dr. Rob Long
- [S104] Gerhard Klimeck, Mathieu Luisier, Rajib Rahman, Seung Park, Hoon Ryu, Sunhee Lee, Neerav Kharche, Lloyd Hollenberg, Sven Rogge, Gabriel Lansbergen, "Atomistic Modeling of Ultra-Scaled Devices", Globalfoundries Workshop on III-V devices for high performance logic, Nov. 2 2010, Host: Dr. Witek Maszara.
- [S103] Gerhard Klimeck, "Atomistic Modeling and Simulation Tools for Nanoelectronics and their Deployment on nanoHUB.org", Purdue University, Department of Physics, Sept 10, 2010, Host: Prof. Michael Manfra
- [S102] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development", Purdue SURF Summer Seminar, July 1, 2010, Host: Vicki Leavitt
- [S101] Gerhard Klimeck, "Atomistic Modeling of Ultra-Scaled III-V, Si/Ge, Graphene, and Single Impurity Devices", Samasung Advanced Institute of Technology, SAIT, Aug. 16, 2010, Host: Dr. Jai Kwang Shin
- [S100] Gerhard Klimeck, "nanoHUB.org / NCN: Future Cyberinfrastructure serving over 90,000 users today & Rappture tool development", University of Rome Tor Vergata, Oct. 12 2009, Host: Prof. Aldo Di Carlo.
- [S99] Gerhard Klimeck, "moving towards atomistic 3-D quantum transport in nano-scale semiconductors", University of Rome Tor Vergata, Oct. 12 2009, Host: Prof. Aldo Di Carlo.
- [S98] Gerhard Klimeck, "Nanoelectronic Modeling: From Quantum Mechanics and Atoms to Realistic Devices", Ph.D. Short Course, University of Pisa, Oct. 5-9 2009, Host: Prof. Gianluca Fiori. 41 individual lecture elements - approximately 16 hours of lectures. All lectures to be published on nanoHUB.org.
- [S97] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development", Norfolk State University, Graduate Student Seminar, Sept. 21, 2009, Host: Prof. Suely Black.
- [S96] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development", Purdue University, ECE 694 Graduate Seminar Class, Aug. 27, 2009.
- [S95] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development", Purdue SURF Summer Seminar, July 28, 2009, Host: Vicki Leavitt.
- [S94] Gerhard Klimeck, "Your Career Choices after Graduate School and The Most-Neglected Item in your Career Development", Purdue SURF Spring Seminar, April 8, 2009, Host: Vicki Leavitt.

- [S93] Gerhard Klimeck, "Modeling and Simulation Tools for Nanoelectronics", University of Duisburg-Essen, Germany, 2:30pm, March 18., 2009, Host. Dr. Werner Prost and Prof. Tegude.
- [S92] Gerhard Klimeck, "Modeling and Simulation Tools for Nanoelectronics", Ruhr University Bochum, Germany, 10:15am, March 18., 2009, Host. Prof. Ulrich Kunze.
- [S91] Gerhard Klimeck, "Quantum Dots 101 and Quantum Dot Lab", Purdue, School of Technology, March 12., 2009, Host. Prof. Helen McNally.
- [S90] Gerhard Klimeck, "Introduction to Quantum Dots on nanoHUB.org", Purdue, School of Technology, Oct. 27, 2008, Host. Prof. Helen McNally.
- [S89] Gerhard Klimeck, "nanoHUB.org simulation tools ranging from semiconductor device education to nanoelectronic research", MIT, MSD Teleseminar Series, Oct. 9, 2008, Host. Prof. Judy Hoyt.
- [S88] Gerhard Klimeck, "nanoHUB.org - Future Cyberinfrastructure serving over 75,000 users today", Purdue-Silicon Valley Symposium, August 26, 2008, Host. Margarita Contreni.
- [S87] Gerhard Klimeck, "nanoHUB.org serving over 6,200 simulation users including NanoElectronic Modeling (NEMO and OMEN)", UT Dallas Seminar, August 22, 2008, Host: Prof. Eric Vogel.
- [S86] Gerhard Klimeck, "Atomistic Nanoelectronic Modeling - NEMO and OMEN", NCSA Director's Seminar, NCSA, University of Illinois Urbana Champaign, April 17, 2008, Host. Prof. Thom Dunning.
- [S85] Gerhard Klimeck, "Introduction to Quantum Dot Lab", Purdue University, School of Technology, Introduction to nanotechnology Course. march 6th, 2008. Host Prof. Helen McNally.
- [S84] Gerhard Klimeck, "Atomistic Modeling of Single Electron Quantum State Control in Silicon using NEMO 3-D", University of New South Wales, Physics Department, Centre for Quantum Electronics, March 3rd, 2008, Host Profs. Michelle Simmons and Bob Clark.
- [S83] Gerhard Klimeck, "Atomistic Quantum Transport in Realistically Extended Devices - nanowires and thin bodies", GRC / SRC Technology Transfer e-workshop, Feb. 21, 2008, Host Dr. Kwok Ng.
- [S82] Gerhard Klimeck, "Algorithms and Parallelization Approaches for Scaling to 23,000 Processors in Nanoelectronic Modeling (NEMO)", Purdue University SIAM student meeting, Feb 7, 2008. Host Mr. Maxim Naumov
- [S81] Gerhard Klimeck, "nanoHUB.org - Future Cyberinfrastructure serving over 26,000 users today", Oak Ridge National Lab, TN, Jan 9, 2008
- [S80] Gerhard Klimeck, "Atomistic NanoElectronic Modeling (NEMO) for Predictive 1D Out-of-Equilibrium Quantum Transport, and Disordered 3D Multi-Million Atom Electronic Structure", Oak Ridge National Lab, TN, Jan 8, 2008
- [S79] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", Northwestern University, Dec. 6, 2007
- [S78] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", Purdue University, School of Technology Student Seminar, Nov. 15, 2007
- [S77] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 25,000 users today", Ruhr University Bochum, Institute for Theoretical Electrical Engineering, Oct. 25, 2007, Hosts: Prof. Kunze and Brinkmann
- [S76] Gerhard Klimeck, "Engineering at the nanometer scale: Is it a new material or a new device?", Purdue University, Material Science and Engineering Seminar, Oct. 19, 2007, Host: Prof. Edwin Garcia.
- [S75] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 25,000 users today", Purdue University, Math Graduate Student Seminar, Oct. 19, 2007
- [S74] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 25,000 users today", Purdue University, Electrical and Computer Engineering Graduate Student Seminar, ECE694, Oct. 18, 2007, Host: Prof. P. Krause
- [S73] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 25,000 users today", Jet Propulsion Laboratory, Section 388 seminar, Pasadena CA, October 4, 2007. Host: Dr. Paul von Allmen
- [S72] Mark Lundstrom, Gerhard Klimeck, "The NCN and the nanoHUB", Lawrence Livermore National Laboratory, April 9, 2007, Host: Dr. Jeff Neaton.
- [S71] Michael McLennan, Gerhard Klimeck, "nanoHUB Demo and Usage Scenarios for Education", Purdue University, Electrical and Computer Engineering, EI2G: The ECE Instructional Innovation Group, March 6th, 2007, Host: Dr. Mark Johnsson.
- [S70] Gerhard Klimeck, "Atomistic Alloy Disorder in Nanostructures", Purdue University, NCN/INAC Tutorial Lecture Feb. 7, 2007, Host: NCN Student Leadership Council.
- [S69] Gerhard Klimeck, Martha Prada, "Electronic Structure of Si/InAs Composite Channels", University of Notre Dame, Electrical Engineering Department January 30, 2007, Host: Prof. Alan Seabaugh.
- [S68] Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "Network for Computational Nanotechnology", Semiconductor Research Corporation e-Workshop, Teleseminar, Nov. 17, 2006, Host: Jim Hutchby

