

Dr. Gerhard Klimeck

Purdue University, School of Electrical and Computer Engineering
465 Northwestern Avenue, West Lafayette, IN 47907

Office: (765) 494-9212
Email: gekco_at_purdue.edu

OBJECTIVE

Provide leadership to the Network for Computational Nanotechnology (NCN) Director and conduct nanoelectronic research, high performance computing, and software engineering.

EDUCATION

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

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

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

Advisor: Professor Daniel S. Elliott, Purdue.

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

EMPLOYMENT

Purdue University, School of Electrical and Computer Engineering

Professor, Director Network for Computational Nanotechnology 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 1,000 annual users in 2003 to over 132,000 users (as of June 2010)
 - Introduction of fully interactive simulations, >8,500 annual users >341,000 simulations
- Lead the development of NEMO 3-D and OMEN towards peta-scale computing applications. Demonstrated scaling to 222,000 processors – enabled multimillion atom electronic structure calculations and atomistic non-equilibrium Green Function treatments of transistors.
- Lead ~15 professional nanoHUB staff members and ~20 researchers in nanoelectronics.

NASA Jet Propulsion Laboratory, California Institute of Technology

Principal Member of Technical Staff (academic part time since 12/03) 9/01-present

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

Senior Member of Technical Staff, High Performance Computing Group 2/98-9/01

- Development of an atomistic nanoelectronic modeling and simulation tool, a genetic algorithm based 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,

Lecturer. Teaching “Advanced Semiconductor Device Theory”, graduate level course 5/97-8/97

Purdue University, School of Engineering 9/90-1/94

Research Assistant - Supervisor: Professor Supriyo Datta

Ruhr-University Bochum, EE, Research Assistant - Supervisor: Professor Eckhard Kneller 2/88-8/88

SELECTED HONORS

- Awarded Proposal Author as PI and lead Co-PI exceeding \$68,3M – including 5 center level grants.
- Co/Author of 125 journal, 121 proceedings, 125 inv. conf., 271 contr. conf., 215 sem./review, 33 Reports
- JPL Dr. Edward Stone Award for Outstanding Research Publication 2002.
- 12 NASA software, NASA board, NASA Space Act, and NASA Tech Brief Awards
- Two US Patents 6,490,193 and 6,667,490, memory cells in RTDs.
- Texas Instruments Award for timely delivery of the Phase II NEMO software.
- DARPA Award to Raytheon-TI Systems: Sustained Excellence by a Performer in FY97.
- Scholarships: Purdue Fee Remission Award, National Science Foundation of Germany.
- Member of ηκν EE Honor Society, τβπ Engineering Honor Society, IEEE (senior) and APS.
- Tae Kwon Do 2nd degree black belt.

PUBLICATION SUMMARY

- The following two pages highlight my research activities with references to publications.

• Publication count (excl. submissions): total			total
-Peer reviewed journals:	143	- Technical Reports:	34
-Peer reviewed proceedings:	140	- Invited Seminars:	107
-Invited conference papers:	147	- Technical Program Reviews	75
-Contributed conference papers:	308	- Technical Briefings	49

•Citation count in Database of Institute for Scientific Information (2/2002: 291) (2/2003: 425) (4/19/2004: 565) (2/16/2005: 672) (2/15/2006: 805) (2/13/2007: 954) (8/24/2008: 1342) (2/7/2009: 1627).

•Citation count in Google Scholar: (8/24/2008: 1710) (2/7/2009: 1916) (1/27/2010: 2516).

•h-index, generated from the web of science citations: (2/9/2009: h-index 22) (1/27/2010: h-index 26), years since PhD: 16

STRATEGIC HIGHLIGHTS (WORK PERFORMED AT JPL AND PURDUE)

- **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 2-7 – annual center renewals.
- **Transformation of the nanoHUB** - 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 1,000 simulation users were served with such 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 7,300 with over 394,000 simulation runs (data as of Jan. 2009). Over 130 interactive tools have been deployed. The key to this increase in user numbers is the usability of the HUB.
- **Nanoelectronic Modeling Research** - Lead a research group of around 20 graduate and undergraduate students plus 3-4 post-doctoral researchers and research faculty in the development of nanoelectronic modeling tools.
- **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 WORK (WORK PERFORMED AT PURDUE)

- **Deployment of interactive Simulation Tools on nanoHUB.org** – personally involved with 33 simulation tools in terms of their development, user interface-redesign, and/or deployment. Over 9,400 users ran over 324,000 simulations with these 33 tools (total count as of Feb 2009). In the last 12 months alone over 3,800 users ran over 185,000 simulations on these 33 tools.
- **Nanotechnology Tutorials on nanoHUB.org** –published 12 on-line contributions in forms of interactive Breeze presentations, pdf presentations, and/or Pod-Casts (on iTunes). Also coauthored over 100 homework and project assignments on nanoHUB in the summer of 2008 – enable “Tool Powered Curricula” on nanoHUB. (the abacus tool released in Aug. 2008 was used by 428 by Feb 2009). All “nanoHUB and more” content items have been used by over 21,000 users in the past 12 months (Feb. 2009) and over 45,000 users in total.

TOOL DEVELOPMENT HIGHLIGHTS (WORK PERFORMED AT TI, JPL AND PURDUE)

- **NEMO 3-D - Development of atomistic Nanoelectronic Modeling in 3-D** – Developed 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 (AT TI, JPL AND PURDUE)

- **Full 3D Atomistic Carrier Transport** – Guided work on combination of NEMO 1-D and NEMO 3-D principles into a quantum transport simulator. Demonstrated capability to model strained InAs/InGaAs/InAlAs HFETS [
- **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** - 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:** 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:** 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.
- **Scattering** - Studied 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).

PROGRAMMING EXPERIENCE

- **Software Project Management** - NEMO is a simulation tool consisting of about 250,000 lines of code. Personally wrote about 80,000 lines of code. Tackled issues of software design, documentation, release 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.
- **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].
- **Systems** - Linux, HP-9000, SUN, IBM-RISC, SGI, IBM SP2, Ardent, and GOULD, MAC, MS.

TEACHING EXPERIENCE

[Fall 09] "Nanoelectronic Modeling: From Quantum Mechanics and Atoms xto 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.

[Fall 09] "ECE 694 - Graduate Student Seminar Course" Mandatory Course for all ECE graduate Students. Purdue University. Instructor Goal: Coordinate presentations by external visitors on professional aspects of life after graduate school.

[Fall 96] "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 15-20 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

- 10/1987 Best in Prediploma Class in Electrical Engineering at the Ruhr University Bochum.
- 10/1990 Second Best in Diploma Class in Electrical Engineering at the Ruhr University Bochum.
- 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 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.

- 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.
- 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.

RESEARCH PROPOSAL AWARDS (PI OR PRIMARY CONTRIBUTOR)

- 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) 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). \$23,447k
- 8) 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. \$24,071k
- 9) 01/2004, NSF Teragrid, friendly user account, 50,000 SUs, "NEMO 3-D on Teragrid", PI: James Bottum, Co- PI: Gerhard Klimeck, Sebastien Goasguen.
- 10) 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. \$26,771k
- 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 though 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 Wasles, "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

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.

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.

PATENTS

- 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.
- 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.
- U.S. patent Application Serial No. 12/858,465, “Tunneling Field-Effect Transistor with Low Leakage Current”, Mathieu Luisier, Samarth Agarwal, Gerhard Klimeck

EDITOR

- Proceedings of the 10th International Workshop on Computational Electronics, Journal of Computational Electronics, Springer, ISSN 1569-8025 (Print) 1572-8137 (Online), Issue Volume 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, 3004. Springer Verlag, 2005.

PROGRAM COMMITTEE, CONFERENCE PREPARATION, CONFERENCE / SESSION CHAIR

- Program Committee, 27th international Symposium on Compound Semiconductors (ISCS), IEEE, (2000), Monterey, CA, Oct 2-5, 2000.
- Session Moderator, Quantum Transport, Advanced Research Workshop on Quantum Transport in Semiconductors, Maratea, Italy, June 17-22, 2001.

- Program Committee, Session Chair, Nanoelectronics Session, Nanospace 2002, Galveston, TX, June 24-28, 2002.
- Session Chair, Superlattices and Resonant Tunneling Structures, March Meeting of American Physical Society, March 16-21, Austin, TX (2003).
- Program Committee, 2nd International Workshop on Quantum Dots for Quantum Computing and Classical Size Effect Circuits, University of Notre Dame, August 7-9, 2003.
- Session Chair, Computational Approaches Toward the Electronic Properties of Quantum Dots Workshop, Chicago, September 22-24, 2003, sponsored by DARPA.
- Session Chair, "Advanced MOS Devices", 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona, Spain. October 16-17 2003.
- Program Committee, IEEE Nano 2004, Munich, Germany, August 16-19, 2004.
- Session Chair, IEEE Nano 2004, Session Nanoelectronics 1, Munich, Germany, August 16-19, 2004.
- Conference Chair, International Workshop for Computational Electronics, Purdue University, October 24-27, 2004.
- Program Committee, 15th Workshop on Modelling and Simulation of Electron Devices (MSED) 4-5 July 2005, Pisa, Italy.
- Program Committee, 14th International Conference on Nonequilibrium Carrier Dynamics in Semiconductors (HCIS-14), Chicago, Illinois, July 24-29, 2005.
- Program Committee, IEEE Nano 2005, Nagoya, Japan, August 11-15, 2005.
- IEEE IEDM Modeling and Simulation Program and Selection Committee, Vancouver, Canada, August 1st, 2005.
- 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.
- Program committee: HPCNano2005 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2005, Nov 12-18, 2005, Seattle, WA.
- Session Chair, IEEE IEDM Modeling and Simulation, Nanowires, Washington DC, Dec. 6th, 2005
- International Advisory Board, IEEE International Workshop for Computational Electronics, Technical University Vienna, May 25-27, 2006.
- "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
- Program committee: HPCNano2006 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2006, Nov 12-17, 2006, Tampa, FL.
- "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.
- Program Committee, MRS 2007 Spring Meeting, Session G, Extending Moore's Law with Advanced Channel Materials.
- 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
- 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
- International Advisory Board, IEEE International Workshop for Computational Electronics, University of Mass Amherst, Oct. 8-10, 2007.
- Workshop Co-Chair: HPCNano2007, Nov. 16, 2007 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2007, Reno, NV.
- "nanoHUB tutorial", IEEE Nano conference, Arlington, TX, August 18, 2008.

- Workshop Advisory Committee: HPCNano2008, Nov. 21, 2008 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2008, Austin TX.
- Workshop Advisory Committee: HPCNano2009, Nov. 15, 2009 (IEEE/ACM International Workshop on High Performance Computing for Nano-science and Technology), Supercomputing 2009, Portland OR.

EXTERNAL REVIEW PANEL SERVICE

- National Science Foundation, Jan 13-14, 2005, Review panel on Electronic Devices, Washington DC.
- National Science Foundation, Oct 31-Nov 1, 2006, Review panel on Electronic Devices, Washington DC.

ADVISORY BOARD SERVICE

- Advisory Board Meeting, NCCR Resource for Macromolecular Modelling and Bioinformatics, May 16, 2005, Chicago IL, PI.: Prof. Klaus Schulten, U Illinois Urbana-Champaign.
- Advisory Board Meeting, NSF NMI project, "nanoHUB Deployment", West Lafayette, IN 47907, PI: Sebastien Goasguen, Oct 2004-2007.
- Non-voting Ex-Officio AdCom member of the IEEE EDS Compact Modeling Committee.
- 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.
- Teragrid governance planning board, June 2007 - present.
- NSF Future of TeraGrid working Group, October 2007 - present.
- 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.
- Advisory Board Meeting, "NanoCMOS – e-Science - EPSRC", Oct 24, 2007, Host Asen Asenov, University of Glasgow.
- Advisory Board Meeting, "NanoCMOS – e-Science - EPSRC", Nov. 12, 2008, Host Asen Asenov, University of Southampton.
- Oak Ridge Leadership Facility (OLCF) User council, Advise OLCF on operational and user aspects, meets throughout the year in conference calls, Aug. 2009-present,
- Advisory Board Meeting, "NanoCMOS – e-Science - EPSRC", Nov. 14, 2009, Host Asen Asenov, University of York.

INDUSTRIAL COMMITTEE SERVICE

- SRC Multi-Scale Modeling Working Group, Feb. 2004 – Fall 08.
- ITRD – ERM (Emerging Research Materials) working group, July 2004 – Fall 08.

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 – present)

STUDENT SERVICES / OUTREACH

- 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: Tillmann Falk, Jannik Emde, Ralf Georg Hetmanczyk
 - AY05/06 students: Monica Siepmann, Markus Kasper, Hayg Dabag, Winfried Schüngel
 - AY06/07 students: Lars Wolleschensky, Martin Schiffner, Martin Oettmeier

- AY07/08 students: Gesine Hinterwalder, Lukas Lohaus, Oliver Mischke
- AY08/09 students: Michael Szelong, Matthias (Yui-Hong) Tan, Martin Beckmann
- AY09/10 students: Matthias (Yui-Hong) Tan, Patrick Wesskamp, Jan Trieschmann, Cornel Reuber
- AY10/11 students: Melanie Schmidt, Hendrik Vogt, Richard Ronig

JOURNAL REVIEWER / REFEREE

- Physical Review B
- physica status solidi b
- Superlattices and Microstructures
- IEEE Transactions on Electron Devices, IEEE Transactions on Nanotechnology
- Journal for Computational Electronics
- VLSI Design

PURDUE SCIENTIFIC MENTOR / ADVISOR

- Current Post-doc advisor to
 - Mathieu Luisier (Feb. 2008 - present)
 - Hong-Hyon Park (July 2009 – present)
 - Michael Povolotskyi (Sept. 2009 – present)
 - Denis Areshkin (June 2010 – present)
- Current Ph.D. student advisor to
 - Hoon Ryu, (July 2006 – present)
 - Sunhee Lee (Aug. 2006 – present)
 - Abhijeet Paul, (Aug. 2006 – present)
 - Saumitra Mehrota, (Aug. 2007 - present)
 - Sung Geun Kim (Aug. 2007 - present)
 - Yaohua Tan (Aug. 2008 – present)
 - Parijat Sengupta (Aug. 2008 – present)
 - Mehdi Salmani (Jan. 2009 – present)
 - Sung Hyon Park (Jan. 2010 – present)
 - Ganesh Hegde (May 2010 - present)
 - Yu He (Aug. 2010 - present)
- Current Master Student advisor to
 - Woo-Suhl Cho (Aug. 2008 – present)
 - Zhengping Jiang (Aug. 2008 – present)
 - Matthias Tan (Aug. 2009 – present)
 - Kai Miao (Aug. 2010 - present)
- Current Undergraduate Research Student advisor to
 - Win Than Aung (Dec. 2008 – present)
- Past Post-doc advisor to
 - 1) Olga Lazarenkova (Feb 2002-Jan 2004)
 - 2) Marek Korkusinski (July 2004-June 2005)
 - 3) Marta Prada (Jan 2006 – Sept. 2006)
 - 4) Clemens Heitzinger (August 2005-December 2006)
 - 5) Shaikh Ahmed (February 2005-Aug. 2007)
 - 6) Ben Haley (Nov. 2006 – Jan. 2010)
 - 7) Jean Michel Sellier (Nov. 2008 – May 2010)
- Graduated 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 Reifenberger (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
- Graduated 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) Sung Hyon Park (continued for PhD) (Aug. 2007 – Dec. 2009)
Hyperfine Mapping of Donor Wave Function Deformations in Silicon Phosphorous Based Quantum Devices
 - 4) 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
 - 5) Xufeng Wang, co-advised with M. Lundstrom (continued for PhD Lundstrom) (Aug. 2008 – present)
nanoMOS 4.0: A tool to explore ultimate Si transistors and beyond.
 - Graduated Undergraduate Research Student advisor to
 - Aaron Christensen June - Aug 04
 - Adrian Rios June - Aug 04
 - Patrick Macnamara June - Aug 04
 - Laurie St. Ange June - Aug 04
 - Muriel Fort June - Aug 04
 - Sameer Hamdan June - Aug 04
 - Akira Matsudaira (June 2005-Jan 2006)
 - Katie Ikuku Kitamura (June 2005-Dec 2005)
 - Matteo Mannino (May 2005-May 2006), (Jan 2007 – June 2007)
 - Anish Dhanekula (June 2006 – Jan 2007)
 - Xufeng Wang (June 2006 – Aug. 2008)
 - Sriraman Damodaran (Sept 2006 – Dec. 2007)
 - Amanda Weitzel (Sept 2006 – May 2007)
 - Thomas Andrews May 08-Aug 08
 - Drew Schuster May 08-Aug 08
 - Gloria Budiman May 08-Aug 08, May 09-Aug. 09
 - Mario Salaomon May 08-Aug 08
 - Naman Chopra (Nov. 2008 – Aug. 09)
 - Gloria Budiman May 09-Aug 09
 - Matthias Tan (Aug. 2008 – May 09)
 - Junzhe Geng May 09-Aug 09
 - Victoria Savikhin May 09-Aug 09
 - Abhinav Sinha <abhinavsinha@iitb.ac.in>, May-Aug. 2010
 - Matthew Buresh <mjburesh@asu.edu>, May-Aug. 2010
 - Lars Bjaalie <bjaalie1@illinois.edu>, May-Aug. 2010
 - Siqi Wang <>wang340@purdue.edu>, May-Aug. 2010
 - Muhammad Zulkifli <mzulkifli@purdue.edu>, May-Aug. 2010
 - Krystal Hoganson <khoganson@miners.utep.edu> May-Aug. 2010
 - Past Ph.D. student advisor to
 - Srikant Srinivasan, Co-advisor with Leonid Rokhinson (Aug. 2005 – Dec. 2006)
 - Abu Naser Zainuddin, (Aug. 2006 – Aug. 2007)

- Past Master Student advisor to
 - Jing Li (Aug 2004 – Aug. 2005).
 - Selvakumaran Vadivelmurugan (Aug 2006 – Jan. 2007).
 - Hemanth Hedge, (Aug. 2006 – May 2007)
 - Rezwan Chowdhury, (Aug. 2006 – May 2007)
 - Seungmin Kim, (Aug. 2007 – Aug. 2008)

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 – present), non-thesis
- Kurtis Cantley (Aug 2005 – present), 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 – present), advised by Prof. Supriyo Datta
 - Ra Seong Kim (Aug 2005 – present), advised by Prof. Mark Lundstrom
 - Stephen Cauley (Aug 2005 – present), 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 – present), advised by Prof. Supriyo Datta
 - Adina Deborah Scott (Aug 2005 – Dec. 08), advised by Prof. David Janes

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.

PUBLICATION SUMMARY

- **Publication count** (excl. submissions): total total
 - Peer reviewed journals: 143 - Technical Reports: 34
 - Peer reviewed proceedings: 140 - Invited Seminars: 107
 - Invited conference papers: 147 - Technical Program Reviews 75
 - Contributed conference papers: 308 - Technical Briefings 49
- Citation count in Database of Institute for Scientific Information (2/2002: 291) (2/2003: 425) (4/19/2004: 565) (2/16/2005: 672) (2/15/2006: 805) (2/13/2007: 954) (8/24/2008: 1342) (2/7/2009: 1627).
- Citation count in Google Scholar: (8/24/2008: 1710) (2/7/2009: 1916) (1/27/2010: 2516).
- h-index, generated from the web of science citations: (2/9/2009: h-index 22) (1/27/2010: h-index 26), years since PhD: 16

Year	Journals	Proceedings	Inv. Conf	Conference	Tech. Rep.	Inv. Sem.	Reviews	Briefings
1990	1			2				
1991	1 / 2				1			
1992	1 / 3			3				
1993	2 / 5		1	3 / 6	1	1		
1994	3 / 8		3 / 4	8 / 16	1 / 3	2 / 3	2	
1995	2 / 10	5	2 / 6	6 / 22	1 / 4		8 / 10	
1996	2 / 12	3 / 8	3 / 9	4 / 26		5 / 8	7 / 17	
1997	5 / 17	8 / 16	6 / 15	9 / 35	1 / 5	3 / 11	4 / 21	
1998	7 / 24	1 / 17	3 / 18	5 / 40	4 / 9	4 / 15		
1999	3 / 27	5 / 22	1 / 19	9 / 49	2 / 11	1 / 16	1 / 22	
2000	2 / 29	5 / 27	2 / 21	8 / 57		3 / 19	2 / 24	
2001	6 / 35	5 / 32	3 / 24	14 / 71		1 / 20	1 / 25	
2002	6 / 41	2 / 34	6 / 30	20 / 91	9 / 20	10 / 30	3 / 28	
2003	5 / 46	8 / 42	9 / 39	15 / 106		4 / 34	1 / 29	
2004	9 / 55	14 / 56	12 / 51	20 / 126	1 / 21	11 / 45	7 / 36	14
2005	11 / 66	11 / 67	17 / 68	20 / 146	3 / 24	10 / 55	6 / 42	9 / 23
2006	7 / 73	12 / 79	18 / 86	36 / 182	2 / 26	13 / 68	9 / 51	3 / 26
2007	17 / 90	10 / 89	19 / 105	29 / 211	3 / 29	11 / 79	4 / 55	11 / 37
2008	21 / 111	21 / 110	14 / 119	31 / 242	3 / 32	11 / 90	8 / 61	5 / 42
2009	14 / 125	17 / 127	8 / 127	34 / 276	1 / 33	10 / 100	8 / 69	7 / 49
2010-current	18 / 143	13 / 140	20 / 147	32 / 308	1 / 34	7 / 107	6 / 75	

BOOK

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

SUBMITTED JOURNAL PUBLICATIONS

[xxx] Muhammad Usman, Yui H. Matthias Tan, Hoon Ryu, Shaikh S. Ahmed, Timothy B. Boykin, Gerhard Klimeck, "Quantitative Excited State Spectroscopy of a Single InGaAs Quantum Dot Molecule through Multi-million Atom Electronic Structure Calculations", submitted for publication.

[xxx] Giuseppe Carlo Tettamanzi, Abhijeet Paul, Sunhee Lee, Saumitra R. Mehrotra, Nadine Collaert, Serge Biesemans, Gerhard Klimeck, Sven Rogge, "Interface Trap Density Metrology of state-of-the-art undoped Si n-FinFETs", submitted for publication

[xxx] Abhijeet Paul, Gerhard Klimeck, "Tuning lattice thermal conductance by porosity control in ultra-scaled Si and Ge nanowires", submitted for publication.

- [xxx] Neerav Kharche, Gerhard Klimeck, Dae-Hyun Kim, Jesoes. A. del Alamo, Mathieu Luisier, "Multiscale Metrology and Optimization of Ultra-Scaled InAs Quantum Well FETs", submitted for publication.
- [xxx] SungGeun Kim, Abhijeet Paul, Mathieu Luisier, Timothy B. Boykin, Gerhard Klimeck, "Full 3D Quantum Transport Simulation of Atomistic Interface Roughness in Silicon Nanowire FETs", submitted for publication (2009).
- [xxx] Rajib Rahman, Seung H. Park, Gerhard Klimeck, Lloyd C. L. Hollenberg, "Stark tuning of the charge states of a two-donor molecule in silicon", submitted for publication (2009).

JOURNAL PUBLICATIONS (WORK PERFORMED AT JPL AND PURDUE)

- [143] Shweta Deora, Abhijeet Paul, Bijesh R, Jeff Huang, Gerhard Klimeck, Gennadi Bersuker, Paul Kirsch, Raj Jammy, "Intrinsic Reliability improvement in Biaxially Strained SiGe p-MOSFETs", IEEE Electron Device Letters, Accepted for publication Dec. 6th, 2010;
- [142] Martha Prada, Gerhard Klimeck, and Robert Joynt, "Spin-orbit splittings in Si/SiGe quantum wells", accepted for publication (2009). Abstract on arXiv:0908.2417
- [141] Tillmann Kubis, Saumitra Raj Mehrotra, Gerhard Klimeck, "Design concepts of terahertz quantum cascade lasers: Proposal for terahertz laser efficiency improvements", Applied Physics Letters Vol.97, Issue 26
- [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
- [138] Rajib Rahman, Richard P. Muller, James E. Levy, Malcolm S. Carroll, Gerhard Klimeck, Andrew D. Greentree, Lloyd C. L. Hollenberg, " Coherent electron transport by adiabatic passage in an imperfect donor chain", Phys. Rev. B. (2010) Vol. 55, Issue 3. arXiv: 1008.1494
- [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 B.Boykin, Mathieu Luisier, Gerhard Klimeck, "Current density and continuity in discretized models", European Journal of Physics, Vol 31, pg:1077(2010).
- [135] Mincheol Shin, Sunhee Lee, and Gerhard Klimeck, "Computational Study on the Performance of Si nanowire pMOSFETs based on the k·p method", IEEE Transactions on Electron Devices, Vol 57, pg: 2274 (2010).
- [134] Neophytos Neophytou, Sung Geun 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 of Appl. Physics, Vol. 107, 113701 (2010).
- [133] Alejandro Strachan, Gerhard Klimeck, Mark S. Lundstrom, Cyber-Enabled Simulations in Nanoscale Science and Engineering INTRODUCTION, Computing in Science and Engineering, Vol. 12, pg: 12-17 (2010)
- [132] Timothy B. Boykin, Mathieu Luisier, Mehdi Salmani-Jelodar, and 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 and Gerhard Klimeck, "Simulations of Nanowire Tunneling Transistors: from the WKB Approximation to Full-Band Phonon-Assisted Tunneling", J of Appl. Physics, 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, pg. 621 (2010)
- [129] Mathieu Luisier and 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 and Gerhard Klimeck, "Performance Prediction of Ultra-scaled SiGe/Si Core/Shell Electron and Hole Nanowire MOSFETs", IEEE Electron Device Letters, Vol. 31 pg. 278-280 (2010).
- [127] Gerhard Klimeck and Mathieu Luisier, "Atomistic Modeling of Realistically Extended Semiconductor Devices with NEMO /OMEN", IEEE Computing in Science and Engineering (CISE) Vol.12, pg. 28-35 (2010).
- [126] Giuseppe C. Tettamanzi, Abhijeet Paul, Gabriel P. Lansbergen, Jan Verduijn, Sunhee Lee, Nadine Collaert, Serge Biesemans, Gerhard Klimeck and Sven Rogge, "Thermionic Emission as a tool to study transport in undoped nFinFETs", IEEE Electron Device Letters, Vol. 518 pg. 2521-2523 (2009).
- [125] Samarth Agarwal, Kyle H. Montgomery, Timothy B. Boykin, Gerhard Klimeck, and Jerry M. Woodall, "Design Guidelines for True Green LEDs and High Efficiency Photovoltaics Using ZnSe/GaAs Digital Alloys", Electrochemical and Solid-State Letters Vol. 13, pp. H5-H7 (2010).
- [124] Mathieu Luisier and Gerhard Klimeck, "Atomistic Full-Band Simulations of Si Nanowire Transistors: Effects of Electron-Phonon Scattering", Phys. Rev. B, Vol. 80, 155430 (2009).
- [123] Rajib Rahman, G. P. Lansbergen, Seung H. Park, J. Verduijn, Gerhard Klimeck, S. Rogge, and Lloyd C. L. Hollenberg, "Orbital Stark effect and quantum confinement transition of donors in silicon", Phys. Rev. B, Vol. 80, 098936 (2009). Xarchive 0904.4281
- [122] Rajib Rahman, Seung H. Park, Timothy B. Boykin, Gerhard Klimeck, Sven Rogge, Lloyd C. L. Hollenberg, "Gate induced g-factor control and dimensional transition for donors in multi-valley semiconductors", Physical Review B, Vol. 80 134935 (2009).
- [121] Seung H. Park, Rajib Rahman, Gerhard Klimeck, Lloyd C. L. Hollenberg, "Mapping donor electron wave function deformations at sub-Bohr orbit resolution", Phys. Rev. Letter, Vol. 103, 106802 (2009). Abstract on Xarchive, PDF on Xarchive
- [120] Benjamin P. Haley, Gerhard Klimeck, Mathieu Luisier, Dragica Vasileska, Abhijeet Paul, Swaroop Shivarajapura, Diane L. Beaudoin, "Computational nanoelectronics research and education at nanoHUB.org", Journal of Computational Electronics, online July 2009, DOI 10.1007/s10825-009-0273-3.
- [119] Rajib Rahman, Seung H. Park, Jared H. Cole, Andrew D. Greentree, Richard P. Muller, Gerhard Klimeck, and Lloyd C. L. Hollenberg, "Atomistic simulations of adiabatic coherent electron transport in triple donor systems", Phys. Rev. B, Vol. 80, 035302 (2009)
- [118] Mathieu Luisier, and Gerhard Klimeck, "Performance analysis of statistical samples of graphene nanoribbon tunneling transistors with line edge roughness", Applied Physics Letters, Vol. 94, 223505 (2009), DOI:10.1063/1.3140505
- [117] Hui Zhao, Raseong Kim, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, Fa-Jun Ma, Subhash C. Rustagi, Ganesh S. Samudra, Navab Singh, Guo-Qiang Lo, and Dim-Lee Kwong, "Characterization and Modeling of Subfemtofarad Nanowire Capacitance Using the CBCM Technique", IEEE Electron Device Letters Vol. 30, pp: 526 - 528 (2009).
- [116] Mathieu Luisier, and Gerhard Klimeck, "Atomistic, Full-Band Design Study of InAs Band-to-Band Tunneling Field-Effect Transistors", IEEE Electron Device Letters, Vol. 30, pp. 602-604 (2009), DOI: 10.1109/LED.2009.2020442 (2009).

- [115] Neophytos Neophytou and Gerhard Klimeck, "Design space for low sensitivity to size variations in [110] PMOS nanowire devices: The implications of anisotropy in the quantization mass", nano letters Vol. 9 (2), pp 623–630 (2009).
- [114] Muhammad Usman, Hoon Ryu, Insoo Woo, David S. Ebert, and Gerhard Klimeck, "Moving towards nano-TCAD through multi-million atom quantum dot simulations matching experimental data", IEEE Transactions on Nanotechnology, Vol. 8, Issue 3, pg. 330-344 (2009), DOI: 10.1109/TNANO.2008.2011900 (2009).
- [113] Neerav Kharche, Seongmin Kim, Timothy B. Boykin, and Gerhard Klimeck, "Valley Degeneracies in (111) Silicon Quantum Wells", Applied Physics Letters, Vol. 94, Issue 4, id. 042101 (3 pages) (2009). (also at cond-mat arXiv:0812.3681v1).
- [112] Timothy B. Boykin, Neerav Kharche, and 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, and Alejandro Strachan, "Structures and energetics of Si nanotubes from molecular dynamics and density functional theory", Phys. Rev. B, Vol. 78, 205315 (2008), selected for Virtual Journal of Nanoscale Science&Technology.
- [110] Mark S. Lundstrom, Gerhard Klimeck, George B. Adams III., Michael McLennan, "HUB is where the heart is", IEEE Nanotechnology Magazine, Vol. 2, Issue 1, March 2008 Page(s):28 – 31.
- [109] Neophytos Neophytou, Abhijeet Paul, and Gerhard Klimeck, "Bandstructure Effects in Silicon Nanowire Hole Transport", IEEE Transactions on Nanoechnology - Special issue on nanowires, Vol. 7, 710 - 719 (2008)
- [108] Nancy Wilkins-Diehr, Dennis Gannon, Gerhard Klimeck, Scott Oster, Sudhakar Pamidighantam, "TeraGrid Science Gateways, Virtual Organizations and Their Impact on Science", IEEE Computer, Vol. 41, Issue 11, Nov. 2008, Page(s):32 - 41.
- [107] Raseong Kim, Neophytos Neophytou, Abhijeet Paul, Gerhard Klimeck, and Mark S. 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, pg 1628 (2008).
- [106] Srikant Srinivasan, Gerhard Klimeck, and Leonid P. Rokhinson, "Valley splitting in Si quantum dots embedded in SiGe", Applied Physics Letters, Vol. 93, pg. 112102 (2008) (Cond-mat <http://arxiv.org/abs/0808.1234>).
- [105] Marek Korkusinski, Pawel Hawrylak, M. Zielinski, W. Sheng, and 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, Steve Clark, Benjamin Haley, Maxim Naumov, Faisal Saied, Marek Korkusinski, Rick Kennel, Michael McLennan, Timothy B. Boykin, and Gerhard Klimeck, "Multimillion Atom Simulations with NEMO 3-D ", accepted in Springer Encyclopedia for Complexity, 2008
- [103] Song Li, Shaikh Ahmed, Gerhard Klimeck, and 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] Timothy B. Boykin, Neerav Kharche and Gerhard Klimeck, "Valley splitting in finite barrier quantum wells", Phys. Rev. B, Vol. 77, 245320 (2007).
- [101] G.P. Lansbergen, R. Rahman, C.J. Wellard, P.E. Rutten, J. Caro, N. Collaert, S. Biesemans, I. Woo, G. Klimeck, L.C.L. Hollenberg, and S. Rogge, "Gate induced quantum confinement transition of a single dopant atom in a Si FinFET", Nature Physics, Vol. 4, pg. 656 (2008).

- [100] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom and Gerhard Klimeck, "Bandstructure Effects in Silicon Nanowire Electron Transport", IEEE Transaction on Electron Devices, Vol. 55, pg. 1286-1297 (2008).
- [99] Yang Liu, Neophytos Neophytou, Gerhard Klimeck, and Mark S. Lundstrom, "Band Structure Effects on the Performance of III-V Ultra-thin-body SOI MOSFETs", IEEE Transaction on Electron Devices, Vol. 55, Issue 5, pg. 1116 - 22 (2008).
- [98] Gianluca Fiori, Giuseppe Iannaccone, and 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, No. 4, pg. 1094-5 (2008).
- [97] Gerhard Klimeck, Michael McLennan, Sean B. Brophy, George B. Adams III, Mark S. Lundstrom, "nanoHUB.org: Advancing Education and Research in Nanotechnology", IEEE Computers in Engineering and Science (CISE), Vol. 10, pg. 17-23 (2008).
- [96] Timothy B. Boykin, and Mathieu Luisier, and Gerhard Klimeck "Multi-band transmission calculations for nanowires using an optimized renormalization method", Phys Rev B, Vol. 77, 165318 (2008).
- [95] Maxim Naumov, Sunhee Lee, Ben Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Steve Clark, and Gerhard Klimeck, "Eigenvalue Solvers for Atomistic Simulations of Electronic Structures with NEMO-3D", Journal of Computational Electronics, Vol. 7, pg. 297–300 (2008).
- [94] Roksana Golizadeh-Mojarad, A.N.M. Zainuddin, Shaikh S. Ahmed, Gerhard Klimeck, and Supriyo Datta, "Atomistic Non-equilibrium Green's Function Simulations of Graphene Nano-Ribbons in the Quantum Hall Regime", Journal of Computational Electronics, Vol. 7, pg. 407–410 (2008).
- [93] Neerav Kharche, Mathieu Luisier, Timothy B. Boykin, and Gerhard Klimeck, "Electronic Structure and Transmission Characteristics of SiGe Nanowires", Journal of Computational Electronics, Vol. 7, pg. 350–354 (2008).
- [92] Neophytos Neophytou, Abhijeet Paul, Mark S. Lundstrom, and Gerhard Klimeck, "Simulation of nanowire transistors: Atomistic vs. Effective Mass Models", Journal of Computational Electronics, Vol. 7, pg. 363–366 (2008).
- [91] Bhaskaran Muralidharan, Hoon Ryu, Z. Huang, and 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).
- [90] Yang Liu, Neophytos Neophytou, Tony Low, Gerhard Klimeck, and Mark S. Lundstrom, "A Tight-binding Study of the Ballistic Injection Velocity for Ultra-thin-body SOI MOSFETs", IEEE Transaction on Electron Devices, Vol. 55, Issue 3, pg. 866-71 (2008).
- [89] Rajib Rahman, Cameron. J. Wellard, Forrest R. Bradbury, Marta Prada, Jared H. Cole, Gerhard Klimeck, and Lloyd C. L. Hollenberg, "High precision quantum control of single donor spins in Si", Physical Review Letters Vol 99, pg 036403 (2007); selected to virtual journal of nano science, also posted on arxiv.org/abs/0705.2079-
- [88] Timothy B. Boykin, Neerav Kharche, and 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 Ali Yanik, Gerhard Klimeck, and Supriyo Datta, "Quantum Transport with Spin Dephasing: A Nonequilibrium Green's function Approach", Phys. Rev. B Vol. 76, 045213 (2007), also posted cond-mat/0605037 .

- [86] INVITED: Gerhard Klimeck, Shaikh Ahmed, Neerav Kharche, Marek Korkusinski, Muhammad Usman, Marta Prada, and Timothy B. Boykin, "Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D: Part II - Applications", Special Issue on Nanoelectronic Device Modeling in IEEE Transactions on Electron Devices, Vol. 54, Issue 9, pg. 2090 - 2099 (2007).
- [85] INVITED: Gerhard Klimeck, Shaikh Ahmed, Hansang Bae, Neerav Kharche, Steve Clark, Benjamin Haley, Sunhee Lee, Maxim Naumov, Hoon Ryu, Faisal Saied, Marta Prada, Marek Korkusinski, and Timothy B. Boykin, "Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D: Part I - Models and Benchmarks", Special Issue on Nanoelectronic Device Modeling in IEEE Transactions on Electron Devices, Vol. 54, Issue 9, pg. 2079 - 2089 (2007).
- [84] Timothy B. Boykin, Neerav Kharche, and Gerhard Klimeck, "Evolution time and energy uncertainty", Eur. J. Phys. 28 (2007) 673-678 (2007).
- [83] Neophytos Neophytou, Shaikh Ahmed and Gerhard Klimeck, "Influence of vacancies on metallic nanotube transport properties", Applied Physics Letters Vol 90, 182119 (2007).
- [82] Gianluca Fiori, Giuseppe Iannacone, and Gerhard Klimeck, "Coupled mode space approach for the simulation of realistic Carbon Nanotube Field Effect Transistors", IEEE Transaction on Nanotechnology, Vol. 6, pg. 475-480 (2007).
- [81] Gengchiao Liang, Jie Xiang, Neerav Kharche, Gerhard Klimeck, Charles M. Lieber, and Mark Lundstrom, "Performance Analysis of a Ge/Si Core/Shell Nanowire Field Effect Transistor", cond-mat/0611226, Nano letters, Vol. 7, 642-646 (2007).
- [80] Shaikh Ahmed, Gerhard Klimeck, Derrick Kearney, Michael McLennan, and M. P. 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, Marta Prada, Timothy B. Boykin, and Gerhard Klimeck, "Valley-splitting in strained Silicon quantum wells modeled with 2 degree miscuts, step disorder, and alloy disorder", Applied Phys. Lett. Vol. 90, 092109 (2007).
- [78] Clemens Heitzinger and Gerhard Klimeck, "Numerical 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, and Gerhard Klimeck, "Transport Calculation of Semiconductor Nanowires Coupled to Quantum Well Reservoirs", Journal of Computational Electronics, Vol. 6, pg. 199-202, 2007.
- [76] Neophytos Neophytou, Shaikh Ahmed, and 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, 2007.
- [75] Vladimir V. Mitin, Nizami Z. Vagidov, Mathieu Luisier, and Gerhard Klimeck, "Energy Dispersion Relations for Holes in Silicon Quantum Wells and Quantum Wires", Journal of Computational Electronics Vol. 6, pg. 227-230, 2007.
- [74] Timothy B. 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).
- [73] Timothy B. Boykin, Mathieu Luisier, Andreas Schenk, Neerav Kharche, Gerhard Klimeck, "Atomistic, random-alloy calculations of the electronic structure and transmission characteristics of AlGaAs nanowires", IEEE Transactions on Nanotechnology, Vol. 6, No. 1, 43-7 (2007).