- [S67] Gerhard Klimeck, "Atomistic Modeling of Ultra-Scaled Si/Ge Devices and Tool Deployment on nanoHUB.org", Samsung Advanced Institute of Technology, Seoul, Korea, October 27, 2006 Host: Dr. Jongsoeb Kim.
- [S66] Sebastien Goasguen, Gerhard Klimeck, Renato Figueiredo, Alain Roy, Krishna Madhavan, "The nanoHUB case: Cyberinfrastructure-enabled Virtual Organization", NSF / OCI (Office of Cyberinfrastructure) seminar, presentation to program directors, NSF, Washington DC, Oct 5, 2006. Host: Dr. Miriam Heller.
- [S65] Gerhard Klimeck, "Why is Nanotechnology Multidisciplinary? - A perspective of one EE", Purdue Multi-Disciplinary Engineering Program, Purdue University, Oct. 3, 2006, Host: Prof. Robin Adams
- [S64] Michael McLennan, Gerhard Klimeck, "HUB Technologies: A Fully Operational Collaborative Cyberinfrastructure for Research, Education, and Outreach Shared Infrastructure Available for You Today!", Cyber Center Seminar, Purdue University, School of Computer Science, September 25, 2006.
- [S63] Gerhard Klimeck, "nanoHUB overview to the MSD/MARCO Center", MIT MSD/MARCO center Teleseminar, Sept 21. 2006, Host: Prof. Judy Hoyd
- [S62] Michael McLennan, Gerhard Klimeck, "HUB Technologies: A Fully Operational Collaborative Cyberinfrastructure for Research, Education, and Outreach Shared Infrastructure Available for You Today! ", University wide presentation, Purdue University, Burton Morgan Center for Entrepreneurship, September 6, 2006.
- [S61] Michael McLennan, Gerhard Klimeck, "Usage Scenarios of and Vision for nanoHUB", Presentation to the teacher summer workshop initiated from SC05, Purdue University, STEW 322 Host: Krishna Madhavan, July, 12, 2006.
- [S60] Michael McLennan, Gerhard Klimeck, "nanoHUB.org: The Computational User Facility Complement to the Birk Nanotechnology Center", Nanotechnology Seminar Series, Purdue University, Birk 1001 June 5, 2006.
- [S59] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Krishna Madhavan, "nanoHUB.org online simulation and more - A fully operational Cyberinfrastructure that is transforming how Students learn, Teachers teach and Researchers and Engineers work ", Presentation to the Northwest Indiana Grid Steering committee, representatives of Purdue West Lafayette, Purdue-Calumet, and Notre Dame. Host Nathan Bohlmann, Chris Hoffmann, Access grid presentation, May 24, 2006.
- [S58] Krishna Madhavan, Sebastien Goasguen, Gary Bertoline, Gerhard Klimeck, "Next-generation Cyberinfrastructure for Bridging Discovery and Learning: nanoHUB", Revolutionizing science and education through cyberinfrastructure. Presentation at the Exploratorium Brown Bag Series, San Francisco, CA, May 18, 2006.
- [S57] Krishna Madhavan, Sebastien Goasguen, Gary Bertoline, Gerhard Klimeck, "Next-generation Cyberinfrastructure for Bridging Discovery and Learning: nanoHUB", April 11, 2006, 10:00am, NSF ENG Cyberinfrastructure Seminar, National Science Foundation, Washington DC, Host: Dr. Gary Gabriele.
- [S56] Gerhard Klimeck, "Computational and Algorithm Challenges for Nanoscience and Nanotechnology", March 1, 2006, 4:00pm, Purdue University, Jointly sponsored by Computing Research Institute (CRI), CSE Spring 2006 Seminar Series, Center for Computational and Applied Mathematics (CCAM), Host: Prof. Dongbin Xiu.
- [S55] Gerhard Klimeck, "Bandstructure in Nanoelectronics", Nov. 2, 2005, 10:30am, Purdue University Nanotechnology Tutorial Series.
- [S54] Gerhard Klimeck, "Development of a Nanowire Simulator at the Network for Computational Nanotechnologies (NCN)", Sept. 20, 2005, 4:30pm, Gerhard Mercator Universität Duisburg, Host: Dr. Werner Prost.
- [S53] Gerhard Klimeck, "Parallel Computing for Realistic Nanoelectronic Simulations", Sept. 12, 2005, 2:30pm, Purdue University, Nanotechnology Tutorial Series.
- [S52] Gerhard Klimeck, "Nano 101 - Quantum Dots", July 20, 2005, 11am, Purdue University, Summer Undergraduate Research Institute (SURI) Host: Prof. Michael Melloch.
- [S51] Gerhard Klimeck, Michael McLennan, "CVS Crashcourse", April 6, 9am, 2005, Purdue University, Burton Morgan Entrepreneurship Center, NCN Student Leadership workshop.
- [S50] Gerhard Klimeck, "NCN Cyberinfrastructure or How can your science software reach thousands of users?", April 6, 2pm, 2005, Purdue University, Burton Morgan Entrepreneurship Center, NCN Student Leadership workshop.
- [S49] Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN) or How can your educational modules contain interactive online simulation? ", Feb 28, 2005, National Center for Learning and Teaching in Nanoscale Science and Engineering, Northwestern University, Purdue University, web-based seminar, Host: Prof. Bob Chang.
- [S48] Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN)", Feb 28, 11am, 2005, Purdue University, STEW 320, ITaP user forum, Host: Steve Dunlop.
- [S47] Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN) and NEMO 1-D transport simulations ", Feb 18, 2005, Morgan State University, Baltimore, Host: Prof. Craig Scott.

- [S46] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, "The Network for Computational Nanotechnology (NCN) or How can your science software reach thousands of users? ", Feb 17, 2005, NIST, Gaithersburg, Host: Dr. David Seiler.
- [S45] Gerhard Klimeck, "NEMO 1-D: The First NEGF-based TCAD Tool and The Network for Computational Nanotechnology", Nov. 4, 2004, Purdue University, EE 694 Graduate Student Seminar, Host: Prof. P. Krause.
- [S44] Gerhard Klimeck, Mark Lundstrom, Sebastien Goasguen, "The Network for Computational Nanotechnology Cyber-Infrastructure and Grid Computing for Nanotechnology Exploration and Education", Sept. 21, 2004, Purdue University, IEEE Computer Society, Host: Mr. Greg Veldman.
- [S43] Gerhard Klimeck, "Computational Nanoelectronics: Towards Design, Analysis, and Fundamental Limits - Development of the Nanoelectronic Modeling Tool NEMO", Sept. 1, 2004, Walter Schottky Institute, Garching, Munich, Host: Prof. Peter Vogl.
- [S42] Gerhard Klimeck, "Computational Nanoelectronics: Towards Design, Analysis, Synthesis, and Fundamental Limits.", August 30, 2004, Gwangju Institute of Technology (GIST), South Korea, Host: Prof. Youngjoo Chung.
- [S41] Gerhard Klimeck, "NEMO 1-D: A NEGF-based CAD Tool, Interactive lecture and software demo.", Lecture on June 14, 2004, Summer School: Introduction to Computational Nanotechnology, June 7-18, 2004, Beckman Institute, University of Illinois at Urbana-Champaign, Host: Prof. Umberto Ravaioli.
- [S40] Gerhard Klimeck, "Numerical Aspects of NEGF: The Recursive Green Function Algorithm", Lecture on June 14, 2004, Summer School: Introduction to Computational Nanotechnology, June 7-18, 2004, Beckman Institute, University of Illinois at Urbana-Champaign, Host: Prof. Umberto Ravaioli.
- [S39] Gerhard Klimeck, "Development of the Nanoelectronic Modeling Tool (NEMO): Towards Design, Analysis, Synthesis, and Fundamental Limits", April 15, 2004, Ball State University, Center for Computational Nanoscience (CCN), Host: Prof. Jin Feng.
- [S38] Gerhard Klimeck, "HPC Challenges for NanoElectronic Modeling (NEMO)s", March 5, 2004, Purdue University, Computing Research Institute (CRI) Advisory Group, Host: Prof. Chris Hoffmann.

INVITED SEMINARS (WORK PERFORMED AT JPL) (25 TOTAL)

- [S37] Gerhard Klimeck, "Development of NEMO 3-D: Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures", Feb. 27, 2004, University of Duisburg-Essen, Germany, Host: Dr. Werner Prost.
- [S36] Gerhard Klimeck, "Development of NEMO 3-D: Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures", Feb. 24, 2004, Ruhr-University Bochum, Germany, Host: Prof. Ulrich Kunze.
- [S35] Gerhard Klimeck, "Development of the Nanoelectronic Modeling Tool (NEMO): Towards Design, Analysis, Synthesis, and Fundamental Limits", Feb. 18, 2004, State University of New York, Buffalo, Host: Prof. Vladimir Mitin.
- [S34] Gerhard Klimeck, "Computational Nanoelectronics: Towards Design, Analysis, Synthesis, and Fundamental Limits ", July 28, 2003, Purdue University, Host: Prof. Mark Lundstrom.
- [S33] Gerhard Klimeck, "Computational Nanoelectronics: Towards Design, Analysis, Synthesis, and Fundamental Limits ", JPL, Division 32 and 38 Seminar, June 18, Host: Dr. Carl Ruoff, Div 32 and 38 Chief Technologist.
- [S32] Gerhard Klimeck, "Computational Nanoelectronics: Towards Design, Analysis, Synthesis, and Fundamental Limits ", JPL, Section 381 Noontime seminar, April 10, 2003, Host Jason Hyon, Section 381 Deputy.
- [S31] Gerhard Klimeck, "Computational Nanoelectronics: Towards Design, Analysis, Synthesis, and Fundamental Limits ", Dr. Ed Stone Award Outstanding Research Publication Award Lecture, JPL, Feb. 18, 2003, Host: Dr. Tom Prince, JPL Chief Scientist.
- [S30] Gerhard Klimeck, "Modeling of Disordered Multimillion Atom Quantum Dot Systems", University of Duisburg, Germany, Nov 13, 2002, Hosts Dr. Werner Prost and Prof. Tegude.
- [S29] Gerhard Klimeck, "Modeling of Disordered Multimillion Atom Quantum Dot Systems", Ruhr-University Bochum, Germany, Nov 11, 2002, Host Prof. Ulrich Kunze.
- [S28] Gerhard Klimeck, "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots ", California State University Northridge, Northridge, CA, March 29, 2002, Host Prof. Nickolas Kioussis.
- [S27] Gerhard Klimeck, "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots ", Purdue University, West Lafayette, IN, March 20, 2002, Host Prof. Supriyo Datta.
- [S26] Gerhard Klimeck, "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots ", Notre Dame, South Bend, IN, March 15, 2002, Host Prof. Wolfgang Porod.
- [S25] Gerhard Klimeck, "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots ", R. G. Herb Memorial Lecture, Physics Dept., University of Wisconsin-Madison, Madison, WI, March 14, 2002, Host Prof. Bob Joynt