- [72] Wei Qiao, Michael McLennan, Rick Kennell, David Ebert, and Gerhard Klimeck, "Hub-based Simulation and Graphics Hardware Accelerated Visualization for Nanotechnology Applications", IEEE Transactions on Visualization and Computer Graphics, Vol. 12, pg. 1061-1068 (2006).
- [71] Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, and Gerhard Klimeck, "Atomistic Simulation of Nanowires in the $sp^3d^5s^*$ Tight-Binding Formalism: from Boundary Conditions to Strain Calculations", Phys. Rev. B 74, 205323 (2006).
- [70] Gianluca Fiori, Giuseppe Iannaccone, and 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, pg 1782 (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 B. 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. P. Drachev, W. Cai, U. Chettiar, H.-K. Yuan, A. K. Sarychev, A. V. Kildishev, G. Klimeck, and V. M. Shalaev, "Experimental verification of an optical negative-index material", Laser Phys. Lett. Vol. 3, 49-55 (2006).
- [66] A. S. Martins, Timothy B. Boykin, Gerhard Klimeck, and Belita Koiller, "A new conduction band tight-binding description for silicon applied to P donors in Si", Phys. Rev. B Vol. 72 pg. 193204 (2005).
- [65] Yong S. Joe, Arkady M. Satanin, and 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), selected for the September 26, 2005 issue of Virtual Journal of Nanoscale Science & Technology.
- [64] Timothy B. Boykin and 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 and Mark Lundstrom, "On the Validity of the Parabolic Effective-Mass Approximation for the Current-Voltage Calculation of Silicon Nanowire Transistors", IEEE Transactions on Electron Devices, Vol. 52 (7): 1589-1595 (2005).
- [62] Yun Zheng, Cristian Rivas, Roger Lake, Khairul Alam, Timothy B. Boykin, and Gerhard Klimeck, "Electronic Properties of Silicon Nanowires", IEEE Transactions on Electron Devices, Vol. 52 (6): 1097-1103 (2005).
- [61] Jeremy Green, Timothy B. Boykin, Corrie D. Farmer, Michel Garcia, Charles N. Ironside, Gerhard Klimeck, Roger Lake, and Colin R. Stanley, "Quantum cascade laser gain medium modeling using a second-nearest-neighbor sp^3s^* tight-binding model", Superlattices and Microstructures, Vol. 37, pg. 410-424 (2005).
- [60] Timothy B. Boykin, Gerhard Klimeck, Paul von Allmen, Seungwon Lee, and Fabiano Oyafuso, "Valley-splitting in V-shaped quantum wells", J. of Appl. Phys, Vol 97, pg. 113702 (2005).
- [59] Carl L. Gardner, Gerhard Klimeck, and 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).
- [58] Jing Wang, Anisur Rahman, Avik Ghosh, Gerhard Klimeck and Mark Lundstrom, "Performance Evaluation of Silicon Nanowire Transistors with Atomic-basis Dispersion Relations", Applied Phys. Lett. Vol. 86 (9): Art. No. 093113 (2005).

- [57] Timothy B. Boykin and Gerhard Klimeck, "Practical Application of Zone-Folding Concepts in Tight-Binding", *Physical Review B*, Vol. 71, 115215 (2004).
- [56] Anisur Rahman, Gerhard Klimeck, Mark Lundstrom, Nizami Vagidov, and Timothy B. Boykin, "Atomistic Approach for Nano-Scale Devices at the Scaling Limit and Beyond - Valley Splitting in Si", *Japanese Journal of Applied Physics* Vol. 44, No. 4B, pp. 2187-2190 (2005).
- [55] Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, K. Birgitta 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). Also selected for *Virtual Journal of Nanoscale Science and Technology*.
- [54] Timothy B. Boykin, Gerhard Klimeck, M. A. Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Valley splitting in low-density quantum-confined heterostructures studied using tight-binding models", *Phys. Rev. B*. Vol. 70, 165325 (2004).
- [53] Olga L. Lazarenkova, Paul von Allmen, Fabiano Oyafuso, Seungwon Lee, and 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 L. Lazarenkova, Fabiano Oyafuso, Paul von Allmen, and 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). Also selected for *Virtual Journal of Nanoscale Science and Technology*.
- [51] Timothy B. Boykin and Gerhard Klimeck, "The discretized Schrödinger equation and simple models for semiconductor quantum wells", *Eur. J. Phys.*, Vol. 25 No 4, 503-514 (2004).
- [50] Olga L. Lazarenkova, Paul von Allmen, Fabiano Oyafuso, Seungwon Lee, and Gerhard Klimeck, "Atomistic model for the simulation of acoustical phonons, strain distribution, and Grüneisen coefficients in zinc-blende semiconductors", *Superlattices and Microstr.*, Vol 34, pg 553-556 (2004).
- [49] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures with empirical tight-binding model", *Phys. Rev. B* 69, 045316 (2004).
- [48] Timothy B. Boykin, Gerhard Klimeck, and Fabiano Oyafuso, "Valence band effective mass expressions in the $sp^3d^5s^*$ empirical tight-binding model applied to a new Si and Ge parameterization", *Phys. Rev. B*. 69, 115201, No 11 (2004)
- [47] Timothy B. Boykin, Gerhard Klimeck, Mark Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and 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 R. Frensley, Gerhard Klimeck, Phillip E. Thompson, Karl D. Hobart, Sean L. Rommel, and Paul R. Berger, "Full Band Modeling of the Excess Current in a Delta-Doped MBE Grown Silicon Tunnel Diode", *J. of Appl. Phys.*, Vol 94, No. 8, pg 5005-5013 (2003).
- [44] Fabiano Oyafuso, Gerhard Klimeck, Paul von Allmen, Tim Boykin, and R. Chris 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, and Wiley Kirk, "Off-Center Electron Transport and Breakdown of Tsu-Esaki Formula in Resonant Tunneling Diodes due to Incoherent Scattering", *Phys. Rev. B.*, Vol 68, 115320 (2002).

- [42] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Paul von 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. Chris Bowen, Timothy B. Boykin, Thomas A. Cwik, Edith Huang, and 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, pp 75-79 (2002).
- [39] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. 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 W. Wilkins, Garnett Bryant, and Gerhard Klimeck, "Many-body levels of multiply charged and laser-excited InAs nanocrystals modeled by empirical tight binding", *Phys. Rev. B* 66, 235307 (2002). Also selected for *Virtual Journal of Nanoscale Science and Technology*.
- [37] Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and, 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 B. Boykin R. Chris Bowen, and, Paul von 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), ISSN: 1526-1492.
- [35] Timothy B. Boykin, R. Chris Bowen, and, 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. Chris Bowen, and Timothy B. 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, and John W. Wilkins, Garnett Bryant, and Gerhard Klimeck, "Electron-hole correlations in semiconductor quantum dots with tight-binding wave functions", *Phys. Rev. B* Vol. 63, 195318 (2001). Also selected for *Virtual Journal of Nanoscale Science and Technology*.
- [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 R. Frensley, Massimo V. Fischetti, Phillip E. Thompson, Sean L. Rommel, and Paul R. Berger, "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. Chris Bowen, and Timothy B. Boykin, "Off Zone Center (Indirect Bandgap Like) Hole Transport in Heterostructures", *Phys. Rev. B.*, Vol. 63, pg. 195310 (2001).
- [29] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Thomas A. Cwik, "sp³s* Tight-Binding Parameters for Transport Simulations in Compound Semiconductors", *Superlattices and Microstructures* Vol. 27, pp. 519-524 (2000).
- [28] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, Carlos Salazar-Lazaro, Thomas A. Cwik, and 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 B. Boykin, R. Chris Bowen, Gerhard Klimeck, and Kevin L. Lear, "Resonant-tunneling diodes with emitter prewells", *Appl. Phys. Lett.*, Vol. 75, 1302 (1999).
- [26] Timothy B. Boykin, Lisa J. Gamble, Gerhard Klimeck, and R. Chris Bowen, "Valence-band warping in tight-binding models", *Phys. Rev. B* Vol. 59, 7301 (1999).
- [25] Timothy B. Boykin, Roger K. Lake, Gerhard Klimeck, and Mukund Swaminathan, "Interface effects in tunneling models with identical real and complex dispersions", *Phys. Rev. B* Vol. 59, 7316 (1999).

JOURNAL PUBLICATIONS (WORK PERFORMED PRIOR TO JPL AT TI)

- [24] Gerhard Klimeck, Dan Blanks, Roger Lake, R. Chris Bowen, Chenjing L. Fernando, Manhua Leng, William R. Frensley, Dejan Jovanovic, and Paul Sotirelis, "Writing Research Software in a Large Group for the NEMO Project", *VLSI Design* Vol. 8, pg 79 (1998).
- [23] Seal L. Rommel, Thomas E. Dillon, M. W. Dashiell, H. Feng, J. Kolodzey, Paul R. Berger, Phillip E. Thompson, Karl D. Hobart, Roger Lake, Alan C. Seabaugh, Gerhard Klimeck and Daniel K. 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 and Daniel K. 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 and Daniel K. 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 K. Lake, R. Chris Bowen, Chenjing L. Fernando and William R. Frensley, "Resolution of Resonances in a General Purpose Quantum Device Simulator", *VLSI Design* Vol. 6, pg. 107 (1998).
- [19] Roger K. Lake, Gerhard Klimeck, R. Chris Bowen, Dejan Jovanovic, Paul Sotirelis and William R. Frensley, "A Generalized Tunneling Formula for Quantum Device Modeling", *VLSI Design*, Vol. 5, pg 9 (1998).
- [18] Gerhard Klimeck, Roger Lake and Daniel K. Blanks, "Role of interface roughness scattering in self-consistent resonant tunneling diode simulation", *Phys. Rev. B*, Vol. 58, 7279 (1998).
- [17] Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and Roger Lake, "Effective Mass Reproducibility of the Nearest-Neighbor sp^3s^* Models: Analytic Results", *Phys. Rev. B* Vol. 56, 4102 (1997).
- [16] Gerhard Klimeck, Roger Lake, Dan Blanks, Chenjing L. Fernando, R. Chris Bowen, Ted Moise, and Y. C. 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. Chris Bowen, Dejan Jovanovic, Dan 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. Chris Bowen and Dejan Jovanovic, "Single and multiband modeling of quantum electron transport through layered semiconductor devices", *J. of Appl. Phys.* 81, 7845 (1997).
- [13] R. Chris Bowen, Gerhard Klimeck, Roger Lake, William R. Frensley and Ted Moise, "Quantitative Resonant Tunneling Diode Simulation", *J. of Appl. Phys.* 81, 3207 (1997).

- [12] Roger K. Lake, Gerhard Klimeck, R. Chris Bowen, Chenjing L. Fernando, Manhua Leng, Ted Moise and Y. C. Kao, "Interface Roughness and Polar Optical Phonon Scattering And the Valley Current in Resonant Tunneling Devices", Superlattices and Microstructures, Vol. 20, p.279 (1996).
- [11] Jim A Tatum, Duncan L. MacFarlane, R. Chris Bowen, Gerhard Klimeck and William R. Frensley, "Ultrafast Characteristics of InGaP/InGaAlP Laser Amplifiers", IEEE J. of Quantum Electronics, Vol. 32, p.664 (1996).
- [10] Gerhard Klimeck, Roger K. Lake, R. Chris Bowen, William R. Frensley and Ted Moise, "Quantum Device Simulation with a Generalized Tunneling Formula", Appl. Phys. Lett., Vol. 67, p.2539 (1995).
- [9] R. Chris Bowen, William R. Frensley, Gerhard Klimeck, Roger K. Lake, "Transmission resonances and zeros in multi-band models", Phys. Rev. B. Vol. 52, p.2754 (1995)

JOURNAL PUBLICATIONS (WORK PERFORMED DURING PH.D. AT PURDUE)

- [8] Gerhard Klimeck, Roger Lake, Supriyo Datta, and 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. H. Chen and W. A. Goddard III, "Resonant Tunneling through Quantum Dot Arrays", Phys. Rev. B, Vol. 50, p.8035 (1994).
- [6] Gerhard Klimeck, Guanlong L. Chen and Supriyo Datta, "Conductance Spectroscopy in Coupled Quantum Dots", Phys. Rev. B, Vol. 50, p.2316 (1994)
- [5] Roger Lake, Gerhard Klimeck, M. P. Anantram, and 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, and 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 J. McLennan, Gerhard Klimeck, Roger Lake and Supriyo Datta, "Quantum Kinetic Analysis of Mesoscopic Systems: Linear Response", Superlattices and Microstructures, Vol. 11, p.137 (1992).
- [2] Gerhard Klimeck, D. S. Elliott and M. W. 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 and D. S. Elliott, "Generation and Intensity Correlation Measurements of the Real Gaussian Field", Phys. Rev. A Vol. 41, p.6376 (1990).

PEER REVIEWED CONFERENCE PROCEEDINGS

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.

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

- [P140] 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;
- [P139] Tillmann Kubis, Gerhard Klimeck, "Rough interfaces in THz quantum cascade lasers", accepted in proceedings of the International Workshop for Computational Electronics, Pisa, Italy, October 2010
- [P138] Zhengping Jiang, Neerav Kharche, Gerhard Klimeck, "Valley Degeneracy in (110) Si Quantum Wells - Strain and Misorientation Effects", accepted in proceedings of the International Workshop for Computational Electronics, Pisa, Italy, October 2010

- [P137] Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Atomistic modeling of the phonon dispersion and lattice properties of free-standing <100> Si nanowires" accepted in proceedings of the International Workshop for Computational Electronics, Pisa, Italy, October 2010,
- [P136] George B. Adams III, Krishna P.C. Madhavan, Michael G. 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
- [P135] Krishna P.C. Madhavan, Diane Beaudoin, Swaroop Shivarajapura, George B. Adams III., Gerhard Klimeck, "nanoHUB.org serving over 120,000 users worldwide: it's first cyber-environment assessment" Proceedings of IEEE Nano 2010, Seoul Korea, Aug. 17-20, 2010
- [P134] Sunhee Lee, Hoon Ryu, Gerhard Klimeck, H.Campbell, S.Mahapatra, M.Y.Simmons, L.C.L.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
- [P133] 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
- [P132] 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
- [P131] 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
- [P130] Hoon Ryu, S. Lee, B. Weber, S. Mahapatra, M. Y. Simmons, L. C. L. Hollenberg, G. 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
- [P129] Mark Rodwell, W. Frensley, S. Steiger, E. Chagarov, S. Lee, H. Ryu, Y. Tan, G. Hegde, L Wang, J. Law, T. Boykin, G. Klimek, P. Asbeck, A. Kummel, J. N. 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
- [P128] K.P.C. Madhavan, G. Klimeck, D. Beaudoin, G.B. Adams III, S. 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, USA.
- [P127] Gerhard Klimeck, Saumitra R Mehrotra, Abhijeet Paul, Mathieu Luisier, "Atomistic simulations for SiGe pMOS devices Bandstructure to Transport" ISDRS 2009, December 9-11, 2009, College Park, MD, USA.
- [P126] Gerhard Klimeck, Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, "Study of Ultra-scaled SiGe/Si Core/Shell Nanowire FETs for CMOS Applications" ISDRS 2009, December 9-11, 2009, College Park, MD, USA.
- [P125] G. C. Tettamanzi, G. P. Lansbergen, Abhijeet Paul, P. A. Deosarran1, N. Collaert, Gerhard Klimeck, S. Biesemans, Sven Rogge, "Subthreshold Study of Undoped Trigate nFinFET", Thin Solid Films, doi:10.1016/j.tsf.2009.10.114
- [P124] Neerav Kharche, Gerhard Klimeck, Dae-Hyun Kim, Jesús. A. del Alamo, and Mathieu Luisier, "Performance Analysis of Ultra-Scaled InAs HEMTs", IEDM 2009, Dec. 7-9, 2009.

- [P123] Mathieu Luisier and 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.
- [P122] Neophytos Neophytou, Gerhard Klimeck, and Hans Kosina, "Diameter, orientation, and bias dependence of injection velocity and capacitance in Si nanowires: An atomistic tight-binding study", accepted in IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009
- [P121] Mathieu Luisier and Gerhard Klimeck, "Investigation of In_xGa_{1-x}As Ultra-Thin-Body Tunneling FETs using a Full-Band and Atomistic Approach", accepted in IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009
- [P120] Mincheol Shin, Sunhee Lee, Gerhard Klimeck, "k•p-based Quantum Transport Simulation of Silicon Nanowire pMOSFETs", accepted in the Proceedings of the IEEE NANO 2009 Conference, Genoa July 26-30 2009.
- [P119] Benjamin P. Haley, Sunhee Lee, Mathieu Luisier, Gerhard Klimeck, Hoon Ryu, Faisal Saied, Steve Clark, Hansang Bae, "Advancing Nanoelectronic Devices through Peta-Scale Computing and Deployment on nanoHUB", Proceedings of the SciDAC Conference, San Diego, June 15-19, 2009.
- [P118] Mathieu Luisier and Gerhard Klimeck, "Performance limitations of graphene nano ribbon tunneling FETS due to line edge roughness", IEEE Device Research Conference, June 22-24, 2009.
- [P117] Kyle Montgomery, Samarth Agarwal, Gerhard Klimeck, and Jerry Woodall, "Proposal of ZnSe/GaAs Digital Alloys for High Band Gap Solar Cells and True Green LEDs", accepted in 2009 IEEE Nanotechnology Materials and Devices Conference (NMDC 2009), June 2-5, 2009, Traverse City, Michigan, USA.
- [P116] Gerhard Klimeck and Dragica Vasileska, "ABACUS and AQME: Semiconductor Device and Quantum Mechanics Education on nanoHUB.org", IEEE proceedings of the 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009, DOI:10.1109/IWCE.2009.5091083.
- [P115] Sunhee Lee, Hoon Ryu, Zhengping Jiang and Gerhard Klimeck, "Million Atom Electronic Structure on Peta-Scale Computers ", to appear in IEEE proceedings of the 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009 , DOI:10.1109/IWCE.2009.5091117.
- [P114] Hoon Ryu, Sunhee Lee, and 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, DOI:10.1109/IWCE.2009.5091082.
- [P113] Muhammad Usman, Hoon Ryu, and Gerhard Klimeck, "Quantum Confined Stark Shift and Ground State Optical Transition Rate in [100] 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.
- [P112] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, and 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.
- [P111] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, and 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

- [P110] Gabriel P. Lansbergen, Rajib Rahman, J. Caro, S. Biesemans, I. Woo, Gerhard Klimeck, L.C.L. Hollenberg, Sven Rogge, "Transport spectroscopy of a single atom in a FinFET", Journal of Physics: Conference Series 2008, Vol 109, pp 012003.
- [P109] Gabriel P. Lansbergen, Rajib Rahman, J. Caro, I. Woo, N. Colleart, S. Biesemans, Gerhard Klimeck, L.C.L. 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.
- [P108] Gabriel P. Lansbergen, Rajib Rahman, C.J. Wellard, J. Caro, N. Colleart, S. Biesemans, Gerhard Klimeck, L.C.L. Hollenberg, Sven Rogge, "Atomistic Understanding of a Single Gated Dopant Atom in a MOSFET", proceedings of the MRS Spring meeting 2008 San Francisco 2008.
- [P107] Gabriel P. Lansbergen, Rajib Rahman, C.J. Wellard, P.E. Rutten, J. Caro, I. Woo, N. Colleart, S. Biesemans, Gerhard Klimeck, L.C.L. 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
- [P106] Gerhard Klimeck and 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, DOI: 10.1109/IEDM.2008.4796647.
- [P105] Gabriel P. Lansbergen, Rajib Rahman, C.J. Wellard, J. Caro, N. Colleart, S. Biesemans, Gerhard Klimeck, L.C.L. Hollenberg, Sven Rogge, "Transport-based dopant mapping in advanced FinFETs", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008, DOI: 10.1109/IEDM.2008.4796794.
- [P104] Mathieu Luisier, Neophytos Neophytou, Neerav Kharche, and Gerhard Klimeck, "Full-Band and Atomistic Simulation of Realistic 40 nm InAs HEMT", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008, DOI : 10.1109/IEDM.2008.4796842.
- [P103] Mathieu Luisier and Gerhard Klimeck, "A multi-level parallel simulation approach to electron transport in nano-scale transistors", Supercomputing 2008, Austin TX, Nov. 15-21 2008, DOI: 10.1145/1413370.1413383, ISBN: 978-1-4244-2835-9, Regular paper - 59 accepted papers, 277 submissions (21%).
- [P102] Hoon Ryu and Gerhard Klimeck, "Contact Block Reduction Method for Ballistic Quantum Transport with Semi-empirical sp³d⁵s* Tight Binding Band Models", Proceedings of the 2008 International Conference on Solid-State and Integrated-Circuit Technology (ICSICT), October 20-23, 2008, Beijing, China.
- [P101] Mathieu Luisier and 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.
- [P100] Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, Timothy B. Boykin, and 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.
- [P99] Gerhard Klimeck, Michael McLennan, Mark S. Lundstrom, George B. 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.
- [P98] Muhammad Usman, Shaikh Ahmed, and 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.
- [P97] Mathieu Luisier and Gerhard Klimeck, "OMEN an atomistic and full-band quantum transport simulator for post-CMOS nanodevices", IEEE nano 2008, Arlington, TX, August 18-21, 2008.

- [P96] 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.
- [P95] Amritanshu Palaria, Alejandro Stracha, 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.
- [P94] Samarth Agarwal, Gerhard Klimeck "1D hetero-structure tool for atomistic simulation of nano-devices", Proceedings of TECHCON 2008, Austin, TX, September 15 - 16, 2008, 50% acceptance rate.
- [P93] Muhammad Usman, Dragica Vasileska, and 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.
- [P92] Gabriel Lansbergen, Rajib Rahman, Cameron Wellard , Nadine Colleart, 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).
- [P91] Hansang Bae, Steve Clark , Ben Haley, Ryu Hoon, Gerhard Klimeck, Sunhee Lee, Mathieu Luisier, and Faisal Saied, "A Nano-electronics Simulator for Petascale Computing: From NEMO to OMEN", Proceedings of TeraGrid 2008, June 9-13, 2008, Reno, NV.
- [P90] Clemens Heitzinger, Rick Kennell, Gerhard Klimeck, Norbert Mauser, Michael McLennan, and 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).
- [P89] Bhaskaran Muralidharan, Hoon Ryu, Z. Huang, and 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
- [P88] Roksana Golizadeh-Mojarad, A.N.M. Zainuddin, Shaikh S. Ahmed, Gerhard Klimeck, and 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
- [P87] Neophytos Neophytou, Abhijeet Paul, Mark S. Lundstrom, and 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
- [P86] Neerav Kharche, Mathieu Luisier, Timothy B. Boykin, and 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
- [P85] Maxim Naumov, Sunhee Lee, Ben Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Steve Clark, and Gerhard Klimeck, "Alternative Sparse Eigensolvers and Performance Optimization for Electronic Structure Simulations with NEMO-3D", Proceedings of The 12th International Workshop on Computational Electronics, University of Massachusetts Amherst, Oct. 7-10, 2007
- [P84] Neophytos Neophytou, Abhijeet Paul, Mark S. Lundstrom, and 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

- [P83] Neophytos Neophytou, Abhijeet Paul, Mark S. Lundstrom, and Gerhard Klimeck, "Self-consistent simulations of nanowire transistors using atomistic basis sets", Proceedings of SRC TECHCON, September 2007
- [P82] Hansang Bae, Steve 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,
- [P81] Mark Lundstrom, Jason V. Clark, Gerhard Klimeck, and 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, Gaithersberg, MD. conference proceedings will be published by AIP in a hardback book.
- [P80] Shaikh Ahmed, Muhammad Usman, Neerav Kharche, Andrei Schliwa, and Gerhard Klimeck, "Atomistic Simulation of Non-Degeneracy and Optical Polarization Anisotropy in Pyramidal Quantum Dots", proceedings of The 2nd Annual 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.
- [P79] Eddie Howell, Clemens Heitzinger, and 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).-
- [P78] Clemens Heitzinger and Gerhard Klimeck, "Investigation of Conventional DNAFETs for Genome-wide Detection of Polymorphisms", Proceedings of Eurosensor Conference, Goteborg, Sweden, September 21, 2006.-
- [P77] Gerhard Klimeck, Timothy Boykin, Mathieu Luisier, Neerav Kharche, Andreas Schenk, "A Study of alloyed nanowires from two perspectives: approximate dispersion diagrams and transmission coefficients", 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 711.
- [P76] Shaikh Ahmed, Muhammad Usman, Clemens Heitzinger, Rajib Rahman, Andrei Schliwa, and 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.
- [P75] Muhammad Usman, Shaikh Ahmed, Marek Korkusinski, Clemens Heitzinger, and 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. 847.
- [P74] Gerhard Klimeck, Michael McLennan, Matteo Mannino, Marek Korkusinski, Clemens Heitzinger, Rick Kennell, and 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.
- [P73] Clemens Heitzinger and Gerhard Klimeck, "Numerical 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.
- [P72] Mathieu Luisier, Gerhard Klimeck, Andreas Schenk, and 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.

- [P71] Gianluca Fiori, Giuseppe Iannaccone, and 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.
- [P70] Neophytos Neophytou, Shaikh Ahmed, M.P. Anantram, and 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.
- [P69] Vladimir V. Mitin, Nizami Z. Vagidov, Mathieu Luisier, and 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.
- [P68] Mark S. Lundstrom and Gerhard Klimeck, "The NCN: Science, Simulation, and Cyber Services", 2006 IEEE Conference on Emerging Technologies - Nanoelectronics, 10-13 Jan. 2006 Page(s):496 - 500.
- [P67] Jing Wang, Anisur Rahman, Gerhard Klimeck and 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 of 120 submitted Modeling and Simulation abstracts).
- [P66] Anisur Rahman, Gerhard Klimeck, and 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 of 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", 2005 IEEE International Electron Devices Meeting, Washington, DC, December 5 - 7, 2005. (One of 27 accepted out of 120 submitted Modeling and Simulation abstracts).
- [P64] Wei Qiao, David S. 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 out of 268 submissions.
- [P63] Gianluca Fiori, Giuseppe Iannaccone, Mark Lundstrom, and 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.
- [P62] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, and Faisal Saied, "Atomistic simulations of long-range strain effects in multimillion-atom quantum dot nanostructures", SISPAD 2005, International Conference on Simulation of Semiconductor Processes and Devices, Komaba Eminence, Tokyo, JAPAN, September 1-3, 2005
- [P61] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, and 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 J. Terrile, H. Aghazarian, M.I. Ferguson, W. Fink, WT.L. Huntsberger, D. Keymeulen, Gerhard Klimeck, Mark A. Kordon, Seungwon Lee, Paul von Allmen, "Atomistic Simulations in Nanostructures Composed of Tens of Millions of Atoms:Importance of long-range Strain Effects in Quantum Dots", Proceedings. 2005 NASA/DoD Conference on Evolvable Hardware, 2005. 29 June-1 July 2005, pg 131-138.

- [P59] Marek Korkusinski, G. Klimeck, H. Xu, S. Lee, S. Goasguen, F. Saied, "Atomistic Simulations in Nanostructures Composed of Tens of Millions of Atoms: Importance of long-range Strain Effects in Quantum Dots", proceedings of 2005 NSTI Nanotechnology Conference and Trade Show, Anaheim, CA, May 8-12, 2005.
- [P58] Sebastien Goasguen, Michael McLennan, Gerhard Klimeck, and Mark S. 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, Mohamed Sayeed, Sebastien Goasguen, and Gerhard Klimeck, "Large Scale Simulations in Nanostructures with NEMO3-D on Linux Clusters", 2005 Linux Cluster Institute Conference, Raleigh, NC, April, 2005
- [P56] Richard J. Terrile, Christoph Adami, Hrand Aghazarian, Savio N. Chau, Van T. Dang, Michael I. Ferguson, Wolfgang Fink, Terrance L. Huntsberger, Gerhard Klimeck, Mark A. Kordon, Seungwon Lee, Paul von Allmen and Joseph Xu, "Evolutionary Computation Technologies for the Automated Design of Space Systems", proceedings of IEEE Aerospace Conference, 5-12 March 2005 pg 1-12.
- [P55] Anisur Rahman, Gerhard Klimeck and Mark Lundstrom, "Bandstructure Effects in Nanoscale MOSFETs", IEEE IEDM, San Francisco, CA, Dec. 6-8 2004.
- [P54] E. Khorenko, W. Prost, F.-J. Tegude, M. Stoffel, R. Duschl, M.W. Dashiell, O.G. Schmidt, and G. 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 von Allmen, Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, S.N. Coppersmith, Mark Friesen, and Mark Erikson, "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.
- [P52] Yun Zheng, Cristian Rivas, Roger Lake, Khairul Alam, Timothy B. Boykin, and 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 B. Boykin, and Mark S. 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", proceedings of IEEE Simulation of Semiconductor Processes and Devices (SISPAD) 2004, Keynote Address, Munich, Germany, September 2-4, 2004; in Simulation of semiconductor processes and devices 2004: SISPAD 2004, pg. 9-12, Gerhard Wachutka and Gabriele Schrag (Eds.), ISBN: 978-3-211-22468-7
- [P49] Ahmet Ali Yanik, Prabhakar Srivastava, Gerhard Klimeck, and Supriyo Datta, "Coherent Transport in SWCNTs with Spin-Orbit Coupling", IEEE Nano 2004, Munich, Germany, August 16-19, 2004.
- [P48] Olga L. Lazarenkova, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, and 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 von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, and 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 von Allmen, and Gerhard Klimeck, "Effect of Wetting Layers on Strain and Electronic Structures of Self-Assembled Quantum Dots", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [P45] Olga L. Lazarenkova, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, and 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 von Allmen, Fabiano Oyafuso, Gerhard Klimeck, and K. B. Whaley, "Electron spin dephasing and decoherence by interaction with nuclear spins in self-assembled quantum dots", accepted in proceedings of Winter International Symposium on Information and Communication Technologies, January 5-8, 2004, Cancun, Mexico.
- [P42] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Conduction band valley splitting in silicon nanostructures", 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 von Allmen, and 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, pages 171-174.
- [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.
- [P39] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche 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 B. Boykin, R. Chris Bowen, and Paul von 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 and R. Chris 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 Koon Lee, Colin Stanley, Charles Ironside, Gerhard Klimeck, and Roger Lake, "Quantum cascade laser simulation using sp3s* full Brillouin zone tight-binding model", IEEE Proceedings of Conference on Lasers and Electro-Optics CLEO/Europe 2003, Munich 22-27 June 2003, pg 182.
- [P35] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, Paul von Allmen, "Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations", Proceedings of Nanotech2003 (including MSM 2003 and ICCN 2003), February 23-27, 2003, San Francisco.
- [P34] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems", IEEE proceedings of Simulation of Semiconductor Processes and Devices (SISPAD) 2002, Kobe, Japan, Sept. 3-6, 2002, pg 163 -166.

- [P33] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, Paul von 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 (IWQDQC), Kochi, Japan, Jan 26-28, 2002.
- [P32] Tom Cwik, Gerhard Klimeck, Myche McAuley, Bob Deen and 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 Simulation 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, Urbana Champaign.
- [P30] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. 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, Urbana Champaign.
- [P29] Tom Cwik, Gerhard Klimeck, Charles Norton, Thomas Sterling, Frank Villegas and 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, Aug. 2001.
- [P28] Tom Cwik, Gerhard Klimeck, and 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).
- [P27] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic simulation of quantum dots including strain and bandstructure and full band simulation of hole transport in 1-D heterostructures", in IEEE proceedings of 7th International Workshop on Computational Electronics (IWCE). Book of Abstract, Glasgow 22-25 May 2000, pp 6-7, (2000)
- [P26] Didier Keymeulen, Gerhard Klimeck, R. 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 ANNIE12000 (Smart Engineering System Design), St. Louis, MO, November 5-8, 2000
- [P25] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Transverse Momentum Dependence of Electron and Hole Tunneling in a Full Band Tight-Binding Simulation", IEEE Proceedings of the 27th international Symposium on Compound Semiconductors (ISCS), IEEE, (2000)
- [P24] Adrian Stoica, Didier Keymeulen, Ricardo Zebulum, Anil Thakoor, 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, and 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, and Anil Thakoor, "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 and Gerhard Klimeck, "Genetically Engineered Microelectronic Infrared Filters", IEEE Proceedings of the First NASA/DoD Workshop on Evolvable Hardware, IEEE 1999 , Page(s): 242 - 246.

- [P20] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, and Thomas Cwik, "Genetically Engineered Nanoelectronics", IEEE Proceedings of the First NASA/DoD Workshop on Evolvable Hardware, IEEE 1999, Page(s): 247 -248.
- [P19] Tom Cwik and Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", IEEE Proceedings of 1999 Aerospace Conference, IEEE Volume: 5, 1999, Page(s): 131 -138.
- [P18] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, and Tom Cwik, "Genetically Engineered" Nanostructure Devices, in "Materials in Space Science, Technology, and Exploration", MRS Symposium Proceedings, Vol. 551, pg. 149 (1999).

CONFERENCE PROCEEDINGS (WORK PERFORMED PRIOR TO JPL)

- [P17] Daniel K. Blanks, Gerhard Klimeck, Roger Lake, R. Chris Bowen, Manhua Leng, Chenjing Fernando, William R. Frensley, and Dejan Jovanovic, "NEMO Quantum Device Simulator", 1998 Government Microcircuit Applications Conference Digest of Papers (GOMAC), March 1998, p. 218.
- [P16] R. Chris Bowen, Chenjing Fernando, Gerhard Klimeck, A. Chatterjee, Daniel Blanks, Roger Lake, J. Hu, J. Davis, M. Kularni, S. Hattangady, and I.C. Chen, "Physical Oxide Extraction and Versification using Quantum Mechanical Simulation", Proceedings of IEDM 1997, IEEE, 869 (1997).
- [P15] R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Amitava Chatterjee, Dan Blanks, Roger Lake, Jerry Hu, Joseph Davis, Mak Kulkarni, Sunil Hattangady, and Ih-Chin Chen, "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 Wilk, Alan Seabaugh, and Gerhard Klimeck, "Resonant Tunneling in Disordered Materials such as SiO₂/Si/SiO₂", IEEE 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 K. Blanks, Gerhard Klimeck, Roger Lake, Dejan Jovanovic, R. Chris Bowen, Chenjing Fernando, William R. Frensley, and Manhua Leng, "NEMO: General Release of a New Comprehensive Quantum Device Simulator", IEEE Proceedings of the 24th International Symposium on Compound Semiconductors (ISCS), IEEE, NJ (1997). Inst. Phys. Conf. Ser. 156: 639-642, 1998.
- [P12] J. P. A. van der Wagt, Alan Seabaugh, Gerhard Klimeck, Ed A. Beam III, Timothy, B. Boykin, R. Chris Bowen, and Roger Lake, "Ultralow Current Density RTDs for Tunneling-based SRAM", IEEE 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] Dan Blanks, Gerhard Klimeck, Roger Lake, R. Chris Bowen, William R. Frensley, Manhua Leng, and Chenjing L. 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 B. Boykin, R. Chris Bowen, Roger Lake, Dan Blanks, Ted Moise, Y. C. Kao, and William R. Frensley, "Quantitative Simulation of Strained InP-Based Resonant Tunneling Diodes", in IEEE Proceedings of the 1997 55th IEEE Device Research Conference Digest, IEEE, NJ, p. 92 (1997).
- [P9] Gerhard Klimeck, Dan Blanks, Chris Bowen, Bobby Brar, Tom Broekaert, Gary Frazier, Dejan Jovanovic, Roger Lake, Ted Moise, Alan Seabaugh, Glen Wilk, and Paul van der Wagt, "Design and Implementation of Resonant Tunneling Devices into Circuits and Applications", in Proceedings of PHASDOM97, Phantoms Strategic Domain Meetings, Aachen, Germany, March 10-13, 1997.
- [P8] Roger Lake, Gerhard Klimeck, "Experimentally Verified Quantum Device Simulations Based on Multiband Models, Hartree Self-consistency, and Scattering Assisted Charging", in IEEE Proceedings of the 1996 54th IEEE Device Research Conference Digest, IEEE, NJ, p. 174, 1996

- [P7] William R. Frensley, R. Chris Bowen, Chenjing Fernando, Gerhard Klimeck, and Roger Lake, "Quantitatively Accurate Simulation of Quantum Semiconductor Devices", IEEE 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, 1996.
- [P6] Gerhard Klimeck, Roger Lake, Chenjing L. Fernando, R. Chris Bowen, Dan Blanks, Manhua Leng, Ted Moise, Y. C. Kao, and William R. Frensley in "Quantum Devices and Circuits" edited by K. Ismail, S. Bandyopadhyay, and J. P. Leburton, Imperial Press London (1996).
- [P5] Gerhard Klimeck, Roger Lake, R. Chris Bowen, William R. Frensley and Daniel Blanks, "Nanoelectronic Modeling (NEMO)", in IEEE Proceedings of the 1995 53rd Device Research Conference Digest, IEEE, NJ p. 52, 1995.
- [P4] R. Chris Bowen, William R. Frensley and Gerhard Klimeck, "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.
- [P3] Supriyo Datta, Gerhard Klimeck, Roger K. Lake and M. P. Anantram, "Resonant Tunneling devices: Effect of Scattering", IEEE Proceedings of International Symposium on Compound Semiconductors (ISCS), San Diego, Sept. 18-24, 1994. Inst. Phys. Conf. Ser. No 141; Chapter 7, p.775, (1995)
- [P2] Gerhard Klimeck, Roger K. Lake, and Supriyo Datta, "The Phonon Peak in Resonant Tunneling Diodes", Journal of the Electrochemical Society, (1995).
- [P1] Gerhard Klimeck, Roger Lake, Supriyo Datta, and Garnett Bryant, "High Bias Transport through Quantum Dots", Journal of the Electrochemical Society, (1995).

INVITED CONFERENCES

- [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, W. Frensley, S. Steiger, E. Chagarov, S. Lee, H. Ryu, Y. Tan, G. Hegde, L Wang, J. Law, T. Boykin, G. Klimek, P. Asbeck, A. Kummel, J. N. 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, Tim 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-Link", The regional nanotech education center, 2nd Annual Conference, Minneapolis, MN, Oct 5-7, 2010
- [I140] Gerhard Klimeck, "Atomistic Graphene Transistors - New Device or New Material", NRI Workshop on Carbon Based Electronics, Albany NY, Sept. 21-22, 2010

- [I139] Tillmann C. Kubis, Gerhard Klimeck, Peter Vogl, "Non-equilibrium Green's functions in quantum cascade lasers: Prediction of novel devices", 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's Multi-Scale Multi-Disciplinary Modeling of Electronic Materials Workshop; Sept 1-2, 2010 Fairfax, Va
- [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, H.Campbell, S.Mahapatra, M.Y.Simmons, L.C.L.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 and 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 and 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] keynote: George B. Adams III and 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, Steve Clark, Hansang Bae, "NEMO 3-D and OMEN: Nanoelectronic Modeling or Advanced Semiconductor Device Studies and their Deployment on nanoHUB.org", TeraGrid Conference, Crystal City, June 21-26, 2009.