- [S24] Gerhard Klimeck, "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", NTT Central Research Laboratory, Erato Project, Feb 8, 2002, Hosts Dr. Michael Stope and Prof. Tarucha.
- [S23] Gerhard Klimeck, "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", University of Tokyo, February 8, 2002, Host Prof. Seigo Tarucha.
- [S22] Gerhard Klimeck, "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", Tokyo Institute of Technology, Feb 6, 2002, Host Prof. Oda.
- [S21] Gerhard Klimeck, "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", Osaka University, January 30m 2002, Host Prof. Hishiro Hamaguchi.
- [S20] Gerhard Klimeck, "Quantum Dot Modeling using NEMO 3-D", JPL, Section 367 Seminar, February 6, 2001, 126-346, 3p.m.
- [S19] Gerhard Klimeck, "Quantum Dot Modeling using NEMO 3-D", University of California Riverside, Department of Electrical and Computer Engineering, Dec 8, 2000.
- [S18] Gerhard Klimeck, R. Bowen, Tom Cwik, Timothy Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Notre Dame, South Bend, IN, April 12, 2000.
- [S17] Gerhard Klimeck, R. Bowen, Tom Cwik, Timothy Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", General Dynamics Information Systems, Minneapolis, MN, March 22, 2000.
- [S16] Gerhard Klimeck, R. Bowen, Tom Cwik, "Simulator Development for Nanoelectronic and Electromagnetic Devices", National Reconnaissance Office, Chantilly, VA, March 31, 1999.
- [S15] Gerhard Klimeck, R. Bowen, Timothy Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", MIT Lincoln Laboratory, Lexington, MA. Dec. 2, 1998.
- [S14] Gerhard Klimeck, R. Bowen, Timothy Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", Gerhard Mercator University Duisburg, Nov 25, 1998.
- [S13] Gerhard Klimeck, R. Bowen, Timothy Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", Ruhr University Bochum, Lehrstuhl fuer Werkstoffe der Elektrotechnik, Nov 23, 1998.

Work Performed at UTD/TI (9 Total)

- [S12] Gerhard Klimeck, "NEMO: A 1-D Heterostructure Design Tool", Center for Integrated Space Microsystems, Jet Propulsion Laboratory, Pasadena, CA, April 24, 1998.
- [S11] Gerhard Klimeck, "NEMO: A General Purpose 1-D Quantum Device Simulator", November 21, 1997, Intel Corporation, Portland, OR.
- [S10] Gerhard Klimeck, "NEMO: A General Purpose 1-D Quantum Device Simulator", October 6, 1997, Jet Propulsion Laboratory, Pasadena, CA.
- [S9] Gerhard Klimeck, "NEMO: Quantitative RTD Simulation", Hitachi Ltd., Cambridge, UK, July 21, 1997.
- [S8] Gerhard Klimeck, Dejan Jovanovic, "NEMO: Quantum Device Modeling (1-D, 2-D and 3-D)", Ultra Electronics Program Review, Estes Park, CO, Oct. 6-10, 1996.
- [S7] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", IMEC, Leuven, Belgium, May 31, 1996
- [S6] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Ruhr-Universität Bochum, Germany, May 30, 1996.
- [S5] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Universität Duisburg, Germany, May 28, 1996.
- [S4] Gerhard Klimeck, Roger Lake, R. Bowen, Daniel Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Texas Instruments Research Colloquium, Dallas, TX, May 23, 1996.

Work Performed in Graduate School (3 Total)

- [S3] Gerhard Klimeck, Roger Lake, Garnett Bryant, Guanlong Chen, Supriyo Datta, R. Bowen, William Frensley, "Elektronen-Elektronen und Elektronen-Phononen Wechselwirkungen in der Nanotechnologie", Ruhr-Universität Bochum, Germany, Dec. 20, 1994.
- [S2] Gerhard Klimeck, Roger Lake, Garnett Bryant, Guanlong Chen, Supriyo Datta, R. Bowen, William Frensley, "Elektronen-Elektronen und Elektronen-Phononen Wechselwirkungen in der Nanotechnologie", Universität Duisburg, Germany, Dec. 15, 1994.

- [S1] Gerhard Klimeck, Roger Lake, Supriyo Datta, "Erhöhter Stromfluss durch Streuprozesse oder überraschende Ergebnisse im Bereich der Quantenbauelemente", Ruhr-Universität Bochum, Germany, Jan. 8, 1993.

PROGRAM REVIEWS (TOTAL 98, STOPPED TRACKING 2015)

I stopped tracking program reviews in 2015.

Work Performed at Purdue (67 total)

The NCN/nanoHUB site visit happened every year since 2004 and I spent about 1-2 months preparing for that including creating the annual reports)

- [R98] Jim Fonseca, Gerhard Klimeck, "NEMO5 on Blue Waters: A Flexible Package for Nanoelectronics Modeling Problems", Blue Waters Symposium, Sunriver, OR, May, 2015
- [R97] Tao Chu, Hesameddin Ilatikhameneh, Rajib Rahman, Gerhard Klimeck, zhihong chen, "Field Controlled Dynamic Bandgap", LEAST annual review, South Bend, IN, 2014
- [R96] Hesameddin Ilatikhameneh, Bozidar Novakovic, Yaohua Tan, zhihong chen, Joerg Appenzeller, Rajib Rahman, Gerhard Klimeck, "Atomistic Modeling of 2D Material Based Steep Subthreshold Field Effect Transistors", LEAST annual review, South Bend, IN, 2014
- [R95] Rifat Ferdous, Yuling Hsueh, Rajib Rahman, Gerhard Klimeck, "Atomistic Modeling of Disordered Silicon Quantum Dots", ARO/LPS Quantum computing program review, Washington DC, Aug 11-15, 2014
- [R94] Rajib Rahman, Yuling Hsueh, Yu Wang, Archana Tankasala, Rifat Ferdous, Lloyd Hollenberg, Gerhard Klimeck, "Components of atomistic modeling for donor devices", ARO/LPS Quantum computing program review, Washington DC, Aug 11-15, 2014
- [R93] Gerhard Klimeck, "Elevating nanoHUB to the Next Level: Project Overview", NCN/nanoHUB reverse Site visit, Washington DC, Feb 22, 2013
- [R92] Gerhard Klimeck, "Elevating nanoHUB to the Next Level: Data Proposal", NCN/nanoHUB reverse Site visit, Washington DC, Feb 22, 2013
- [R91] Michael Povolotskyi, Tillmann Kubis, Jim Fonseca, Gerhard Klimeck, "Advanced Quantum Device Simulation using NEMO5", Semiconductor Research Corporation Review, Santa Barbara, CA, April 8 - 11, 2013
- [R90] Zhengping Jiang, Yu He, Kai Miao, Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Gerhard Klimeck, "Quantum Transport in Tunneling Field Effect Transistors", Nanoelectronic Research Initiative (NRI) review, MIND center (Midwest Institute for Nanoelectronics Discovery), Notre Dame, Aug. 15, 2012
- [R89] Jim Fonseca, Tillmann Kubis, Michael Povolotskyi, Jean Sellier, Gerhard Klimeck, "Advanced Simulations of Nanoelectronic Devices with NEMO5", Semiconductor Research Corporation Review, Santa Barbara, Ca, April, 2012
- [R88] Gerhard Klimeck, "Quantum Simulation of Advanced Transistors", MSD / FCRP All hands meeting, Stanford University, Pre-review March 1, full review May 5-6, 2012.
- [R87] Gerhard Klimeck, "Preparation Meeting, Technology Transfer for a proposed STC", UCSB, Oct. 5-6, 2012
- [R86] Gerhard Klimeck, "Advanced Quantum Device Simulation using NEMO5", SRC Annual Executive Review, Ronler Acres, Intel Oregon, Feb. 2-3, 2012.
- [R85] Gerhard Klimeck, "Technology Transfer for a proposed STC", UCSB, Oct. 24-26, 2012
- [R84] Gerhard Klimeck, "Advanced Quantum Device Simulation using NEMO5", SRC Program Review, Urbana Champaign, Aug. 31, 2011.
- [R83] Gerhard Klimeck, "3D Quantum Transport Modeling", MIND - Annual Review Meeting, (Midwest Institute for Nanoelectronics Discovery), Notre Dame, Aug. 17-18, 2011.
- [R82] Gerhard Klimeck, "Quantum Simulation of Advanced Transistors", MSD / FCRP All hands meeting, Stanford University, Pre-review March 7-8, full review May 10-11, 2011.
- [R81] Gerhard Klimeck, "HUBzero: Future Sociology and Cybertechnology that empowers over 170,000 Annual Users in Research, Education, and Industry Today", NCN all hands meeting, Feb. 10-11.
- [R80] Hoon Ryu, Sunhee Lee, Zhengping Jiang, Yui-Hong Tan, Michael Povolotskyi, Neerav Kharche, Mark Eriksson, Timothy Boykin, Gerhard Klimeck, Bent Weber, Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, W. Lim, H. Yang, N. Lai, F. Mohiyaddin, Andrea Morello, Andrew Dzurak, Michelle Simmons, Lloyd Hollenberg, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / IARPA / ARO Quantum Computing Technology Workshop, Denver, August 11-12, 2011.
- [R79] Hoon Ryu, Sunhee Lee, Zhengping Jiang, Yui-Hong Tan, Michael Povolotskyi, Neerav Kharche, Mark Eriksson, Timothy Boykin, Gerhard Klimeck, Bent Weber, Martin Fuechsle, Jill Miwa, Suddhasatta Mahapatra, Wee Lim, H. Yang, N. Lai, F. Mohiyaddin, Andrea Morello, Andrew Dzurak, Michelle Simmons, Lloyd Hollenberg, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / IARPA / ARO Quantum Computing Technology Workshop, Denver, August 16-17, 2011
- [R78] Gerhard Klimeck, Mathieu Luisier, "3D Quantum Transport Modeling", NRI Annual Review, MIND, Gaithersburg, Oct 27, 2010.
- [R77] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Rajib Rahman, Seung Park, Neerav Kharche, Zhengping Jiang, Timothy Boykin, Lloyd Hollenberg, Gabriel Lansbergen, Sven Rogge, Bent Weber, Michelle Simmons,

- "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / IARPA / ARO Quantum Computing Technology Workshop, Minneapolis, August 19-20, 2010.
- [R76] Gerhard Klimeck, Mathieu Luisier, "3D Quantum Transport Modeling", MIND - Annual Review Meeting, (Midwest Institute for Nanoelectronics Discovery), Notre Dame, Aug. 10-11, 2010.
- [R75] Gerhard Klimeck, "NCN Director's Overview", NCN annual review, April 28-29, 2010.
- [R74] Gerhard Klimeck, "Quantum Simulation of Advanced Transistors", MSD / FCRP All hands meeting, Stanford University, Pre-review March 1, full review May 5-6, 2010.
- [R73] George Adams III., Rick Kennel, Gerhard Klimeck, Michael McLennan, Debbie Perouli, Mehdi Salmani-Jelodar, "Instant on Computing", Strategic Technologies for CyberInfrastructure STCI and Software Development for CI (SDCI) PI Meeting on January 28-29, 2010 at NSF in Arlington, Virginia
- [R72] Gerhard Klimeck, "Cyber-Enabled Knowledge Transfer", NSF STC proposal site visit, Norfolk State University, Oct. 26, 2009.
- [R71] Gerhard Klimeck, "Knowledge Transfer using nanoHUB.org", Norfolk State University, NSF STC proposal dry run and team reaview Sept. 21, 2009.
- [R70] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Rajib Rahman, Benjamin Haley, Seung Park, Neerav Kharche, Zhengping Jiang, Timothy Boykin, Cameron. Wellard, Lloyd Hollenberg, Gabriel Lansbergen, Sven Rogge, Bent Weber, Michelle Simmons, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / IARPA / ARO Quantum Computing Technology Workshop, Minneapolis, August 21-22, 2009.
- [R69] Gerhard Klimeck, Mathieu Luisier, "3D Quantum Transport Modeling", MIND - Annual Review Meeting, (Midwest Institute for Nanoelectronics Discovery), Notre Dame, Aug. 20, 2009.
- [R68] Gerhard Klimeck, "Full 3-D quantum transport modeling of realistically extended devices", SRC - Semiconductor Research Corporation, Annual Review Austin, Tx, June 24, 2009.
- [R67] Michael McLennan, Gerhard Klimeck, "nanoHUB and HUBzero overview and demo", NCN annual review, June 17-18, 2009.
- [R66] Gerhard Klimeck, "NCN Director's Overview", NCN annual review, June 17-18, 2009.
- [R65] Gerhard Klimeck, "Software Customization and Deployment on the nanoHUB", MSD / FCRP All hands meeting, Stanford University, May 4-5, 2009.
- [R64] Gerhard Klimeck, Neerav Kharche, Rajib Rahman, Benjamin Haley, Timothy Boykin, Cameron. Wellard, Lloyd Hollenberg, Gabriel Lansbergen, Sven Rogge, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / DTO / ARO Quantum Computing Technology Workshop, Atlanta, August 11-13, 2008.
- [R63] Gerhard Klimeck, Michael McLennan, "nanoHUB overview and demo", NCN annual review, June 26-27, 2008.
- [R62] Gerhard Klimeck, Diane Beaudoin, "nanoHUB metrics, statistics, and assessment", NCN annual review, June 26-27, 2008.
- [R61] Gerhard Klimeck, "Full 3-D quantum transport modeling of realistically extended devices", SRC - Semiconductor Research Corporation, Annual Review, Austin, Tx, June 24, 2008.
- [R60] Gerhard Klimeck, "3D Atomistic Modeling. from NEMO to OMEN", MIND - Kickoff and Review Meeting, (Midwest Institute for Nanoelectronics Discovery), Notre Dame, June 4-5th, 2008.
- [R59] Gerhard Klimeck, Michael McLennan, George Adams III., Mark Lundstrom, "nanoHUB - future cyberinfrastructure serving over 62,000 users today", Birck Nanotechnology Research Review 2008, April 14th, 2008.
- [R58] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN all hands meeting, External Advisory Board meeting, April 2nd and 3rd, 2008.
- [R57] Gerhard Klimeck, "Software Customization and Deployment on the nanoHUB", MSD / FCRP All hands meeting, Stanford University, March 4, 2008.
- [R56] Gerhard Klimeck, Neerav Kharche, Rajib Rahman, Srikant Srinivasan, Leonid Rokhinson, Martha Prada, Benjamin Haley, Timothy Boykin, Cameron. Wellard, Lloyd Hollenberg, Gabriel Lansbergen, Sven Rogge, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / DTO / ARO Quantum Computing Technology Workshop, Minneapolis, August 12-17, 2007.
- [R55] Gerhard Klimeck, "Full 3-D quantum transport modeling of realistically extended devices", SRC - Semiconductor Research Corporation, Annual Review, Durham, NC, June 26, 2007.
- [R54] Gerhard Klimeck, Michael McLennan, "nanoHUB overview and demo", NCN annual review, June 19-21, 2007.
- [R53] Gerhard Klimeck, Michael McLennan, "nanoHUB overview, metrics, and plans", NCN all hands meeting, External Advisory Board meeting, April 4rd and 5th, 2007.
- [R52] Gerhard Klimeck, Martha Prada, Neerav Kharche, Rajib Rahman, Timothy Boykin, Seungwon Lee, Paul Allmen, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", LPS / ARO Site visit to University of Wisconsin, Madison, Sept. 19, 2006.