- [I124] Gerhard Klimeck, Mathieu Luisier, Benjamin P. Haley, Sunhee Lee, Hoon Ryu, Faisal Saied, Steve Clark, Hansang Bae, "Advancing Nanoelectronic Devices through Peta-Scale Computing and Deployment on nanoHUB", SciDAC Conference, San Diego, June 15-19, 2009.
- [I123] Mathieu Luisier, Gerhard Klimeck, "Full-Band and Atomistic Modeling of Nanoelectronic Devices", Nanotech Conference and Expo, Houston, TX, May 7-9, 2009.
- [I122] 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.
- [I121] George B. Adams III, Mark Lundstrom, Gerhard Klimeck, and 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, and 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, "Transport-based dopant mapping in advanced FinFETs", IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008.
- [I117] Mathieu Luisier and Gerhard Klimeck, "Full-Band Simulation of Realistic Nanoelectronic Devices at the Atomic Scale" 4th International Workshop on High Performance Computing for Nanoscience and Technology, HPCNano|08, in conjunction with Supercomputing 2008, Purdue University Exhibition Booth, Workshop Program, Presentation, Nov 21, 2008, Austin, TX.
- [I116] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 75,000 users today" Supercomputing 2008, Purdue University Exhibition Booth, Presentation Schedule, Presentation, 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 B. 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 S. Lundstrom, George B. 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 S. Lundstrom, George B. 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 the TeraGrid Planning Process Steering 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, "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, "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, and George Adams, "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, and George Adams, "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, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today", NSF nano 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, Presentation Schedule, Presentation, Nov 13, 2007, Reno, NV.
- [I100] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 26,000 users today" Supercomputing 2007, Purdue University Exhibition Booth, Presentation Schedule, Presentation, Nov 13, 2007, Reno, NV.
- [I99] Alejandra Magana, Alissa Nedossekina and 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.

- [194] Gerhard Klimeck, "nanoHUB, a Fully Operational Science Gateway", Science Gateways TeraGrid Planning Process Workshop, University of Wisconsin Memorial Union, Madison, Wisconsin, June 7, 2007.
- [193] Gerhard Klimeck, "Atomistic Modeling of Nanoelectronic devices", Si nanoelectronics, Leiden, Netherlands, May 21-25, 2007.
- [192] 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.
- [191] Mark Lundstrom, J.C. Clark, G. Klimeck, and A. 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, Gaithersberg, MD. Conference proceedings will be published by AIP in a hardback book.
- [190] Gerhard Klimeck and Michael McLennan, "nanoHUB.org and High Performance Computing", Purdue-Industry High-Performance Computing Workshop, March 20, 2007, Purdue Computing Research Institute (CRI).
- [189] Michael McLennan and 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.
- [188] Gerhard Klimeck, "Atomistic Nanoelectronic Modeling", Forum on the Frontiers in Computational Nanoelectronics February 20-21, 2007, Indianapolis, IN.
- [187] Gerhard Klimeck and 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.
- [186] Mark Lundstrom and Gerhard Klimeck, "The Network for Computational Nanotechnology: Shared Infrastructure for the NNI", NSF Grantees, Conference, Washington, D.C., Dec. 4-6, 2006.
- [185] Michael McLennan and Gerhard Klimeck, "nanoHUB - overview and usage scenarios", FutureTECH Conference Nov 18, 2006, Norfolk State University
- [184] Gerhard Klimeck and Michael McLennan, "nanoHUB - overview", Supercomputing 2006, Two Presentations in the TeraGrid Booth, Nov 11-17, 2006, Tampa, FL.
- [183] 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.
- [182] Gerhard Klimeck, Michael McLennan, Wei Qiao, David Ebert, and Rick Kennel, "nanoVIZ Server", Supercomputing 2006, Presentation in the Purdue Booth, Nov 11-17, 2006, Tampa, FL.
- [181] Gerhard Klimeck, Michael McLennan, and 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
- [180] Gerhard Klimeck, Rick Kennel, Michael McLennan, Stephen Clark, Clemens Heitzinger, Shaikh S. 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.
- [179] Gerhard Klimeck and 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, and Timothy B. Boykin, "Quantum Dot, Nanowire, and 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 and Gerhard Klimeck, "The Network for Computational Nanotechnology", International Nanotechnology Conference on Communication and Cooperation: NSF/NNI Symposium, Arlington, VA, May, 15, 2006.
- [I72] Krishna P.C. Madhavan, Gerhard Klimeck, Sebastien Goasguen, Michael McLennan, Mark S Lundstrom, "New frontiers in nano-education through the nanoHUB", Annual ECE Department Heads Association, Oahu, HI, March 10-14, 2006.
- [I71] Krishna P.C. Madhavan, Gerhard Klimeck, Mark S 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 S Lundstrom, Michael McLennan, Sebastien Goasguen, Krishna Madhavan, "The Network for Computational Nanotechnology", MERLOT Mid-year Directors Conference, San Diego, CA, Jan 27 - 29, 2006.
- [I69] Mark Lundstrom and 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 S 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 and 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, and Mark Lundstrom, "nanoHUB.org – A Service-Oriented Gateway for the nano Science Community", HPCNano2005 (IEEE/ACM International Workshop on High Performance Computing for Nanoscience and Technology), Supercomputing 2005, Nov 12-18, 2005, Seattle, WA.
- [I65] Gerhard Klimeck, Sebastien Goasguen, Michael McLennan, Faisal Saied, Krishna Madhavan, and 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,

- [164] 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,
- [163] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, and 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.
- [162] Shaikh Ahmed, Gerhard Klimeck, Sebastien Goasguen, Faisal Saied, Marek Korkusinski, Haiying Xu, and 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.
- [161] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, and Faisal Saied, "Building and Deploying Community Nanotechnology Software Tools on nanoHUB.org x Atomistic simulations of multimillion-atom quantum dot nanostructures", 5th IEEE Conference on Nanotechnology, July 11-15, 2005, Nagoya Congress Center, Nagoya, Japan.
- [160] Sebastien Goasguen, Mark S. Lundstrom, Gerhard Klimeck, Michael McLennan, Jose Fortes and Renato Figueiredo, "The nanoHUB a portal to TeraGrid and OSG for nanotechnology", Open Science Grid Application workshop, SLAC June 1-2, 2005.
- [159] Mark S Lundstrom and 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.
- [158] Gerhard Klimeck, Mark S 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.
- [157] Sebastien Goasguen, Mark S Lundstrom, Gerhard Klimeck, and Michael McLennan, "The nanoHUB a Cyberinfrastructure for Computational Nanotechnology", Gridchem Computational Chemistry Workshop, April 17-19, 2005.
- [156] Gerhard Klimeck, Marek Korkusinski, Fabiano Oyafuso, Seungwon Lee, Timothy B. Boykin, Paul von Allmen, R. Chris Bowen, and Olga Lazarenkova, Mark Friesen, Susan Coppersmith, Mark Eriksson, Anisur Rahman, Mark S. 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.
- [155] Gerhard Klimeck, MS Lundstrom, M Korkusinski, H Xu, F Saied, S Goasguen, TB Boykin, F Oyafuso, S Lee, H Hua, O Lazarankova, RC Bowen, P von Allmen, "nanoHUB.org - Towards On-Line Simulation for Materials and Nanodevices by Design", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [154] 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.
- [153] Gerhard Klimeck, Mark S Lundstrom, Michael McLennan, and Sebastien Goasguen "The Network for Computational Nanotechnology", Inaugural NWICG HPC Workshop, Envision Center, Purdue University, W. Lafayette, March 8-9, 2005

- [152] Marek Korkusinski, Gerhard Klimeck, Fabiano Oyafuso, Seungwon Lee, Timothy B. Boykin, Paul von Allmen, R. Chris Bowen, and 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.
- [151] Gerhard Klimeck, Mark S Lundstrom, Michael McLennan, and Sebastien Goasguen, "The Network for Computational Nanotechnology", 2004 Nanoscale Science and Engineering Grantee Conference, Washington DC, December 13-15, 2004.
- [150] Gerhard Klimeck, Sebastien Goasguen, Haiying Xu, Faisal Saied, Mohammed Sayeed, Hook Hua, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, and Paul von 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.
- [149] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Mohamed Sayeed, Faisal Saied, Sebastien Goasguen, Anisur Rahman, Mark Lundstrom, Fabiano Oyafuso, Seungwon Lee, Timothy Boykin, Paul von Allmen, R. Chris Bowen, and 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.
- [148] Gerhard Klimeck with Anisur Rahman, Nizami Vagidov, Timothy B. Boykin, and Mark S. 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.
- [147] Gerhard Klimeck, "NEMO 1-D: the first NEGF-based TCAD tool", IEEE Simulation of Semiconductor Processes and Devices (SISPAD) 2004, Keynote Speaker, Munich, Germany, September 2-4, 2004,
- [146] Gerhard Klimeck, Mark Lundstrom, and Sebastien Goasguen, "The Network for Computational Nanotechnology: Cyber-Infrastructure and Grid Computing for Nanotechnology Exploration and Education ", Grid Forum Korea Summer Workshop, Seoul, Korea, Aug. 26-27, 2004
- [145] Gerhard Klimeck with Ahmet Ali Yanik, Prabhakar Srivastava, Supriyo Datta, "Coherent Transport in SWCNTs with Spin-Orbit Coupling", IEEE Nano 2004, Munich, Germany, August 16-19, 2004.
- [144] Gerhard Klimeck, Fabiano Oyafuso, Seungwon Lee, Timothy B. Boykin, Paul von Allmen, R. Chris Bowen, Olga Lazarenkova , Mark Friesen, Susan Coppersmith, Mark Eriksson, Anisur Rahman, Mark S. Lundstrom, K. Birgitta 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.
- [143] 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.
- [142] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Susan Coppersmith, Mark Friesen, "Empirical Atomic Level Simulations for QC Applications", CQDT Workshop, Potsdam, NY, May 17-21, 2004.
- [141] Gerhard Klimeck and Mark Lundstrom, "The Network for Computational Nanotechnology", National Nanotechnology Initiative: From Vision to Commercialization, Keynote Address, Washington DC, March 31-April 2, 2004.
- [140] Mark Lundstrom and Gerhard Klimeck, "The Network for Computational Nanotechnology", Nanotech 2004, Keynote Address, Boston, MA, March 8-11, 2004.
- [139] Mark Lundstrom and 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 and 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.
- [I37] Gerhard Klimeck, Fabiano Oyafuso, Seungwon Lee, Timothy B. Boykin, Paul von Allmen, R. Chris Bowen, and 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 von Allmen, Timothy B. Boykin, and R. Chris 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 B. Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul von Allmen, Seungwon Lee, and K. Birgitta 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. Chris Bowen, Tim Boykin, Dan Blanks, William R. Frensley, Fabiano Oyafuso, Seungwon Lee, Paul von Allmen, Olga Lazarenkova, Thomas A. 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 von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, Tim Boykin, "Empirical Atomic Level Simulations for QC Applications", THINQC, June 9-10, 2003, Harpers Ferry.
- [I32] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche McAuley, Eric DeJong, and 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 von Allmen, Timothy B. Boykin, and R. Chris 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 B. Boykin, R. Chris Bowen, and Paul von 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 von Allmen, Timothy B. Boykin, and R. Chris 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 von Allmen and 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 B. Boykin, and Paul von 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 B. Boykin, R. Chris Bowen, and Paul von 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 B. Boykin, R. Chris Bowen, Paul von 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 (IWQDQC), 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, TNT 2001 Conference, 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. Chris Bowen, Timothy B. 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. Chris Bowen, Thomas A. Cwik, and Timothy B. 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. Chris Bowen, Timothy B. Boykin, Carlos Salazar-Lazaro, Thomas A. Cwik, and Adrian Stoica, "Simulator Development for Nanoelectronic Device", 3rd NASA Workshop on Device Modeling, NASA Ames Research Center, August 26-29, 1999.
- [I18] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Carlos Salazar-Lazaro, Adrian Stoica, and Tom Cwik, "Nanoelectronic Modeling at JPL", DARPA Ultra Electronics Program Review, Oct 18-21, 1998, Estes Park, CO.
- [I17] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and 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 H. Salazar-Lazaro, Adrian Stoica, and 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.

INVITED CONFERENCES (WORK PERFORMED PRIOR TO JPL)

- [I15] Gerhard Klimeck, Daniel K. 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, 1997
- [I14] Gerhard Klimeck, Roger Lake, Daniel K. Blanks, "NEMO: Quantitative Resonant Tunneling Diode Simulation", 1997 DARPA ULTRA Electronics and Advanced Microelectronics Program Review, October 26-31, Santa Fe, NM (1997).
- [I13] R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Amitava Chatterjee, Dan Blanks, Roger Lake, Jerry Hu, Joseph Davis, Mak Kulkarni, Sunil Hattangady, and Ih-Chin Chen, "Dopant Fluctuations and Quantum Effects in Sub-0.1µm CMOS", 1997 International Semiconductor Device Research Symposium, Virginia, Dec. 1997.
- [I12] Gerhard Klimeck, Dan Blanks, Roger Lake, R. Chris Bowen, William R. Frensley, Manhua Leng, and 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. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, William R. Frensley, Dejan Jovanovic, Paul Sotirelis, "The NEMO Project or Writing Software in a Large Research Group", International Workshop on Computational Electronics, Notre Dame, South Bend, IN, May 1997.
- [I10] Gerhard Klimeck, Dan Blanks, Chris Bowen, Bobby Brar, Tom Broekaert, Gary Frazier, Dejan Jovanovic, Roger Lake, Ted Moise, Alan Seabaugh, Glen Wilk, and Paul van der Wagt, "Design and Implementation of Resonant Tunneling Devices into Circuits and Applications", PHASDOM97, Phantoms Strategic Domain Meeting, Aachen, Germany, March 10-13, 1997.
- [I9] William R. Frensley, R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Manhua Leng, Dan Blanks and 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. Chris Bowen, Chenjing L. Fernando, Ted Moise, Daniela Francovicchio, and Y. C. 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 L. Fernando, R. Chris Bowen, Ted Moise, Y. C. Kao, and 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 R. Frensley, R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Roger Lake and Dan 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 R. Frensley, James R. Hellums, Chenjing L. Fernando, R. Chris Bowen, and 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 R. Frensley, Chenjing L. Fernando, R. Chris Bowen, and Gerhard Klimeck, "Modeling Tools for the Development of Quantum and Conventional Semiconductor Heterostructure Devices", Government Microcircuit Applications Conference (GOMAC), San Diego, CA, Nov. 1994.
- [I3] Supriyo Datta, Gerhard Klimeck, Roger Lake, Yong Lee and Michael J. McLennan, "Quantum Device Simulation Including Interactions", International Workshop on Computational Electronics, Portland, May 18-20 1994.
- [I2] Supriyo Datta, Gerhard Klimeck, and Roger Lake, "Resonant tunneling diodes: Effects of Scattering on the Valley Current", International Symposium on Compound Semiconductors, San Diego, Sept. 18-24, 1994.
- [I1] Supriyo Datta, Roger Lake, and 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 (WORK PERFORMED AT PURDUE)

- [C308] 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

- [C307] 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
- [C306] 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
- [C305] 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
- [C304] George B. Adams III, Krishna P.C. Madhavan, Michael G. 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
- [C303] Dragica Vasileska, Gerhard Klimeck, A. Magana, S. M. Goodnick, "Tool-Based Curricula and Visual Learning", European Conference on Electronic Learning, Porto, Portugal, Nov. 4-5 2010
- [C302] Saumitra Mehrotra, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "Valley Degeneracy in (110) Si Quantum Wells: Strain and Misorientation Effects", TECHCON, Sept. 13-14, Austin, Texas (2010)
- [C301] 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
- [C300] 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
- [C299] Saumitra Mehrotra, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, "A Tight-Binding approach for SiGe Bandstructure Calculations", TECHCON, Austin, Texas, Sept. 13-14, 2010
- [C298] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, Timothy B. Boykin, Gerhard Klimeck, "Strain Engineering of Trigated Silicon Nanowire FinFETs for Improved Device Performance", TECHCON, Austin, Texas, Sept. 13-14, 2010
- [C297] Woo-Suhl Cho, Mathieu Luisier, Gerhard Klimeck, "Full-band Simulations of Band-to-Band Tunneling Diodes", TECHCON, Austin, Texas, Sept. 13-14, 2010
- [C296] 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
- [C295] Abhijeet Paul and G. Klimeck, "Atomistic modeling of the thermoelectric power factor in ultra-scaled silicon nanowires", 2010 IEEE Silicon Nanoelectronics Workshop, June 13.14, 2010 Hilton Hawaiian Village, Honolulu, HI
- [C294] Gerhard Klimeck and Mathieu Luisier, "Scattering in Si-nanowires – Where does it matter?", 2010 IEEE Silicon Nanoelectronics Workshop, June 13.14, 2010 Hilton Hawaiian Village, Honolulu, HI
- [C293] Hoon Ryu, S. Lee, B., Weber, S. Mahapatra, M. Y. Simmons, L. C. L. Hollenberg and G. Klimeck, "Quantum transport in ultra-scaled phosphorous-doped silicon nanowires", 2010 IEEE Silicon Nanoelectronics Workshop, June 13.14, 2010 Hilton Hawaiian Village, Honolulu, HI

- [C292] B. Weber, S. Mahapatra, W. R. Clarke, H. Ryu, S. Lee, G. Klimeck, L. C. L. Hollenberg and M. Y. Simmons, "Quantum transport in atomic-scale silicon nanowires", 2010 IEEE Silicon Nanoelectronics Workshop, June 13-14, 2010 Hilton Hawaiian Village, Honolulu, HI
- [C291] K.P.C. Madhavan, G. Klimeck, D. Beaudoin, G.B. Adams III, S. 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
- [C290] Sunhee Lee, Hoon Ryu, Gerhard Klimeck, H.Campbell, S.Mahapatra, M.Y.Simmons, L.C.L.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.
- [C289] N. Kharche, M. Luisier, S. Lee, S. Steiger and G. Klimeck, "Study on Ultra-scaled InAs Channel Devices", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 5-6, 2010.
- [C288] Amrit Palaria, Yumi Park, Gerhard Klimeck and Alejandro Strachan, "Atomic and electronic structure properties of Si/Ge heterostructures", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 5-6, 2010.
- [C287] Abhijeet Paul, Saumitra R. Mehrotra, Zhengping Jiang, Mathieu Luisier and 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.
- [C286] Sung Geun Kim, Abhijeet Paul, Mathieu Luisier, Gerhard Klimeck, Timothy B. Boykin, "Full 3D Quantum Transport Simulation of Interface Roughness in Nanowire FETs", American Physical Society, March Meeting, March 15–19, 2010; Portland, Oregon (2010).
- [C285] 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).
- [C284] Muhammad Usman, Gerhard Klimeck, "Wavelength engineered InAs quantum dots", American Physical Society, March Meeting, March 15–19, 2010; Portland, Oregon (2010).
- [C283] 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).
- [C282] 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).
- [C281] David Lifka, Gerhard Klimeck, Michael McLennan, "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.
- [C280] Gerhard Klimeck, George B. Adams III, and Michael J. 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.
- [C279] 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.
- [C278] Bent Weber, S. Mahapatra, Hoon Ryu, Sunhee Lee, Gerhard Klimeck and Michelle Y. Simmons, "Atomic-scale Si:P dopant wires", 2010 International Conference On Nanoscience and Nanotechnology (ICONN), Sydney, 22-26th Feb. 2010.