- [R51] Gerhard Klimeck, Michael McLennan, "nanoHUB overview and Usage Scenarios", Purdue University, Discovery Park Advisory Council Meeting, September 15, 2006.
- [R50] Gerhard Klimeck, Martha Prada, Neerav Kharche, Rajib Rahman, Timothy Boykin, Seungwon Lee, Paul Allmen, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARO Quantum Computing Technology Workshop, Atlanta, August 14-16, 2006.
- [R49] Gerhard Klimeck, Michael McLennan, "Full 3-D quantum transport modeling of realistically extended devices", SRC - Semiconductor Research Corporation, Annual Review Durham, NC, June 26-28, 2006.
- [R48] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN annual review, June 20-22, 2006.
- [R47] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN all hands meeting, External Advisory Board meeting, April 3rd and 4th, 2006.
- [R46] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Krishna Madhavan, "The NCN cyber infrastructure strategic plan", NCN advisory board meeting, Purdue University, Feb 6 and 7th, 2006.
- [R45] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN advisory board meeting, Purdue University, Feb 6 and 7th, 2006.
- [R44] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Krishna Madhavan, "The nanoHUB: a demo", NCN advisory board meeting, Purdue University, Feb 6 and 7th, 2006.
- [R43] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Neerav Kharche, Marek Korkusinski, Jing Wang, Timothy Boykin, Fabiano Oyafuso, Paul Allmen, Seungwon Lee, "The NCN: science, simulation, and cyber services and Transport in Si Nanowires", SRC Review, The New York Center for Advanced Interconnect Science and Technology (NYCAIST), Packaging / Interconnect and BEP Fall Review, October 2-6, 2005, University at Albany-SUNY, Albany Nanotech Campus, NanoFab 300S.
- [R42] Gerhard Klimeck, Paul Allmen, Rajib Rahman, Neerav Kharche, Timothy Boykin, Seungwon Lee, Fabiano Oyafuso, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Tampa, FL, August 22-26, 2005.
- [R41] Mark Lundstrom, Jing Wang, Anisur Rahman, Gerhard Klimeck, "NEGF Transistor Simulations", SRC Modeling and Simulation / Compact Modeling Research Review, June 27-29, 2005, Research Triangle Park, NC
- [R40] Gerhard Klimeck, "Network for Computational Nanotechnology and Nanowire Simulation", SRC Modeling and Simulation / Compact Modeling Research Review, June 27-29, 2005, Research Triangle Park, NC
- [R39] Gerhard Klimeck, "NCN Infrastructure Development", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 21-22, 2005.
- [R38] Gerhard Klimeck, "HPC and Visualization for multimillion atom simulations", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 21-22, 2005.
- [R37] Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul Allmen, Seungwon Lee, K. Whaley, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Orlando, FL, August 16-20, 2004.
- [R36] Sebastien Goasguen, Marek Korkusinski, Michael McLennan, Gerhard Klimeck, Mark Lundstrom, "The nanoHUB a TeraGrid Science Gateway", TeraGrid Grid Infrastructure Group Review Argonne National Lab, IL, November 17-19, 2004.
- [R35] Gerhard Klimeck, "Top-Down Approaches: 1) Tight binding, 2) System Synthesis, 3) Software Infrastructure", DARPA, PROM kickoff meeting, July 18-19, 2004, California Institute of Technology.
- [R34] Anisur Rahman, Mark Lundstrom, Gerhard Klimeck, "Bandstructure effects in Ultra-thin Body MOSFETs", SRC Research Annual Review, June 30, 2004.
- [R33] Gerhard Klimeck, "NCN Computational Research Overview", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 24-25, 2004.
- [R32] Gerhard Klimeck, "NCN Infrastructure Development", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 24-25, 2004.

Work Performed at JPL (9 total)

- [R31] Paul Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Susan Coppersmith, Mark Friesen, "Empirical Atomic Level Simulations for QC Applications", ARDA Kickoff Meeting, Madison, WI, June 3, 2004.
- [R30] Gerhard Klimeck, Timothy Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul Allmen, Seungwon Lee, K. Whaley, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 18-22, 2003.
- [R29] Gerhard Klimeck, Fabiano Oyafuso, E. Tisdale, Hook Hua, R. Bowen, "Development of a Parallel Eigensystem Solver for Beowulf Clusters", Oct 31 2002, JPL ESTO-CT program review.
- [R28] Gerhard Klimeck, Akos Czikmantory, Hook Hua, "WIGLAF – A Web Interface Generator and Legacy Application Facade", Oct 31 2002, JPL ESTO-CT program review.

- [R27] Gerhard Klimeck, Timothy Boykin, Fabiano Oyafuso, Paul Allmen, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 19-23, 2002.
- [R26] Nikzad Toomarian, R. Bowen, Gerhard Klimeck, "Quantum Dot Modeling – Development of a Bottom-Up Nanoelectronic Modeling Tool", May 9, 2001, JPL CISM (Center for Integrated Space Microelectronics) zero-base review of RCT (Revolutionary Computing Technologies) program.
- [R25] R. Bowen, Gerhard Klimeck, "Quantum Dot Modeling – Development of a Bottom-Up Nanoelectronic Modeling Tool", September 2000, JPL CISM (Center for Integrated Space Microelectronics) review of RCT (Revolutionary Computing Technologies) program.
- [R24] R. Bowen, Gerhard Klimeck, "Quantum Dot Modeling – Development of a Bottom-Up Nanoelectronic Modeling Tool", August 1 2000, JPL CISM (Center for Integrated Space Microelectronics) review of RCT (Revolutionary Computing Technologies) program.
- [R23] R. Bowen, Gerhard Klimeck, "3-D Quantum Device Simulator Development", March 18, 1999, JPL CISM (Center for Integrated Space Microelectronics) review of RCT (Revolutionary Computing Technologies) program

Work Performed at UTD/TI (22 total)

- [RR1-R22] The National Reconnaissance Office, sponsor of the NEMO program, required a quarterly program review. Prof. David Ferry (ASU), Prof. George Haddad (U. of Michigan), and Dr. Harold Grubin (SRA) were hired as scientific reviewers by the program sponsor. In addition, program managers from other agencies such as ONR, DARPA, and NSA were typically present. The reviews were generally held in the Central Research Lab of Texas Instruments or at the DFW Hilton. Individual presentations listed below lasted typically 25-45 minutes.
- [R22] Gerhard Klimeck, "NanoElectronic MOdeling-Software Development Approach", Dec., 1997.
- [R21] Gerhard Klimeck, "Program Status, Activities Overview", May 19, 1997.
- [R20] Gerhard Klimeck, "Software Development – Theory",
- [R19] Gerhard Klimeck, "Software Demo", May 19, 1997.
- [R18] Daniel Blanks, Gerhard Klimeck, "Software / Interface Development", 1996
- [R17] Gerhard Klimeck, "Test Matrix Results", Nov., 1996.
- [R16] NEMO DC, "NEMO Software Summary", May, 1996.
- [R15] NEMO DC, "NEMO Software Tutorial" (3 hours)", May, 1996.
- [R14] Gerhard Klimeck, "NEMO: Software Development", Feb. 7, 1996.
- [R13] Gerhard Klimeck, "NEMO: GUI Development", Feb. 7, 1996.
- [R12] R. Bowen, Gerhard Klimeck, "Multiband Simulations", Feb. 7, 1996.
- [R11] Gerhard Klimeck, "GUI and Theory Interaction - A Dynamic Design", October 11, 1995.
- [R10] Gerhard Klimeck, "NEGF Code Development", October 11, 1995.
- [R9] Gerhard Klimeck, R. Bowen, "Multiband Simulation Results", October 11, 1995.
- [R8] Gerhard Klimeck, William Frensley, Chenjing Fernando, R. Bowen, "Non-Equilibrium Green Function Approach – Software Development", June 27, 1995.
- [R7] R. Bowen, Gerhard Klimeck, William Frensley, "Multiband Simulations", June 27, 1995.
- [R6] Chenjing Fernando, Gerhard Klimeck, William Frensley, "Polar Optical Phonon Scattering Simulations", June 27, 1995.
- [R5] Gerhard Klimeck, William Frensley, Chenjing Fernando, R. Bowen, "Non-Equilibrium Green Function Approach – Software Development", Feb. 23, 1995.
- [R4] Gerhard Klimeck, William Frensley, Chenjing Fernando, R. Bowen, "Non-Equilibrium Green Function Approach – Software Development", Feb. 23, 1995.
- [R3] William Frensley, Gerhard Klimeck, Chenjing Fernando, R. Bowen, "Non-Equilibrium Green Function Approach – Software Development", fall 1994.
- [R2] William Frensley, Gerhard Klimeck, Chenjing Fernando, R. Bowen, "Non-Equilibrium Green Function Approach – Software Development", summer 1994.
- [R1] William Frensley, Gerhard Klimeck, Chenjing Fernando, R. Bowen, "Non-Equilibrium Green Function Approach – Software Development", spring 1994.

TECHNICAL BRIEFINGS (2003-2014, RESTARTED DOCUMENTING IN 2021, SPECIFICALLY WITH ONLINE RECITATIONS FOR FACULTY MEMBERS)

The technical briefing list has been started in December 2003, to account for various Technical Briefings given to possible sponsors or partners of the NCN. I stopped tracking in 2014 and restarted in 2021 as we started online recitation sessions for faculty members globally.

- [B111] Briefing to Microsoft, Jan 13, 2023
- [B110] Briefing to AMD, Jan 13, 2023
- [B109] Briefing to AMD, Nov. 19, 2023
- [B108] Briefing to Synopsis, "Semiconductor workforce development through immersive simulations on nanoHUB.org", Nov. 11, 2022
- [B107] Briefing to Cadence, "nanoHUB", Oct. 24, 2022
- [B106] Gerhard Klimeck, Briefing to AMD on nanoHUB. Oct. 14, 2022
- [B105] **Briefing to Secretary of State Anthony Blinken and Secretary of Commerce Gina M. Raimondo, Gerhard Klimeck "Semiconductor Device Modeling", Purdue University, Sept. 13, 2022**
- [B104] Briefing to Cadence representatives, David Junkin, "nanoHUB", Sept. 8, 2022
- [B103] Briefing to Cadence representatives, "nanoHUB", August. 30, 2022
- [B102] Briefing to Director of Engineering NSF. June 2, 2022.
- [B101] Gerhard Klimeck, "MOSFETs", nanoHUB Online Recitation Series for Semiconductor Education and Workforce Development, <https://nanohub.org/events/details/2176> , <https://nanohub.org/resources/36071> May 25, 2022.
- [B100] Gerhard Klimeck, "MOS Capacitors", nanoHUB Online Recitation Series for Semiconductor Education and Workforce Development, <https://nanohub.org/events/details/2175> , <https://nanohub.org/resources/36070> . May 16, 2022.
- [B99] Gerhard Klimeck, "Bipolar Junction Transistors", nanoHUB Online Recitation Series for Semiconductor Education and Workforce Development, <https://nanohub.org/events/details/2174>, <https://nanohub.org/resources/36069> May 11, 2022.
- [B98] Gerhard Klimeck, "Drift-Diffusion-Lab with Bias and Light", nanoHUB Online Recitation Series for Semiconductor Education and Workforce Development, <https://nanohub.org/events/details/2173> , <https://nanohub.org/resources/36068> May 2, 2022.
- [B97] Gerhard Klimeck, "Bandstructure Models", nanoHUB Online Recitation Series for Semiconductor Education and Workforce Development, <https://nanohub.org/events/details/2172> , <https://nanohub.org/resources/36067> April 27, 2022.
- [B96] Gerhard Klimeck, "PN Junctions", nanoHUB Online Recitation Series for Semiconductor Education and Workforce Development, <https://nanohub.org/events/details/2171>, <https://nanohub.org/resources/36066> April 18, 2022.
- [B95] Gerhard Klimeck, "ABACUS Overview and Crystal Structures", nanoHUB Online Recitation Series for Semiconductor Education and Workforce Development, <https://nanohub.org/events/details/2169> , <https://nanohub.org/resources/36065> April 11, 2022
- [B94] Gerhard Klimeck, "MOSFETs", nanoHUB Online Recitation Series for Semiconductor Education, <https://nanohub.org/events/details/2120> , <https://nanohub.org/resources/35687> Feb. 2, 2022.
- [B93] Gerhard Klimeck, "MOS Capacitors", nanoHUB Online Recitation Series for Semiconductor Education, <https://nanohub.org/events/details/2119> , <https://nanohub.org/resources/35686> . Jan 26, 2022.
- [B92] Gerhard Klimeck, "Bipolar Junction Transistors", nanoHUB Online Recitation Series for Semiconductor Education, <https://nanohub.org/events/details/2157>, <https://nanohub.org/resources/35685> Jan. 19, 2022.
- [B91] Gerhard Klimeck, "Drift-Diffusion-Lab with Bias and Light", nanoHUB Online Recitation Series for Semiconductor Education, <https://nanohub.org/events/details/2116> , <https://nanohub.org/resources/35684> Jan. 12, 2022.
- [B90] Gerhard Klimeck, "Bandstructure Models", nanoHUB Online Recitation Series for Semiconductor Education, <https://nanohub.org/events/details/2115> , <https://nanohub.org/resources/35683> Dec. 16, 2021.
- [B89] Gerhard Klimeck, "PN Junctions", nanoHUB Online Recitation Series for Semiconductor Education, <https://nanohub.org/events/details/2113>, <https://nanohub.org/resources/35682> Dec. 8, 2021.
- [B88] Gerhard Klimeck, "ABACUS Overview and Crystal Structures", nanoHUB Online Recitation Series for Semiconductor Education, <https://nanohub.org/events/details/2112> , <https://nanohub.org/resources/35679> Dec. 1, 2021.
- [B87] Gerhard Klimeck, "Mythbusting Scientific Knowledge Transfer with nanoHUB.org ", Host: Vice President for Research and Partnerships, Simiomo Corporation, Japan, May 14
- [B86] Gerhard Klimeck, "Mythbusting Scientific Knowledge transfer with nanoHUB.org ", Yegor Gaidar Summer Leadership Program, July 14, 2014

- [B85] Gerhard Klimeck, "Nanohub Summary", Briefing to Krishna Shenai, Ph.D. Principal Electrical Engineer, Process Technology Research, Energy Systems Division, Argonne National Laboratory, December 12, 2013
- [B84] Gerhard Klimeck, "nanoHUB.org", Briefing to Dr. Germán Guido-Lavalle Provost Instituto Tecnológico Buenos Aires (ITBA). Oct 8, 2013
- [B83] Gerhard Klimeck, "nanoHUB.org", Briefing to Dr. Dennis Buss, Oct 1 2013
- [B82] Gerhard Klimeck, "nanoHUB", Briefing to Intel Manufacturing site, Chengdu, China, Aug. 2nd, 2013
- [B81] Gerhard Klimeck, "nanoHUB.org", Briefing to Dr. Germán Guido-Lavalle Provost Instituto Tecnológico Buenos Aires (ITBA). Oct 8, 2013
- [B80] Gerhard Klimeck, "nanoHUB", Briefing to Intel Manufacturing site, Dalian, China, July 26, 2013
- [B79] Gerhard Klimeck, "Transferability of nanoHUB", briefing to Thomas Hertel, Nelson Villoria, Krannert School of Business, Thursday May 9, 2013
- [B78] Gerhard Klimeck, "nanoHUB Impact Metrics", Briefing to Teaching and Learning Technology Leadership team. Host Donna Cumberland, Attendees: Donalee H. Attardo, Mathew Pistilli, Bethany, James Willins, Tuesday May 7, 2013
- [B77] Gerhard Klimeck, "nanoHUB.org and NEMO for topological Insulators", Briefing to Dan Green, ONR, Jan 22, 2013, Purdue University
- [B76] Gerhard Klimeck, "Updates on NCN and nanoHUB", Discovery Park Leadership Meeting, Jan. 8, 2012
- [B75] Gerhard Klimeck, "Purdue HUB Collaboratory", Briefing to Frank Cepollina, NASA, Host. Prof. Melba Crawford, Purdue, Feb. 9, 2012
- [B74] Gerhard Klimeck, "nanoHUB.org powered by HUBzero® – A Platform for Collaborative Research with Quantifiable Impact on Research and Education", Briefing to Tang Zhen An, Hui Hung, Shufeng Xia, Dalian University, China, Host. Prof. Mark Lundstrom, Purdue, March. 8, 2012
- [B73] Gerhard Klimeck, "nanoHUB.org: A Global Cyberinfrastructure Serving Over 180,000 Users - What are all these people doing? Customized User Experiences?", Briefing to Nori, CEO Art Norins, VP: Sanjay Wahi, and Data Scientist Morteza Shahram, Sunnyvale, CA, Oct. 28, 2011
- [B72] Gerhard Klimeck, George Adams III., "nanoHUB – Cyberinfrastructure Impact, Network of HUBS – Manufacturing/Materials, Compute Cycles", Briefing to DARPA TTO, Mr. Barry Ives, Deputy Director, LTC Nathan Wiedenman, Deputy Program Manager, Oct. 3, 2011, Arlington VA.
- [B71] Gerhard Klimeck, "nanoHUB Impact and your impact in grad school", Briefing to NCN Graduate student body, Host: Dr. Lynn Zentner, Sept 19, 2011
- [B70] Monica Allain, Gerhard Klimeck, "Colombia-Purdue Institute for Advanced Scientific Research: Fronteras de Educación", Universidad de Nacional, Medellin, March 15, 10am, Medellin, Colombia, presentation to Deans and Faculty.
- [B69] Gerhard Klimeck, Monica Allain, "Colombia-Purdue Institute for Advanced Scientific Research: Fronteras de Educación", Universidad de Bolivariana, March 15, 2pm, Medellin, Colombia - presentation to Deans and Faculty.
- [B68] Gerhard Klimeck, Monica Allain, "Colombia-Purdue Institute for Advanced Scientific Research: Fronteras de Educación", Universidad de Antioquia, March 16, 9am, Medellin, Colombia, – presentation to Dr. Alfonso Monsalve Solórzano, Vice-president for Research and Faculty.
- [B67] Gerhard Klimeck, Monica Allain, "Cyberinfrastructure for Colombia - Colombia-Purdue Institute for Advanced Scientific Research", Universidad de EAFIT, March 16, 1pm, Medellin, Colombia, – presentation to Vice Rector General Julio Acosta and Dean of Engineering Alberto Rodriguez, and Faculty.
- [B66] Gerhard Klimeck, Monica Allain, "Colombia-Purdue Institute for Advanced Scientific Research: Fronteras de Educación", Universidad Nacional, March 17, 9am, Bogota, Colombia – presentation to Deans and Faculty.
- [B65] Gerhard Klimeck, "nanoHUB.org – Purdue Global Impact", Universidad Javeriana, March 17, 3pm, Bogota, Colombia – presentation to Deans and Faculty
- [B64] Gerhard Klimeck, "nanoHUB.org – Cyberinfrastructure For Education and Research", private dinner event at the home of Purdue alum Gilberto Gomez, Universidad Javeriana, March 17, 3pm, Bogota, Colombia – briefing to Colombia's Minister of Education: María Fernanda Campo.
- [B63] Gerhard Klimeck, "nanoelectronics research in the Klimeck research group", Universidad de Los Andes, March 18, 9am, Bogota, Colombia, presentation to nanoelectronics and materials faculty.
- [B62] Gerhard Klimeck, "SME Update, Compute Cycles, Education HUB", April 20, 2011, Briefing Mr. Aneesh Chopra, US Chief Technology Officer (CTO), U.S. OSTP.
- [B61] Gerhard Klimeck, "Multi-Scale and Multi-Expertise HUB-based Virtual Organizations", April 20, 2011, Briefing Mr. Thomas Kalil, Deputy Director for Policy, U.S. OSTP.
- [B60] Gerhard Klimeck, Krishna Madhavan, George Adams III., "Learning Flow Informatics as an Instrumentation Paradigm within Cyberlearning Environments", April 21, 2011, Briefing Dr. Barbara Olds, NSF EHR.
- [B59] Gerhard Klimeck, "Concept: National Center / Lab for Cyberinfrastructure", May 12, 2011, Briefing Kei Koizumi, U.S. OSTP.