- [C277] Chris C. Escott, Andrea Morello, Jarryd Pla, Rajib Rahman, Gerhard Klimeck, Andrew S. Dzurak, and Lloyd C. L. Hollenberg, "Tunnelling rates in silicon qubit devices", 2010 International Conference On Nanoscience and Nanotechnology (ICONN), Sydney, 22-26th Feb. 2010.
- [C276] Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Rajib Rahman, B Haley, S.H Park, Neerav Kharche, Z Jiang, Timothy B. Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabri Lansbergen, Sven Rogge, Bent Weber, M 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.
- [C275] Saumitra R Mehrotra, Abhijeet Paul, Mathieu Luisier, and Gerhard Klimeck, "Atomistic simulations for SiGe pMOS devices Bandstructure to Transport", ISDRS 2009, December 9-11, 2009, College Park, MD, USA.
- [C274] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, and 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.
- [C273] Neerav Kharche, Gerhard Klimeck, Dae-Hyun Kim, Jesús. A. del Alamo, and Mathieu Luisier, "Performance Analysis of Ultra-Scaled InAs HEMTs", accepted in IEDM 2009, Dec. 7-9, 2009.-
- [C272] Mathieu Luisier and Gerhard Klimeck, "Performance Comparisons of Tunneling Field-Effect Transistors made of InSb, Carbon, and GaSb-InAs Broken Gap Heterostructures", accepted in IEDM 2009, Dec. 7-9, 2009.-
- [C271] J. Verduijn, G. P. Lansbergen, G. C. Tettamanzi, R. Rahman, S. Biesemans, N. Colleart, G. Klimeck, L. C. L. Hollenberg, and S. 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.
- [C270] G. C. Tettamanzi, G. P. Lansbergen, Abhijeet Paul, P. A. Deosarran1, N. Collaert, Gerhard Klimeck, S. Biesemans, and Sven Rogge, "Subthreshold Study of Undoped Trigate nFinFET", 2009 Silicon Nanoelectronics Workshop, Rihga Royal Hotel Kyoto, Kyoto, Japan, June 13-14, 2009.
- [C269] G. C. Tettamanzi, G. P. Lansbergen, Abhijeet Paul, P. A. Deosarran1, N. Collaert, Gerhard Klimeck, S. Biesemans, and Sven Rogge, "Subthreshold Study of Undoped Trigate nFinFET", E-MRS (European Materials Research Society) Conference, Strasbough, France, June 8-12, 2009.
- [C268] Woo-Suhl Cho, Hoon Ryu, Seung-Hyun 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.
- [C267] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier and Gerhard Klimeck, "On the Validity of Top of the Barrier Quantum Transport Model for Ballistic Nanowire MOSFETs", accepted in TECHCON 2009 to be held at the Renaissance Hotel in Austin, Texas, September 14 - 15, 2009.
- [C266] Neophytos Neophytou, Gerhard Klimeck, and Hans Kosina, "Diameter, orientation, and bias dependence of injection velocity and capacitance in Si nanowires: An atomistic tight-binding study", accepted in IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009-
- [C265] Mathieu Luisier and Gerhard Klimeck, "Investigation of $\text{In}_x\text{Ga}_{1-x}\text{As}$ Ultra-Thin-Body Tunneling FETs using a Full-Band and Atomistic Approach", accepted in IEEE SISPAD 2009, San Diego, Sept. 9 - 11, 2009
- [C264] W. Pok, G. Scappucci, W. C. T. Lee, D. W. Thompson, H. Buech, B. Weber, S. Mahapatra, L.C.L. Hollenberg, M.Y. Simmons, H. Ryu, S. Lee, G. Klimeck, M. Friesen, and M. A. Eriksson "Precision control of tunneling in STM-patterned Si:P devices", Silicon Qubit Workshop, Univeristy of California Berkeley, Aug. 24-25, 2009.

- [C263] 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", Silicon Qubit Workshop, Univeristy of California Berkeley, Aug. 24-25, 2009.
- [C262] Hoon Ryu, Gerhard Klimeck, Sunhee Lee, Rajib Rahman, B Haley, S.H Park, Neerav Kharche, Z Jiang, Timothy B. Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabri Lansbergen, Sven Rogge, Bent Weber, M Simmons, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", Silicon Qubit Workshop, Univeristy of California Berkeley, Aug. 24-25, 2009.-
- [C261] Gerhard Klimeck, Rajib Rahman, Seung-Hyon Park, Hoon Ryu, Neerav Kharche, G. P. Lansbergen, J. Verduijn, Bent Weber, Lloyd C. L. Hollenberg, Sven Rogge, Michelle Simmons, Richard Muller, "Million-Atom Electronic Structure Simulations for Realistically Large Si-Based Quantum Devices", Silicon Qubit Workshop, Univeristy of California Berkeley, Aug. 24-25, 2009.
- [C260] Mincheol Shin, Sunhee Lee, Gerhard Klimeck, "k•p-based Quantum Transport Simulation of Silicon Nanowire pMOSFETs", accepted in the Proceedings of the IEEE NANO 2009 Conference, Genoa July 26-30 2009.
- [C259] Mathieu Luisier and Gerhard Klimeck, "Performance limitations of graphene nano ribbon tunneling FETS due to line edge roughness", IEEE Device Research Conference, June 22-24, 2009.
- [C258] Kyle Montgomery, Samarth Agarwal, Gerhard Klimeck, and Jerry Woodall, "Proposal of ZnSe/GaAs Digital Alloys for High Band Gap Solar Cells and True Green LEDs", accepted in 2009 IEEE Nanotechnology Materials and Devices Conference (NMDC 2009), June 2-5, 2009, Traverse City, Michigan, USA .
- [C257] Quin Zhang, 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.
- [C256] Amrit Palaria, Ya Zhou, Gerhard Klimeck and 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.
- [C255] Neerav Kharche, Mathieu Luisier, and 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.
- [C254] Sung Geun Kim, Mathieu Luisier, and 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.
- [C253] Abhijeet Paul, Mathieu Luisier, and Gerhard Klimeck, "Bandstructure Lab: Scientific Impact and Tool Development", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 7, 2009.
- [C252] Gerhard Klimeck and Dragica Vasileska, "Semiconductor Device and Quantum Mechanics Education on nanoHUB.org", 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009.
- [C251] Sunhee Lee, Hoon Ryu, Zhengping Jiang and Gerhard Klimeck, "Million Atom Electronic Structure on Peta-Scale Computers ", submitted to 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009.
- [C250] Hoon Ryu, Sunhee Lee, and Gerhard Klimeck, "A Study of Temperature-dependent Properties of n-type delta-doped Si Band-structures in Equilibrium", submitted to 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009.

- [C249] Muhammad Usman, Hoon Ryu, and Gerhard Klimeck, "Quantum Confined Stark Effect in Biased InAs/GaAs Quantum Dots", submitted to 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009.
- [C248] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, and Gerhard Klimeck, "On the validity of the top of the barrier quantum transport model for ballistic nanowire MOSFETs", submitted to 13th International Workshop on Computational Electronics, Tsinghua University, Beijing, May 27-29 2009.
- [C247] Abhijeet Paul, Saumitra Mehrotra, Mathieu Luisier, and 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
- [C246] 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.
- [C245] Muhammad Usman and 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.
- [C244] Abhijeet Paul, Saumitra Mehrotra and Gerhard Klimeck, "Study of Electronic Charge Distribution in Silicon Nanowire Transistors: An Atomistic Approach", American Physical Society, March Meeting, March 16-20, Pittsburgh, PA, 2009.
- [C243] 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.
- [C242] Gabriel P. Lansbergen, Rajib Rahman, C.J. Wellard, P.E. Rutten, J. Caro, I. Woo, N. Collaert, S. Biesemans, Gerhard Klimeck, L.C.L. 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.
- [C241] Gabriel P. Lansbergen, Rajib Rahman, C.J. Wellard, J. Caro, N. Collaert, S. Biesemans, Gerhard Klimeck, LLOYD C.L. Hollenberg, Sven Rogge, "Transport-based dopant mapping in advanced FinFETs", accepted in IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008; approx. 10% acceptance.
- [C240] Mathieu Luisier, Neophytos Neophytou, Neerav Kharche, and Gerhard Klimeck, "Full-Band and Atomistic Simulation of Realistic 40 nm InAs HEMT", accepted in IEEE IEDM, San Francisco, USA, Dec. 15-17, 2008; approx. 10% acceptance rate.
- [C239] 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 and Nanostructures Workshop, Hapuna Beach, Hawaii, Dec. 7-12, 2008.
- [C238] Hoon Ryu, Muhammad Usman, Shaikh Ahmed, and 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.
- [C237] Mathieu Luisier and 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%).
- [C236] Gerhard Klimeck, Mathieu Luisier, Saumitra Mehrotra, Xufeng Wang, SungGeun Kim, Neophytos Neophytou, Abhijeet Paul, Ben Haley, "Nanowire Simulations from atomistic tool development to deployed tools on nanoHUB.org", 3rd nanowire growth workshop, Duisburg, Germany, Sept. 14-16, 2008.

- [C235] 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.
- [C234] Amritanshu Palaria, Alejandro Stracha, 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.
- [C233] 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.
- [C232] Mathieu Luisier and 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.
- [C231] Mathieu Luisier, Andreas Schenk, Wolfgang Fichtner, Timothy B. Boykin, and 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.
- [C230] Gerhard Klimeck, "nanoHUB.org tutorial", IEEE nano 2008, Arlington, TX, August 18-21, 2008.
- [C229] Muhammad Usman, Shaikh Ahmed, and 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.
- [C228] Mathieu Luisier and Gerhard Klimeck, "OMEN an atomistic and full-band quantum transport simulator for post-CMOS nanodevices", IEEE nano 2008, Arlington, TX, August 18-21, 2008.
- [C227] Muhammad Usman, Dragica Vasileska, and 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).-
- [C226] Gabriel Lansbergen, Rajib Rahman, Cameron Wellard, Nadine Colleart, 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).
- [C225] Gerhard Klimeck, "nanoHUB.org in Science Gateways on Parade", Tutorial Session, TeraGrid 2008, June 9-13, 2008, Las Vegas.
- [C224] Hansang Bae, Steve Clark, Ben Haley, Ryu Hoon, Gerhard Klimeck, Sunhee Lee, Mathieu Luisier, and Faisal Saied, "A Nano-electronics Simulator for Petascale Computing: From NEMO to OMEN", TeraGrid 2008, June 9-13, 2008, Las Vegas.
- [C223] Gerhard Klimeck, Neerav Kharche, Muhammad Usman, and Mathieu Luisier, "Atomistic Simulation of Realistically Sized Nanodevices Using NEMO 3-D and OMEN", Nanoelectronics Days, Aachen, Germany, May 13-16, 2008.
- [C222] Gerhard Klimeck, Michael McLennan, Mark Lundstrom, and George B. Adams III., "nanoHUB.org - online simulation and more serving annually over 60,000 users", Nanoelectronics Days, Aachen, Germany, May 13-16, 2008.
- [C221] Abhijeet Paul, Neophytos Neophytou, and Gerhard Klimeck, "Effects of Bandstructure in Nanostructures: Physics and Tool Development", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.

- [C220] Kaushik Balamukundhan, Samarth Agarwal, Tuna Toksoz, and Gerhard Klimeck, "Development of a 1D hetero-structure tool", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.
- [C219] Saumitra R Mehrotra, Ben Haley, and Gerhard Klimeck, "Development and Enhancement of Nanowire on nanoHUB.org", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.
- [C218] Sung G. Kim, Sriraman Damodaran, Ben Haley and Gerhard Klimeck, "MuGFET: Multigate FETs simulated with drift-diffusion models at the nano-scale", MSD, FCRP Annual Review, Student Poster, MIT, Boston, MA, May 8, 2008.
- [C217] Hansang Bae, Stephen 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.
- [C216] Faisal Saied, Hansang Bae, Steve Clark, Ben Haley, Gerhard Klimeck, Sunhee Lee, and Maxim Naumov, "A Massively Parallel Schroedinger Solver for Nano-Electronics", SIAM Conference on Parallel Processing for Scientific Computing, Atlanta, March 12-14 2008,
- [C215] Neerav Kharche, Seungmin Kim, Timothy B. Boykin, Gerhard Klimeck, "Substrate orientation dependence of valley-splitting in Silicon nanostructures", American Physical Society, March Meeting 2008,
- [C214] Muhammed 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,
- [C213] Neophytos Neophytou, Abhijeet Paul, Gerhard Klimeck, "Atomistic Treatment of Electronic Transport: The Effect of Bandstructure", American Physical Society, March Meeting 2008,
- [C212] Timothy B. Boykin, Neerav Kharche, Mathieu Luisier, Gerhard Klimeck, "Zone Unfolding and Approximate Bandstructure Calculations in Tight-Binding", American Physical Society, March Meeting 2008,
- [C211] Neophytos Neophytou, Abhijeet Paul, Mark Lundstrom, and 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), Conference site, Nov. 18-23, 2007.
- [C210] Gerhard Klimeck, "Rapture Tool Development: s/w Environment That Enabled 50+ Applications in Two Years", Supercomputing 2007, Purdue University Exhibition Booth, Presentation Schedule, Presentation, Nov 13, 2007, Reno, NV.
- [C209] Gerhard Klimeck, "generation-nano.org: Engagement K-12", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [C208] Gerhard Klimeck, "From nanoHUB to HUBzero: Roadmap to New HUBs", Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [C207] Gerhard Klimeck, "nanoHPC: Multimillion Atom Simulations Using NEMO 3D". Supercomputing 2007, Purdue University Exhibition Booth, Nov 13, 2007, Reno, NV.
- [C206] Maxim Naumov, Sunhee Lee, Benjamin Haley, Hansang Bae, Stephen Clark, Rajib Rahman, Hoon Ryu, Faisal Saied and 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.

- [C205] Gerhard Klimeck, Faisal Saied, Steven Clark, Ben Haley, Hansang Bae, and 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.
- [C204] Hoon Ryu , Rajib Rahman and Gerhard Klimeck, "Efficient Calculation of Long-Range Coulomb interactions", Supercomputing 2007, Reno, NV, electronic poster at Purdue University Exposition Booth, Nov. 13-16, 2007.
- [C202] Hansang Bae, Stephen 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.
- [C202] Maxim Naumov, Sunhee Lee, Benjamin Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Stephen Clark, and 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.
- [C201] Bhaskaran Muralidharan, Hoon Ryu, Z. Huang, and 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
- [C200] Rokhsana Golizadeh-Mojarad, A.N.M. Zainuddin, Shaikh S. Ahmed, Gerhard Klimeck, and 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
- [C199] Neophytos Neophytou, Abhijeet Paul, Mark S. Lundstrom, and 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
- [C198] Neerav Kharche, Mathieu Luisier, Timothy B. Boykin, and 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
- [C197] Maxim Naumov, Sunhee Lee, Ben Haley, Rajib Rahman, Hoon Ryu, Faisal Saied, Steve Clark, and 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
- [C196] Neophytos Neophytou, Abhijeet Paul, Mark S. Lundstrom, and 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
- [C195] Neophytos Neophytou, Abhijeet Paul, Mark S. Lundstrom, and Gerhard Klimeck, "Self-consistent simulations of nanowire transistors using atomistic basis sets", SRC TECHCON, September 2007
- [C194] Tuna Toksoz, Gerhard Klimeck, Samarth Agarwal, "Implementation of a GUI for a Resonant Tunneling Diode Simulator", Purdue SURF Conference, (Summer Undergraduate Research Fellowship), July 31, 2007.
- [C193] Raseong Kim, Mathieu Luisier, Neophytos Neophytou, Michal McLennan, Jing wang, Anisur Rahman, Gerhard Klimeck, and 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.

- [C192] Sunhee Lee, Hansang Bae, Steve Clark, Ben Haley, Gerhard Klimeck, Maxim Naumov, Hoon Rye, and Faisal Saied, "Multi-Million Atom Electronic Structure simulations Towards Petaflop Operation", Network for Computational Nanotechnology annual site visit, June 18-20, 2007, Purdue University.
- [C191] Hansang Bae, Steve 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,
- [C190] Gerhard Klimeck, Michael McLennen, "Science Gateway Building Blocks: nanoHUB", Teragrid 2007 Conference, Madison WI, June 2007.
- [C189] Michael McLennen, Rick Kennell, Dongyan Xu, Paul Ruth, Gerhard Klimeck, Alain Roy, Renato Figueiredo, "TeraGrid'07 Tutorial: Using nanoHUB.org as a Science Gateway", Teragrid 2007 Conference, Madison WI, June 2007.
- [C188] Sriraman Damodaran, Selvakumaran Vadivelmurugan, Quoc Thai Do, Clemens Heitzinger, and Gerhard Klimeck, "Investigation of the Conductance of Silicon Nanowire Biosensors Using the 2D Drift-diffusion Model", Accepted to NSTI Nanotech 2007, Santa Clara, CA, May 20-24 2007,
- [C187] Marta Prada, Neerav Kharche, Gerhard Klimeck, "Electronic Structure of Si/InAs Composite Channels", Accepted as oral presentation in MRS Spring conference 2007, Symposium G: Extending Moore's Law with Advanced Channel Materials. Accepted as one of 10 oral presentations in 54 submissions.
- [C186] Michael McLennen, Mark Lundstrom, Gerhard Klimeck, "GOMACTech Tutorial: Using nanoHUB for Scientific Computing, Education, and Outreach", GOMACTech Conference, Orlando, FL, March 19, 2007,
- [C185] Hansang Bae, Steve Clark, Ben 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.
- [C184] Neerav Kharche, Marta Prada, Timothy B. Boykin, Gerhard Klimeck, "Valley-splitting in strained Silicon quantum wells on a miscut substrate using tight-binding model", American Physical Society, March Meeting 2007,
- [C183] Shaikh Ahmed, Muhammad Usman, Neerav Kharche, Andrei Schliwa, and 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.
- [C182] Michael McLennan, Wei Qiao, Rick Kennell, and Gerhard Klimeck, "Visualizing Current Flow in Quantum Wires and other Devices on nanoHUB.org", Advanced Heterostructure Workshop, Hawaii, Dec. 3 - 8, 2006.
- [C181] Gerhard Klimeck, Timothy B. Boykin, Mathieu Luisier, Neerav Kharche, Andreas Schenk, "Electronic structure and transport in random alloy AlGaAs nanowires", Advanced Heterostructure Workshop, Hawaii, Dec. 3 - 8, 2006.
- [C180] Wei Qiao, Michael McLennan, Rick Kennell, David S. 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.

- [C179] Eddie Howell, Clemens Heitzinger, and 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
- [C178] K.P.C. 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.
- [C177] Clemens Heitzinger and Gerhard Klimeck, "Investigation of Conventional DNAFETs for Genome-wide Detection of Polymorphisms", Eurosensor Conference, Goteborg, Sweden, September 21, 2006.
- [C176] Shaikh Ahmed and 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
- [C175] 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.
- [C174] Muhammad Usman, Shaikh Ahmed, Clemens Heitzinger, Rajib Rahman, and 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.
- [C173] 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.
- [C172] Gerhard Klimeck, Mathieu Luisier, Timothy B. Boykin, Neerav Kharche, and Andreas Schenk, "A Study of alloyed nanowires from two perspectives: approximate dispersion diagrams and transmission coefficient" International Conference on the Physics of Semiconductors, ICPS 2006, Vienna, Austria, July 24-28 2006.
- [C171] Mathieu Luisier, Raseong Kim, Neophytos Neophytou, Michael McLennan, Jing Wang, Anisur Rahman, Gerhard Klimeck, and Mark Lundstrom, "Bandstructure Lab", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C170] Ahmet A. Yanik, Gerhard Klimeck, Supriyo Datta, "Impurity Effects in Magnetic Tunnel Junctions", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C169] Neerav Kharche, Mathieu Luisier, Timothy B. 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.
- [C168] Neophytos Neophyto, Shaikh Ahmed, and 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.
- [C167] Rajib Rahman, Marta Prada, and Gerhard Klimeck, "Si:P Quantum Computer Architecture", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C166] Neerav Kharche, Marta 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.