- [B58] Gerhard Klimeck, "nanoHUB.org powered by HUBzero® : A Platform for Collaborative Research - Mythbusting Scientific Knowledge Transfer", July 15, 2011, Briefing Dr. Katherine Stevens, Director, Materials and Manufacturing Directorate, Dr. Barry Farmer, Wright Patterson Air Force Base, Directorate RX
- [B57] Gerhard Klimeck, "HUBzero ® ", July 15, 2011, Briefing Mr. Brian Stucke and Mr. Bryon Foster, CTO, Materials and Manufacturing Directorate, Dr. Barry Farmer, Wright Patterson Air Force Base, Directorate RX
- [B56] Gerhard Klimeck, George Adams III., "Briefing to Purdue Decadal Planning Committee", July 27, 2011, led by Provost Prof. Tim Sands
- [B55] Gerhard Klimeck, "nanoHUB Cyberinfrastructure for Colombian Technology Growth", Sept 8th, 2011, Secretary of economic development if the Bogota district, President of the science and technology council, Codiciti, Hernando Gomez, Colombia.
- [B54] Jean Allain, Gerhard Klimeck, "An EPICS Program for Colombia", Sept 9th, 2011, Briefing to Colombia's Minister of Education: María Fernanda Campo.
- [B53] Gerhard Klimeck, "Response to Educator's Prime Interests - Guidance into nanoHUB.org", NCN Workshop on Simulation-Based Learning, Nov. 5-6, Big Ten Conference Center, Chicago.
- [B52] Gerhard Klimeck, "nanoHUB.org overview", NCN Workshop on Simulation-Based Learning, Nov. 5-6, Big Ten Conference Center, Chicago.
- [B51] Mathieu Luisier, Gerhard Klimeck, "OMEN: a Quantum Transport Modeling Tool for Nanoelectronic Devices", Briefing to Dr. Andrew Skipo, Motorola Inc., June 29, 2009, Purdue University.
- [B50] Gerhard Klimeck, "nanoHUB.org Demo and Content Development Options", Briefing to Dr. Deb. Newberry, Dakota County Technical College, Feb. 23, 2009, Purdue University.
- [B49] Gerhard Klimeck, "Atomistic Nanoelectronic Modeling and Deployment on nanoHUB.org", Briefing to Dr. Steve Hillenius (SRC) and Dr. Mark Pinto (Applied Materials), Feb. 21, 2009, Purdue University.
- [B48] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 90,000 users today", Briefing to Prof. Fire Tom. Wada, University of the Ryukyus, Okinawa, Japan, Feb. 13, 2009, Purdue University.
- [B47] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 89,000 users today", Briefing to EAFIT University, Medellin, Colombia, Alberto Rodríguez García, Dean of Engineering, Oscar E. Ruiz, Director of PhD programs, January 28, 2009, Purdue University.
- [B46] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 85,000 users today", Briefing to the NCN Education Advisory Board, November 20, 2008, Purdue University.
- [B45] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 85,000 users today", Briefing to Kwang-Ryeol Lee, Hyung-Min Rho, and Jung-Ho Kim, Korean Institute of Science and Technology (KIST), November 20, 2008, Purdue University.
- [B44] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 68,000 users today", Briefing to GLCPC Virtual School of Computational Science and Engineering Planning Meeting, July 1-2, 2008, University of Michigan, Ann Arbor.
- [B43] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 58,000 users today", Briefing to Purdue IGERT proposal team, Feb. 14, 2008.
- [B42] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 58,000 users today", Briefing to KIST visitors to the Purdue Cyber Center, Host: Barbara Fossum, Monday, Feb. 11, 2008.
- [B41] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", Briefing to Shalaev Research Group, Host: Prof. Vlad Shalaev, Friday, Nov. 29, 2007.
- [B40] Gerhard Klimeck, "nanoHUB.org opportunities", Briefing Purdue ECE untenured faculty, Host: Head of ECE, Prof. Mark Smith , Friday, Nov. 16, 2007.
- [B39] Gerhard Klimeck, "nanoHUB.org", Briefing to IEEE Spectrum Editor Glen Zorpette, Host: Purdue CIO Gerry McCartney, Friday, Nov. 7, 2007.
- [B38] Gerhard Klimeck, "Blue Ocean Opportunity", Briefing Purdue ECE external Avisory board, Host: Head of ECE, Prof. Mark Smith , Friday, Nov. 1, 2007.
- [B37] Gerhard Klimeck, "nanoHUB.org demo", Briefing Purdue ECE Industrial Advisory Board, Host: Head of ECE, Prof. Mark Smith , Sept. 10, 2007.
- [B36] Gerhard Klimeck, "nanoHUB.org demo", Briefing to Lockheed Martin, Drs. Richard Barto, Anna L Paulson , Host. Dr. George Adams, Purdue Discovery Park, Wednesday, May 16, 2007.
- [B35] Gerhard Klimeck, Michael McLennan, "NCN overview and nanoHUB.org demo", Briefing to Purdue University, Discovery Park Key Issues Meeting, Host. Prof. Al Rebar, Director Discovery Park, Wednesday, May 16, 2007.
- [B34] Gerhard Klimeck, Michael McLennan, "nanoHUB.org demo", Briefing to Steven Kahn, Stanford University, Host. Prof. Chris Hoffmann, Purdue Rosen Center for Advanced Computing. April 19, 2007.
- [B33] Gerhard Klimeck, "nanoHUB.org demo", Briefing to Brian R. Wilson, Distinguished Director, CTO, SUN micorsystems, Host. Ahmed Elmargamid, Purdue Cyber Center. April 2, 2007.
- [B32] Gerhard Klimeck, "nanoHUB.org demo", Briefing to Winslow Sargeat, Venture Investors LLC, Host. Barbara Fossum, Purdue Cyber Center. April 2, 2007.