- [C165] Amritanshu Palaria, Arvind Arumbakkam, Gerhard Klimeck, and Alejandro Strachan, "nanoMaterials simulations toolkit and sample learning module", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C164] Clemens Heitzinger and Gerhard Klimeck, "Theory of DNAFETs and BioFETs", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C163] Wei Qiao, Michael McLennan, Rick Kennell, David Ebert, and Gerhard Klimeck, "nanoHUB Visualization Tools", Network for Computational Nanotechnology annual site visit, June 19-22, 2006, Purdue University.
- [C162] Clemens Heitzinger and 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.
- [C161] Sebastien Goasguen, Jon Camden, Muhammad Usman, Steven Clark, Jaime Frey, Clemens Heitzinger, and Gerhard Klimeck, "nanoHUB - nanoscience gateway to the TeraGrid", Teragrid 2006, Indianapolis, IN June 12-15, 2006
- [C160] Michael McLennan, Sebastien Goasguen, Krishna Madhavan, Derrick Kearney, Joe Cychosz, Alicia Goodman, Shaikh Ahmed, Swaroop Shivarajapura, Shawn Rice, Carol Song, Steve 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.
- [C159] 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.
- [C158] Clemens Heitzinger and 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.-
- [C157] Mathieu Luisier, Gerhard Klimeck, Andreas Schenk, and Wolfgang Fichtner, "Transport Calculation of Semiconductor Nanowires Coupled to Quantum Well Reservoirs", 11th International Workshop on Computational Electronics (IWCE 11), Vienna, Austria, May 2006.-
- [C156] Gianluca Fiori, Giuseppe Iannaccone, and 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.
- [C155] Neophytos Neophytou, Shaikh Ahmed, M.P. Anantram, and 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.
- [C154] Vladimir V. Mitin, Nizami Z. Vagidov, Mathieu Luisier, and 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.
- [C153] Neerav Kharche, Mathieu Luisier, Timothy B. 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
- [C152] Elizabeth A Gardner, Mark S Lundstrom, and Gerhard Klimeck, "NCN NanoHUB: a resource for nanotechnology education", Presentation at 2006 Materials Research Society Spring Meeting, April 17-21, 2006.

- [C151] Elizabeth A Gardner, Mark S Lundstrom, and Gerhard Klimeck, "NCN NanoHUB: a resource for nanotechnology education", Poster at American Chemical Society Meeting and Exposition, March 26-30, 2006, Atlanta, GA USA.
- [C150] 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.
- [C149] 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.
- [C148] 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.
- [C147] 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.
- [C146] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, and 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-Dec 2, 2005
- [C145] Jing Wang, Anisur Rahman, Gerhard Klimeck and 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).
- [C144] Anisur Rahman, Gerhard Klimeck, and 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).
- [C143] 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).
- [C142] Wei Qiao, David S. 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.
- [C141] Jing Wang, Neophytos Neophytou, Avik Ghosh, Gerhard Klimeck, and Mark Lundstrom, "Full Band Simulation of Silicon Nanowire Transistors," presented at SRC TECHCON, September, 2005
- [C140] Gianluca Fiori, Giuseppe Iannaccone, Mark Lundstrom, and 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.
- [C139] 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, Sept. 7-8, 2005.

- [C138] Sebastien Goasguen, Gerhard Klimeck, Suma Adabala, Rick Kennell, Renato Figueiredo, Alain Roy, Steve Clark, Wendy Lin, Jose Fortes, Dongyan Xu, 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.
- [C137] Gerhard Klimeck, "Parallel Applications in Nanoelectronics", joint CRI/RCAC HPC Training Workshop, Purdue University, September 7-8, 2005.
- [C136] Gerhard Klimeck, Marek Korkusinski, Haiying Xu, Seungwon Lee, Sebastien Goasguen, and Faisal Saied, "Atomistic simulations of long-range strain effects in multimillion-atom quantum dot nanostructures", SISPAD 2005, International Conference on Simulation of Semiconductor Processes and Devices, Komaba Eminence, Tokyo, JAPAN, September 1-3, 2005
- [C135] Sebastien Goasguen, Krishna Madhavan, Michael McLennan, Mark S. Lundstrom and Gerhard Klimeck, "The nanoHUB: A Science Gateway for nanotechnology", Global Grid Forum 14, Science Gateways workshop, June 28, 2005.
- [C134] Marek Korkusinski, G. Klimeck, H. Xu, S. Lee, S. Goasguen, F. 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.
- [C133] Sebastien Goasguen, Michael McLennan, Gerhard Klimeck, and Mark S. Lundstrom, "What do Mambo, VNC, UML and Grid computing have in common?", 2005 Linux Cluster Institute Conference, Raleigh, NC, April, 2005.
- [C132] Marek Korkusinski, Faisal Saied, Haiying Xu, Seungwon Lee, Mohamed Sayeed, Sebastien Goasguen, and Gerhard Klimeck, "Large Scale Simulations in Nanostructures with NEMO3-D on Linux Clusters", 2005 Linux Cluster Institute Conference, Raleigh, NC, April, 2005
- [C131] Olga L. Lazarenkova, S. Lee, P. von Allmen, F. Oyafuso, G. Klimeck, M. 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.
- [C130] Fabiano Oyafuso, Paul von 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.
- [C129] Marek Korkusinski, G. Klimeck, H. Xu, S. Lee, S. Goasguen, F. Saied, "Atomistic simulations in nanostructures composed of tens of millions of atoms", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C128] A. M. Satanin, Y. S. Joe, and G. Klimeck, "Fano quadrupole in a nanoscale ring", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C127] Timothy B. Boykin, Gerhard Klimeck, S. N. Coppersmith, Mark Friesen, Paul von Allmen, Seungwon Lee, and Fabiano Oyafuso, "Valley splitting in low-density quantum-confined heterostructures: Superposition, not Spin!", APS March Meeting, Los Angeles, CA, March 21-25, 2005.
- [C126] Anisur Rahman, Gerhard Klimeck and Mark Lundstrom, "Bandstructure Effects in Nanoscale MOSFETs", IEEE IEDM, San Francisco, CA, Dec. 6-8 2004.
- [C125] Fabiano A Oyafuso, Paul von Allmen, Seungwon Lee and Gerhard Klimeck, "Nonequilibrium Transport in Silicon Nanowires", 2004 MRS Fall Meeting, Boston, MA, Nov. 29 - Dec. 3, 2004.
- [C124] E. Khorenko, W. Prost, F.-J. Tegude, M. Stoffel, R. Duschl, M.W. Dashiell, O.G. Schmidt, and G. 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.

- [C123] Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, S.N. Coppersmith, Mark Friesen, and Mark Erikson, "Electron Exchange Interaction in Electronically Confined Si Quantum Dots", 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, 2004.
- [C122] Yun Zheng, Cristian Rivas, Roger Lake, Khairul Alam, Timothy B. Boykin, and Gerhard Klimeck, "Electronic Properties of Silicon Nanowires", 10th International Workshop for Computational Electronics (IWCE), Purdue University, West Lafayette, Oct. 24-27, 2004.
- [C121] Faisal Saied, Haiying Xu, Mohamed Sayeed, Sebastien Goasquen, and 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.
- [C120] Olga L. Lazarenkova, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, and 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 in St Petersburg, Russia.
- [C119] Olga L. Lazarenkova, Paul von Allmen, Fabiano Oyafuso, Seungwon Lee, and 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.
- [C118] Sebastien Goasquen, 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.

CONTRIBUTED CONFERENCES (WORK PERFORMED AT JPL)

- [C117] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, and 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.
- [C116] Seungwon Lee, Olga Lazarenkova, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Effect of Wetting Layers on Strain and Electronic Structures of Self-Assembled Quantum Dots", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C115] Olga L. Lazarenkova, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, and Gerhard Klimeck, "Atomistic-Level Simulation of the Vibration Spectrum of Quantum Dot Crystals", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C114] Gerhard Klimeck, T. B. Boykin, M. Eriksson, M. Friesen, S. N. Coppersmith, P. von Allmen, F. Oyafuso, S. Lee, "Conduction band valley splitting in Si", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C113] Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, K Birgitta 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).
- [C112] Seungwon Lee, Fabiano Oyafuso, Paul von 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).
- [C111] Paul von 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).
- [C110] Paul von 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).

- [C109] Olga L. Lazarenkova, Paul von 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).
- [C108] Mark Kordon, Gerhard Klimeck, Dave Hanks, and Hook Hua, "Evolutionary Computing for the Design Search and Optimization of Space Vehicle Power Subsystems", IEEE Aerospace Conference, Big Sky, Montana, March 2004. Proceedings P43.
- [C107] Gerhard Klimeck, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Timothy B. 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).
- [C106] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, and Gerhard Klimeck, "Simulation of Hydrogen Sensors using Pd Nanowires", JPL conference on internal research and development, December 4, 2003, Pasadena, CA.
- [C105] Richard J. Terrile, Chris Adami, Michael Ferguson, Wolfgang Fink, Terry 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.
- [C104] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Conduction band valley splitting in silicon nanostructures", 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.
- [C103] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and 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.
- [C102] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, Paul von Allmen, Seungwon Lee, and 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 Convalescència) 16, 17 October 2003.
- [C101] 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.
- [C100] Seungwon Lee, Gerhard Klimeck, K. Birgitta Whaley, "Electron-spin g-factor engineering with SiGe heterostructures", Spintech II International Conference and School, Semiconductor Spintronics and Quantum Information Technology. August 4-8, 2003 Brugge, Belgium.
- [C99] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche 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.
- [C98] Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, and Paul von 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.
- [C97] Gerhard Klimeck, Phillip Stout and R. Chris Bowen, "Quantum and semi-classical transport in RTDs using NEMO 1-D", International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.

- [C96] Jeremy Green, Corrie Farmer, Michel Garcia, Hock Koon Lee, Colin Stanley, Charles Ironside, Gerhard Klimeck, and Roger Lake, "Quantum cascade laser simulation using sp³s* full Brillouin zone tight-binding model", IEEE Conference on Lasers and Electro-Optics CLEO/Europe 2003, Munich 22-27 June 2003.
- [C95] Titus Sandu, Gerhard Klimeck, and Wiley P. 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).
- [C94] Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, and Paul von 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)
- [C93] Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and 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).
- [C92] Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, Timothy B. Boykin, and Paul von 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.
- [C91] Paul von Allmen and Gerhard Klimeck, "Transport simulation of precessing spin distribution across semiconductor heterojunctions", Materials Research Society Meeting, Boston, MA, Dec 1-6, 2002.
- [C90] Gerhard Klimeck, "NEMO: A User-friendly Quantum Device Design Tool", Twenty-Five Years Ultra-Small Electronics Research, Larry Cooper Symposium, November 29, 2002, Hapuna Beach, Hawaii.
- [C89] Gerhard Klimeck, Fabiano Oyafuso, Chris Bowen, Paul von Allmen, Tom Cwik, Ed Vinyard, Edith Huang, Tim 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.
- [C88] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Tim Boykin, Paul von 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.
- [C87] Gerhard Klimeck, Fabiano Oyafuso, Paul von 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 Barbara, CA, Oct. 28, 2002.
- [C86] Akos (Joey) 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.
- [C85] Paul von Allmen, Gerhard Klimeck, and Fabiano Oyafuso, "Simulation of the electric field dependent spin dynamics in semiconductor thin films", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C84] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Tim Boykin, Paul von Allmen, "Modeling of Disordered Multimillion Atom Quantum Dot Systems", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C83] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche McAuley, Eric DeJong, Fabiano Oyafuso, "Image Correlation Quality Control enabled by Cluster Computing", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.

- [C82] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Paul von 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.
- [C81] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems", proceedings of IEEE Simulation of Semiconductor Processes and Devices (SISPAD) 2002, Kobe, Japan, Sept. 3-6, 2002, pg 163 -166.
- [C80] Gerhard Klimeck, Fabiano Oyafuso, E. Bob Tisdale, Akos Czikmantory, "Eigensolver and Cluster Middleware Development", Computational Technology Project Meeting, NASA Goddard Space flight center, MD, July 10, 2002.
- [C79] Gerhard Klimeck and Thomas A. Cwik, "GENES: Genetically Engineered Nanostructures", Nanospace 2002, Galveston, TX, June 24-28, 2002.
- [C78] Paul von Allmen and Gerhard Klimeck, "Transport Simulation of Precessing Spin Distribution across Semiconductor Heterojunctions", Nanospace 2002, Galveston, TX, June 24-28, 2002.
- [C77] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, and R. Chris Bowen, "Quantum Dot Simulation", AFRL-JPL workshop on Nanotechnology, Pasadena, CA, May 8-10, 2002.
- [C76] Myche 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.
- [C75] 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.
- [C74] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, and R. Chris Bowen, "Multi-million Atom Electronic Structure Simulations using NEMO 3-D", March Meeting of American Physical Society, March 17-22, Indianapolis, IN (2002)
- [C73] Seungwon Lee, Lars Jönsson, Jeongnim Kim, John W. Wilkins, Garnett W. Bryant, and 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)
- [C72] 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
- [C71] Gerhard Klimeck "Full Brillouin-Zone, Charge Self-consistent Quantum Transport Simulation 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, Urbana Champaign.
- [C70] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. 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, Urbana Champaign.
- [C69] Tom Cwik, Gerhard Klimeck, Myche McAuley, Bob Deen and Eric Dejong, "Applications on High Performance Cluster Computers Production of Mars Panoramic Mosaic Images", 2001 AMOS Technical Conference, September 10-14, 2001, Maui.
- [C68] Tom Cwik, Gerhard Klimeck, Charles Norton, Thomas Sterling, Frank Villegas and 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.

- [C67] Tom Cwik, Gerhard Klimeck, and 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).
- [C66] Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, R. Chris Bowen, Timothy B. Boykin, Thomas A. 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).
- [C65] Gerhard Klimeck, R. Chris Bowen, Fabiano Oyafuso, Tom Cwik, Section 385, Edith Huang, Section 366, "IT Challenges in Nanoscale Electronic Devices Modeling", JPL IT Symposium, Pasadena, CA, May 9 (2001),
- [C64] Gerhard Klimeck, Myche 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).
- [C63] Tom Cwik, Viktor Decyk, Daniel S. Katz, Gerhard Klimeck, Nooshin Meshkaty, Charles Norton, Fabiano Oyafuso, Paul Springer, Thomas Sterling, Bob Tisdale, Frank Villegas, Ed Vinyard, Ping Wang, High Performance Computing Group, "The Use of Cluster Computer Systems for NASA/JPL Applications", Section 385, JPL IT Symposium, Pasadena, CA, May 9 (2001),
- [C62] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Fabiano Oyafuso, "Atomistic Quantum Dot Simulation using NEMO-3D", Nanospace 2001, Galveston, Texas, March 13-16 (2001).
- [C61] Lars Jönsson, Seungwon Lee, John W. Wilkins, Garnett W. Bryant, and 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),
- [C60] Timothy B. Boykin, Gerhard Klimeck, and R. Chris Bowen, "A tiger by the tail: the momentum operator in tight-binding", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001),
- [C59] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Quantum Dot Modeling using NEMO 3-D", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001),
- [C58] Seungwon Lee, Lars Jönsson, John W. Wilkins, Garnett W. Bryant, and Gerhard Klimeck, "Long-range electron-hole exchange in semiconductor quantum dots", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001).
- [C57] D. Keymeulen, Gerhard Klimeck, R. Zebulum, Adrian Stoica, Yili Jin, Carlos-Salazar Lazaro, "EHWPack: an Evolvable Hardware Environment using the Spice Simulator and the Field Programmable Transistor Array", ANNIE12000 (Smart Engineering System Design), St. Louis, MO, November 5-8, 2000.
- [C56] Gerhard Klimeck, R. Chris Bowen, and Timothy B. 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),
- [C55] Didier Keymeulen, Gerhard Klimeck, Ricardo Zebulum, Adrian Stoica, and 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.
- [C54] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Simulation of Quantum Dots Including Strain and Bandstructure", Electronic Materials Conference, Denver, CO, June 21-23, 2000.

- [C53] Gerhard Klimeck, R. Chris Bowen, and Timothy B. 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,
- [C52] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and 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,
- [C51] Gerhard Klimeck, R. Chris Bowen, Tom Cwik, and Timothy B. Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Nanospace 2000, Houston, TX Jan. 23-28, 2000.
- [C50] Timothy B. Boykin, Gerhard Klimeck, and R. Chris Bowen, "Nanoelectronic Device Calculation from an atomistic point of view: Empirical Tight-Binding Models for Semiconductor Heterostructures", Nanospace 2000, Houston, TX Jan. 23-28, 2000.
- [C49] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Development of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Surfaces and Interfaces in Mesoscopic Devices, Maui, Hawaii, Dec. 5-10, 1999.
- [C48] Gerhard Klimeck and R. Chris Bowen, "Nanoelectronic Modeling (NEMO 1-D and NEMO 3-D)", Supercomputing 99, Portland Oregon, Nov. 13-19, 1999, demo exhibit in NASA booth.
- [C47] Tom Cwik and Gerhard Klimeck, "Genetically Engineered Microelectronic Infrared Filters", First NASA/DoD Workshop on Evolvable Hardware, July 19-21, 1999, Pasadena, CA.
- [C46] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, and Tom Cwik, "Genetically Engineered Nanoelectronics", First NASA/DoD Workshop on Evolvable Hardware, July 19-21, 1999, Pasadena, CA.
- [C45] Adrian Stoica, Gerhard Klimeck, Carlos Salazar-Lazaro, Didier Keymeulen, and Anil Thakoor, "Evolutionary design of electronic devices and circuits", 1999 Congress on Evolutionary Computation, Washington, D.C. July 6-9, 1999.
- [C44] Tom Cwik and Gerhard Klimeck, "Optimization of Microelectronic Devices for Sensor Applications", Micro and NanoTechnology 99, Pasadena, CA, April 12, 1999.
- [C43] Timothy B. Boykin, Lisa J. Gamble, Gerhard Klimeck, R. Chris Bowen, "Valence-band warping in tight-binding models and its effect on heterostructure electronic states", American Physical Society Centennial Meeting, March 22-26, Atlanta, GA (1999).
- [C42] Gerhard Klimeck, R. Chris Bowen, Tom Cwik, and Timothy B. Boykin, "Tight Binding sp³s* Material Parameters from Genetic Algorithms", American Physical Society Centennial Meeting, March 22-26, Atlanta, GA (1999).
- [C41] Tom Cwik and Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", IEEE Aerospace Conference, March 15-19, 1999, Aspen, CO.
- [C40] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, Tom Cwik, and Timothy B. Boykin, "Material Parameter Analysis using quantum mechanical electron transport simulations and genetic algorithms", Material Research Society Meeting, Symposium JJ, Materials in Space - Science, Technology, and Exploration November 29 - December 2, 1998, Boston MA.
- [C39] Gerhard Klimeck, Carlos H. 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.