- [B31] Gerhard Klimeck, "nanoHUB.org A fully operational Science Gateway for the nano Science Community", Briefing to Jake Chen, UIPUI, Host. Barbara Fossum, Purdue Cyber Center. Feb. 15, 2007.
- [B30] Gerhard Klimeck, "The nanoHUB: a demo", Argonne National Lab, October 30, 2006.
- [B29] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Krishna Madhavan, "The nanoHUB: a demo", NCN Purdue University Advisory Board, Purdue University, Jan 5, 2006.
- [B28] Gerhard Klimeck, "Atomistic simulations of long-range strain and close-range electronic structure in self-assembled quantum dot systems and Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org", Briefing to Rebecca Cortez, Robert Fitch, Mark Calcaterra, Air Force Research Lab, Host. Dr. Edgar Martinez, Purdue University, Jan 13, 2006.
- [B27] Gerhard Klimeck, "The Network For Computational Nanotechnology and Bandstructure Effects in Nanoelectronics", Briefing to Mark Foisy and Brian Winstead of Freescale Semiconductor, Purdue University, Nov 17, 2005.
- [B26] Gerhard Klimeck, "The Network For Computational Nanotechnology", Briefing to Dennis Buss, Chris Bowen, Ramesh Venugopal, Texas Instruments, Purdue University, Nov 10, 2005.
- [B25] Gerhard Klimeck, "The Network For Computational Nanotechnology", Briefing to Ralph Roskies, Pittsburgh Supercomputing Center, Purdue University, Nov 4, 2005.
- [B24] Gerhard Klimeck, "The Network For Computational Nanotechnology", Briefing to Klaus Schulten Computational Biology Research Group, University of Illinois Urbana Champaign, Beckmann Institute. Sept. 16, 2005.
- [B23] Gerhard Klimeck, "Nanowire Simulations and The Network For Computational Nanotechnology", Briefing to Alan Seabaugh (Notre Dame) and Lars-Erik Wernersson (Lund). Sept. 14, 2005.
- [B22] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, "The Network For Computational Nanotechnology", Briefing to Oak Ridge National Laboratory, Dr. John Cobb, May. 19th, 2005.
- [B21] Marek Korkusinski, Gerhard Klimeck, Haiying Xu, Seungwon Lee, Sebastien Goasguen, Faisal Saied, "Atomistic simulations in nanostructures composed of tens of millions of atoms", Briefing to Intel, Dr. Robert Chau, March 31st, 2005.
- [B20] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, "The Network For Computational Nanotechnology", Briefing to Lockheed Martin, Sharon L. Smith, Raj. K. Jain, Feb. 11th, 2005.
- [B19] Gerhard Klimeck, "The Network For Computational Nanotechnology", Briefing to Raytheon, Jill Pate and Dr. Zaher Bardai, Feb. 3rd, 2005.
- [B18] Gerhard Klimeck, "Building the Infrastructure, lessons from the Network for Computational Nanoscience", Planning meeting for NIH Center for design of biomimetic nanoconductors, Organized by Eric Jakobson, University of Illinois Urbana-Champaign, Dec. 17-19, 2004.
- [B17] Gerhard Klimeck, "nanoHUB infratructure for NCLT simulations", Briefing to Bob Chang, NCLT, Northwestern University, Dec. 8, 2004.
- [B16] Gerhard Klimeck, "NEGF details in NEMO 1-D and Multimillion atom simulations", Briefing to Intel, Mark Stettler, and Borna Obradovic, Oct. 28, 2004.
- [B15] Gerhard Klimeck, Michael McLennan, "Computing, Software, and Cyberinfrastructure", Briefing to Intel, Mark Stettler, Martin Giles, and Borna Obradovic, Oct. 28, 2004.
- [B14] Gerhard Klimeck, "Spin Effects in Quantum Dots", Briefing to Nanotechnology Research Initiative, Gurtej Sandu (Micron), Joerg Appenzeler for Tom Theis (IBM), Pushkar Apte (SIA), George Bourianoff (Intel), Sept 20, 2004.
- [B13] Mark Lundstrom, Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN)", Briefing to Intel, JoZell Johnsson, Sept. 21, 2004.
- [B12] Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN)", Briefing to EMC, Deborah Snow and Gael Keough, Sept. 21, 2004.
- [B11] Anisur Rahman, Jing Wang, Ali Yannik, Gerhard Klimeck, "Bandstructure and Spintronics Research", Briefing to Intel Corp., Dmitry Nikonov, Sept. 21, 2004.
- [B10] Mark Lundstrom, Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN) and Intel", Briefing to Intel Corp., Kevin Kahn, Sept. 10, 2004.
- [B9] Gerhard Klimeck, "The Nanoelectronic Modeling tool (NEMO): Possible Release to the Nanotechnology Community and Nanoelectronic Modeling (NEMO): Is it Device or Material Modeling?", Briefing to Raytheon, Gary Valentine, Neil Peterson, at Purdue University, July 27, 2004.
- [B8] Gerhard Klimeck, "The Network for Computational Nanotechnology and Nanoelectronic Modeling (NEMO): Is it Device or Material Modeling?", Briefing to Micron Corporation, at Purdue University, July 13, 2004.
- [B7] Gerhard Klimeck, "The Network for Computational Nanotechnology", Briefing to High Performance Computing Modernization Program, Steve Goodnick, Paul Sotirelis, and Marco Santorini, at Purdue University, June 25, 2004.
- [B6] Gerhard Klimeck, "Development of the Nanoelectronic Modeling tool (NEMO)", Briefing to ARO, Barry Perlman, May 3, 2004.

- [B5] Gerhard Klimeck, "Computational Nanoelectronics, Towards: Design, Analysis, Synthesis, and Fundamental Limits", Briefing to Accelrys Corp., Gerhard Goldbeck-Wood, Scott Kahn, Amitesh Maiti, Presentation at Purdue, Jan 21, 2004.
- [B4] Gerhard Klimeck, "nanoHUB", Briefing to Intel Manufacturing site, Dalian, China, July 26, 2013

OTHER PRINTED PUBLICATIONS

- [O1] Mark Lundstrom, Gerhard Klimeck, Sebastien Goasguen, and Michael McLennan, .The Network for Computational Nanotechnology: A Vision for Theory, Simulation, and Computation,. Facets, International Union of Materials Research Societies, 2005.

PANEL PARTICIPATION (18 TOTAL)

- [18] Susanne Yelin, Mikhail Lukin, Marco Pistoia, Gerhard Klimeck, & Mariia Mykhailova, "Panel on Quantum Education and Outreach", Quantum Science Center, 2nd Annual Quantum Summer School, Purdue University, May 8-12, 2022.
- [17] NITRD Big Data Interagency Virtual Workshop on Pioneering the Future of Federally Supported Data Repositories Wednesday Jan 13th - Friday Jan 15th, 2021 <https://www.orau.gov/bdworkshop21>
- [16] 2021 NNI Strategic Planning Stakeholder Workshop, January 11-13, 2021, National Nanotechnology Coordination Office
- [15] Gerhard Klimeck, "Broadening - Materials Genome", Discovery Park Panel Discussion, sept 15, 2014, Host : Prof. Alan Rebar
- [14] Gerhard Klimeck, "nanoHUB with Global impact", Discovery Park Panel Discussion, sept 15, 2014, Host : Prof. Alan Rebar
- [13] Dennis Buss, Mark Lundstrom, Muhammad Alam, Supriyo Datta, Joerg Appenzeller, Gerhard Klimeck, "A Forum on the Future of Electronics", Fowler Hall, Purdue, Oct. 1, 2013
- [12] Micah Altman, Gerhard Klimeck, Mark Hahnel, Denis Tenen, Kenneth Crews, "Research Data Symposium at Columbia University, Panel 4: Discover, Share, & Impact", Panel 4: Discover, Share, & Impact, Feb 27, 2013
- [11] "Symposium: Learning and Discovery in the Connected Age", Michigan Theatre, Oct. 8, 2012
- [10] "What do get out of a post-doc position", Panel Discussion organized by the Purdue Postdoctoral Association, Sept 22, 2011
- [9] "Open Source Developments in Nanotechnology", Host and Moderator: Dr. Rajinder Khosla, NSF Program Director Panelists: Chuck Bouldin (NSF Program Director, DMR), Sandip Tiwari (Director NNIN), Gerhard Klimeck (NCN Associate Director) NSF nano Grantee's Meeting, Dec. 4th, 2007
- [8] "Quantum Electronics", Host and Moderator: Dr. Gerhard Klimeck, Panelists: Kang Wang, Dragica Vasileska, Dmitri Nikonov, and Susan Coppersmith, NSF Workshop on Quantum, Molecular and High Performance Modeling and Simulation for Devices and Systems (QMHP), April 17, 2007.
- [7] "Cyber Infrastructure Roundtable Discussion, Host and Moderator: Ahmed Elmagarmid, Director Cyber Center", Panelists: Brian Wilson (SUN micorsystems, CTO), Gerhard Klimeck, Rudolf Eigenmann, David Ebert, Thomas J. Hacker
- [6] "Nano Frontiers Workshop", by invitation only, Meeting sponsored by NSF, NIH, Pew Charitable Trust, Wilson Center for International Scholars, Feb. 9-10, 2006.
- [5] "Panel Discussion: Nanotechnology in the Americas", GNN 2005, 3rd International Workshop to Develop a Global Nanotechnology Network, May 25-27, 2005, Saarbrücken, Germany.
- [4] "Panel discussion: Interaction with Industry", 2004 NSF Nanoscale Science and Engineering Grantees Conference, Washington, DC, Dec. 15, 2004.
- [3] "Opportunities on International Collaborations on Grid Computing", Grid Forum Korea (GFK) Summer Workshop, Seoul, Korea, Aug. 26-27, 2004, Moderator: Prof. Chan-Hyun Youn (ICU, Korea).
- [2] "Bird of a Feather Panel on HPC Innovation for Nanotechnology", Supercomputing Conference 2003, Phoenix, AZ, November 16-21, 2003, Moderator: Dr. David Kahaner (ATIP, Japan).
- [1] "Software Development at Academia, Government Labs, Industry", John Barker Agenda/Questions: How can the three share development? Possibly cooperation like designer chemistry software? What are the technical challenges? What is the software we are talking about anyways?, Glasgow, Scotland, UK, May 22-25, 2000, Moderator: Prof. John Barker (U. of Glasgow).