CONTRIBUTED CONFERENCES (WORK PERFORMED PRIOR TO JPL)

- [C38] Gerhard Klimeck, Daniel K. Blanks, Roger Lake, Timothy B. Boykin, R. Chris Bowen, "NEMO: A 1-D Heterostructure Design Tool", March Meeting of the American Physical Society, March 16-20, Los Angeles, CA (1998).
- [C37] Timothy B. Boykin, Gerhard Klimeck, Roger Lake, and R. Chris 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).
- [C36] Harold Grubin, Gerhard Klimeck, and Daniel K. Blanks, "NEMO-PC", 1997 DARPA ULTRA Electronics and Advanced Microelectronics Program Review, October 26-31, Santa Fe, NM (1998).
- [C35] Gerhard Klimeck, Roger Lake and Daniel K. 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.
- [C34] Roger Lake, Gerhard Klimeck and Daniel K. 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.
- [C33] R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Amitava Chatterjee, Dan Blanks, Roger Lake, Jerry Hu, Joseph Davis, Mak Kulkarni, Sunil Hattangady, and Ih-Chin Chen, "Physical Oxide Thickness extraction and Verification using Quantum Mechanical Simulation", IEEE IEDM, Washington, DC, Dec. 8-10 1997.
- [C32] J. P. A. van der Wagt, A. C. Seabaugh, Gerhard Klimeck, E. A. Beam III., T. B. Boykin, R. C. Bowen, and R. Lake, "Ultralow current density RTDs for tunneling-based SRAM", IEEE International Symposium on Compound Semiconductors, San Diego, CA, Sept. 8-11 1997.
- [C31] Roger Lake, Berinder Brar, Glen D. Wilk, Alan C. Seabaugh, and 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.
- [C30] Daniel K. Blanks, Gerhard Klimeck, Roger Lake, R. Chris Bowen, Manhua Leng, Chenjing Fernando, William R. 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.
- [C29] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Timothy B. Boykin, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, William R. Frensley, Ted Moise, and Y. C. Kao, "The effects of self-consistent charging, incoherent scattering and realistic bandstructure on the non-equilibrium transport of electrons in resonant tunneling diodes.", Non-equilibrium Carrier Dynamics in Semiconductors (HCIS-10), Berlin, Germany, July 28 - August 1 1997.
- [C28] Roger Lake, Gerhard Klimeck, R. Chris Bowen, and Dejan Jovanovic, "Numerical Modeling of Non-Equilibrium Incoherent Scattering in Quantum Devices", Non-equilibrium Carrier Dynamics in Semiconductors (HCIS-10), Berlin, Germany, July 28 - August 1 1997.
- [C27] Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, Roger Lake, Dan Blanks, Ted Moise, Y. C. Kao, and William R. Frensley, "Quantitative Simulation of Strained InP-Based Resonant Tunneling Diodes", The 1997 55th IEEE Device Research Conference Digest, IEEE, NJ (1997).
- [C26] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, William R. Frensley and Dejan Jovanovic, "NEMO: A General Purpose 1-D Quantum Device Simulator", Texas Instruments Corporate Research and Development Conference Aug. 19-20, 1996.
- [C25] Roger Lake, Gerhard Klimeck, "Experimentally Verified Quantum Device Simulations Based on Multiband Models, Hartree Self-consistency, and Scattering Assisted Charging", Proceedings of the 1996 54th IEEE Device Research Conference, Santa Barbara, CA, June 24-26, 1996.

- [C24] Gerhard Klimeck, R. Chris Bowen, Roger Lake, Daniel Blanks, Manhua Leng, Dejan Jovanovic, Chenjing Fernando, William R. Frensley, and Paul Sotirelis, "NEMO: A General Purpose 1-D Quantum Device Simulator", International Conference on Quantum Devices and Circuits, Alexandria, Egypt, June 4-8, 1996.
- [C23] Dan Blanks, Gerhard Klimeck, Roger Lake, Manhua Leng, Dejan Jovanovic, Paul Sotirelis, "NEMO", March Meeting of the American Physical Society, St. Louis, March 1996.
- [C22] Roger K. Lake, Gerhard Klimeck, Chenjing L. Fernando, R. Chris Bowen, Ted Moise and Y. C. 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.
- [C21] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Chenjing L. Fernando and William R. 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. Chris Bowen, Dejan Jovanovic, Paul Sotirelis and William R. 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, Dan Blanks, Paul Sotirelis, R. Chris Bowen, Chenjing Fernando, and Manhua Leng, "Quantum Mechanical Simulation Tools For Semiconductor Devices", Texas Instruments Corporate Research and Development Conference, Aug. 1995
- [C18] R. Chris Bowen, William R. Frensley and Gerhard Klimeck, "Efficient Multiband I-V simulations for quantum devices", IEEE Cornell Device Conference, Ithaca, NY Aug. 7-9, 1995.
- [C17] Gerhard Klimeck, Roger Lake, R. Chris Bowen, William R. Frensley and Daniel Blanks, "Nanoelectronic Modeling (NEMO)", 1995 53rd Device Research Conference, Charlottesville, VA, June 19-21, 1995.
- [C16] William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, and 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. Chris Bowen, William R. 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.
- [C14] Gerhard Klimeck, Roger Lake, and 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, and 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, and Garnett Bryant, "High Bias Transport through Quantum Dots", Workshop on Surfaces and Interfaces, Hawaii, April 24-29, 1994.
- [C11] Gerhard Klimeck, Roger Lake, Garnett W. Bryant, and 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, and 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, and 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, and 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, and 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] Gerhard Klimeck, Roger Lake, and 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, and 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] Gerhard Klimeck, Roger Lake, and Supriyo Datta, "Quantum devices: Where Scattering May Enhance Transport", Purdue Electrical Engineering Industrial Institute Fall Workshop, LED's, HBT's, MBE's, ETC.: What's New in Solid State, October 18-20, 1992.
- [C3] Roger Lake, Gerhard Klimeck, and 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 S. 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 S. Elliott, "Nonlinear Interactions Involving The Real Gaussian Field", Optical Society of America Annual Meeting, 1990.

TECHNICAL REPORTS (WORK PERFORMED AT JPL)

- [T34] Gerhard Klimeck, Michael McLennan, George B. Adams III, "Network for Computational Nanotechnology" Annual Report, May 2010
- [T33] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, George B. Adams III, "Network for Computational Nanotechnology", Network for Computational Nanotechnology
- [T32] Gerhard Klimeck, Mark S. Lundstrom, Venkatamaran Balakrishnan, Cheng-Kok Koh, Timothy B. 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 2008.
- [T31] Mark Lundstrom, Gerhard Klimeck, Michael McLennan, "Network for Computational Nanotechnology", Annual Report, May 2008.
- [T30] Hoon Ryu and Gerhard Klimeck, "Contact Block Reduction Method for transport in Multimillion Atom Systems", Annual Research report to NSF, April 1, 2008.
- [T29] Gerhard Klimeck, Mark S. Lundstrom, Venkatamaran Balakrishnan, Cheng-Kok Koh, Timothy B. 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 and 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, posted on cond-mat arXiv:0709.3310.

- [T26] Gerhard Klimeck, Mark S. Lundstrom, Venkatamaran Balakrishnan, Cheng-Kok Koh, Timothy B. 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, "Network for Computational Nanotechnology", Annual Report, May 2005.
- [T23] Mark S Lundstrom, Gerhard Klimeck, Sebastien Goasguen, Michael McLennan, Renato J. Figueiredo and Jose A. B. 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 von Allmen, and 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.
- [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. Robert 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 A. Cwik, Akos Czikmantory, Gerhard Klimeck, Fabiano Oyafuso, Hook Hua, Edward S. 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. Robert Tisdale, Fabiano Oyafuso, R. Chris Bowen, "Parallel Complex Hermitian Sparse Matrix Eigensolvers", Oct. 3, 2002, NTR 30834, JPL New Technology Report.
- [T15] Gerhard Klimeck, Gary M. 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-Real-time Image Correlation", April 1, 2002, NTR 30631, JPL New Technology Report.
- [T13] Gerhard Klimeck, Robert Deen, Michael McAuley, "Parallel Algorithms for Near-Real-time Mosaic Generation", April 1, 2002, NTR 30630, JPL New Technology Report.
- [T12] Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, Timothy B. Boykin, "Nanoelectronic Modeling 3-D (NEMO 3-D) upgrade", Jan. 6, 2002, NTR 30520, JPL New Technology Report.
- [T11] Gerhard Klimeck, "Tightgen - genetic algorithm-based tight binding parameter generation", Oct. 3, 1999, NTR 20877, JPL New Technology Report.
- [T10] Thomas A. Cwik, Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", Dec. 16, 1998, NTR 20625, JPL New Technology Report.
- [T9] Gerhard Klimeck, "JPL NEMO, Benchmarks including Compiler-Based Parallelization", Sept. 23, 1998, NTR 20552, JPL New Technology Report.

- [T8] Gerhard Klimeck, "JPL NEMO extension for Hole transport", Aug. 1998, JPL New Technology Report.
- [T7] Gerhard Klimeck, "Nanotechnology", Annual report of the Center for Integrated Space Microsystems (CISM) 1999.
- [T6] Gerhard Klimeck, "NEMO Benchmarks on SUN, HP, SGI, and Intel Pentium II", <http://hpc.jpl.nasa.gov/PEP/gekco/parallel/benchmark.html> (1998)

TECHNICAL REPORTS (WORK PERFORMED PRIOR TO JPL)

- [T5] Gerhard Klimeck, Roger Lake, Daniel K. Blanks, "NEMO 3.0 User's, Theory and Technical Guide", Raytheon Corporation, <http://www.raytheon.com/rtis/nemo/pubs/nemopubs.htm> (1997)
- [T4] Gerhard Klimeck, Roger Lake, Daniel K. Blanks, "NEMO 2.0 User's and Theory Guide", Texas Instruments Incorporated, 1995.
- [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 J. McLennan, and Supriyo Datta; "QUEST User's Manual", Technical Report TR-EE 93-17, Purdue University, April 1993.
- [T1] Michael J. McLennan, Gerhard Klimeck and 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

- [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, S-H Park, Hoon Ryu, Sunhee Lee, Neerav Kharche, Lloyd Hollenberg, Sven Rogge, G. 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 of Physics, Sep 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" Samsung 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, "From NEMO1D and NEMO3D to OMEN: 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, Hosts: Dr. Baudilio Teherina and Prof. Mark Ratner.
- [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] "The NCN and the nanoHUB", Mark Lundstrom and Gerhard Klimeck, Lawrence Livermore National Laboratory, April 9, 2007, Host: Dr. Jeff Neaton.
- [S71] "nanoHUB Demo and Usage Scenarios for Education", Michael McLennan and Gerhard Klimeck, Purdue University, Electrical and Computer Engineering, EI2G: The ECE Instructional Innovation Group, March 6th, 2007, Host: Dr. Mark Johnsson.
- [S70] "Atomistic Alloy Disorder in Nanostructures", Gerhard Klimeck, Purdue University, NCN/INAC Tutorial Lecture Feb. 7, 2007, Host: NCN Student Leadership Council.
- [S69] "Electronic Structure of Si/InAs Composite Channels", Gerhard Klimeck and Mara Prada, University of Notre Dame, Electrical Engineering Department Januaray 30, 2007, Host: Prof. Alan Seabaugh.
- [S68] "Network for Computational Nanotechnology", Mark Lundstrom, Gerhard Klimeck, and Michael McLennan, Semiconductor Research Corporation e-Workshop, Teleseminar, Nov. 17, 2006, Host: Jim Hutchby
- [S67] "Atomistic Modeling of Ultra-Scaled Si/Ge Devices and Tool Deployment on nanoHUB.org", Gerhard Klimeck, Samsung Advanced Institute of Technonlogy, Seoul, Korea, October 27, 2006 Host: Dr. Jongsoeb Kim.
- [S66] "The nanoHUB case: Cyberinfrastructure-enabled Virtual Organization", Sebastien Goasguen, Gerhard Klimeck, Dongyan Xu, Renato Figueiredo, Alain Roy, Krishna Madhavan, NSF / OCI (Office of Cyberinfrastructure) seminar, presentation to program directors, NSF, Washington DC, Oct 5, 2006. Host: Dr. Miriam Heller.
- [S65] "Why is Nanotechnology Multidisciplinary? - A perspective of one EE", Gerhard Klimeck, Purdue Multi-Disciplinary Engineering Program, Purdue Univerisy, Oct. 3, 2006, Host: Prof. Robin Adams
- [S64] "HUB Technologies: A Fully Operational Collaborative Cyberinfrastructure for Research, Education, and Outreach Shared Infrastructure Available for You Today!", Michael McLennan and Gerhard Klimeck, Cyber Center Seminar, Purdue University, School of Computer Science, Sept. 25, 2006.

- [S63] "nanoHUB overview to the MSD/MARCO Center", Gerhard Klimeck, MIT MSD/MARCO center Teleseminar, Sept 21. 2006, Host: Prof. Judy Hoyd
- [S62] "HUB Technologies: A Fully Operational Collaborative Cyberinfrastructure for Research, Education, and Outreach Shared Infrastructure Available for You Today!", Michael McLennan and Gerhard Klimeck, University wide presentation, Purdue University, Burton Morgan Center for Entrepreneurship, September 6, 2006.
- [S61] "Usage Scenarios of and Vision for nanoHUB", Michael McLennan and Gerhard Klimeck, Presentation to the teacher summer workshop initiated from SC05, Purdue University, STEW 322 Host: Krishna Madhavan, July, 12, 2006.
- [S60] "nanoHUB.org: The Computational User Facility Complement to the Birck Nanotechnology Center", Michael McLennan and Gerhard Klimeck, Nanotechnology Seminar Series, Purdue University, Birck 1001 June 5, 2006.
- [S59] "nanoHUB.org online simulation and more - A fully operational Cyberinfrastructure that is transforming how Students learn, Teachers teach and Researchers and Engineers work ", Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Krishna Madhavan, 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] "Next-generation Cyberinfrastructure for Bridging Discovery and Learning: nanoHUB", Krishna P.C. Madhavan, Sebastien Goasguen, Gary Bertoline, and Gerhard Klimeck, Revolutionizing science and education through cyberinfrastructure. Presentation at the Exploratorium Brown Bag Series, San Francisco, CA, May 18, 2006.
- [S57] "Next-generation Cyberinfrastructure for Bridging Discovery and Learning: nanoHUB", Krishna P.C. Madhavan, Dongyan Xu, Sebastien Goasguen, Gary Bertoline, and Gerhard Klimeck, April 11, 2006, 10:00am, NSF ENG Cyberinfrastructure Seminar, National Science Foundation, Washington DC, Host; Dr. Gary Gabriele.
- [S56] "Computational and Algorithm Challenges for Nanoscience and Nanotechnology", Gerhard Klimeck, 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] "Bandstructure in Nanoelectronics", Gerhard Klimeck, Nov. 2, 2005, 10:30am, Purdue University Nanotechnology Tutorial Series.
- [S54] "Development of a Nanowire Simulator at the Network for Computational Nanotechnologies (NCN)", Gerhard Klimeck, Sept. 20, 2005, 4:30pm, Gerhard Mercator Universiät Duisburg, Host: Dr. Werner Prost.
- [S53] "Parallel Computing for Realistic Nanoelectronic Simulations", Gerhard Klimeck, Sept. 12, 2005, 2:30pm, Purdue University, Nanotechnology Tutorial Series.
- [S52] "Nano 101 - Quantum Dots", Gerhard Klimeck, July 20, 2005, 11am, Purdue University, Summer Undergraduate Research Institute (SURI) Host: Prof. Michael Melloch.
- [S51] "CVS Crashcourse", Gerhard Klimeck and Michael McLennan, April 6, 9am, 2005, Purdue University, Burton Morgan Entrepreneurship Center, NCN Student Leadership workshop.
- [S50] "NCN Cyberinfrastructure or How can your science software reach thousands of users?", Gerhard Klimeck, April 6, 2pm, 2005, Purdue University, Burton Morgan Entrepreneurship Center, NCN Student Leadership workshop.

- [S49] "The Network for Computational Nanotechnology (NCN) or How can your educational modules contain interactive online simulation? ", Gerhard Klimeck, 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] "The Network for Computational Nanotechnology (NCN)", Gerhard Klimeck, Feb 28, 11am, 2005, Purdue University, STEW 320, ITaP user forum, Host: Steve Dunlop.
- [S47] "The Network for Computational Nanotechnology (NCN) and NEMO 1-D transport simulations", Gerhard Klimeck, Feb 18, 2005, Morgan State University, Baltimore, Host: Prof. Craig Scott.
- [S46] "The Network for Computational Nanotechnology (NCN) or How can your science software reach thousands of users?" Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Feb 17, 2005, NIST, Gaithersburg, Host: Dr. David Seiler.
- [S45] "NEMO 1-D: The First NEGF-based TCAD Tool and The Network for Computational Nanotechnology", Gerhard Klimeck, Nov. 4, 2004, Purdue University, EE 694 Graduate Student Seminar, Host: Prof. P. Krause.
- [S44] "The Network for Computational Nanotechnology Cyber-Infrastructure and Grid Computing for Nanotechnology Exploration and Education", Gerhard Klimeck, Mark Lundstrom, Sebastien Goasguen, Sept. 21, 2004, Purdue University, IEEE Computer Society, Host: Mr. Greg Veldman.
- [S43] "Computational Nanoelectronics: Towards Design, Analysis, and Fundamental Limits - Development of the Nanoelectronic Modeling Tool NEMO", Gerhard Klimeck, Sept. 1, 2004, Walter Schottky Institute, Garching, Munich, Host: Prof. Peter Vogl.
- [S42] "Computational Nanoelectronics: Towards Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, August 30, 2004, GIST at Gwangju, South Korea, Host: Prof. Youngjoo Chung.
- [S41] "NEMO 1-D: A NEGF-based CAD Tool, Interactive lecture and software demo", Gerhard Klimeck, 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] "Numerical Aspects of NEGF: The Recursive Green Function Algorithm", Gerhard Klimeck, 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] "Development of the Nanoelectronic Modeling Tool (NEMO): Towards Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, April 15, 2004, Ball State University, Center for Computational Nanoscience (CCN), Host: Prof. Jin Feng.
- [S38] "HPC Challenges for NanoElectronic Modeling (NEMO)s", Gerhard Klimeck, March 5, 2004, Purdue University, Computing Research Institute (CRI) Advisory Group, Host: Prof. Chris Hoffmann.
- [S37] "Development of NEMO 3-D: Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures", Gerhard Klimeck, Feb. 27, 2004, Ruhr-University University Bochum, Germany, Host: Prof. Ulrich Kunze.
- [S36] "Development of NEMO 3-D: Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures", Gerhard Klimeck, Feb. 24, 2004, University of Duisburg-Essen, Germany, Host: Dr. Werner Prost.
- [S35] "Development of the Nanoelectronic Modeling Tool (NEMO): Towards Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, Feb. 18, 2004, State University of New York, Buffalo, Host: Prof. Vladimir Mitin.

- [S34] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, Purdue University, July 28, 2003, Host: Prof. Mark Lundstrom.
- [S33] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, JPL, Division 32 and 38 Seminar, June 18, 2003, Host: Dr. Carl Ruoff, Div 32&38 Chief Technologist.
- [S32] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, JPL, Section 381 Noontime seminar, April 10, 2003, Host Jason Hyon, Section 381 Deputy.
- [S31] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, Dr. Ed Stone Award Outstanding Research Publication Award Lecture, JPL, Feb. 18, 2003, Host: Dr. Tom Prince, JPL Chief Scientist.
- [S30] "Modeling of Disordered Multimillion Atom Quantum Dot Systems", Gerhard Klimeck, University of Duisburg, Germany, Nov 13, 2002, Hosts Dr. Werner Prost and Prof. Tegude.
- [S29] "Modeling of Disordered Multimillion Atom Quantum Dot Systems", Gerhard Klimeck, Ruhr-University Bochum, Germany, Nov 11, 2002, Host Prof. Ulrich Kunze.
- [S28] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots", Gerhard Klimeck, California State University Northridge, Northridge, CA, March 29, 2002, Host Prof. Nickolas Kioussis.
- [S27] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots", Gerhard Klimeck, Purdue University, West Lafayette, IN, March 20, 2002, Host Prof. Supriyo Datta.
- [S26] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots", Gerhard Klimeck, Notre Dame, South Bend, IN, March 15, 2002, Host Prof. Wolfgang Porod.
- [S25] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots", Gerhard Klimeck, University of Wisconsin, Madison, WI, March 14, 2002, Host Prof. Bob Joynt
- [S24] "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", Gerhard Klimeck, NTT Central Research Laboratory, Erato Project, Feb 8, 2002, Hosts Dr. Michael Stopa and Prof. Tarucha.
- [S23] "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", Gerhard Klimeck, University of Tokyo, February 8, 2002, Host Prof. Seigo Tarucha.
- [S22] "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", Gerhard Klimeck, Tokyo Institute of Technology, Feb 6, 2002, Host Prof. Oda.
- [S21] "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", Gerhard Klimeck, Osaka University, January 30, 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, Chris Bowen, Tom Cwik, and Timothy B. Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Notre Dame, South Bend, IN, April 12, 2000.

- [S17] Gerhard Klimeck, Chris Bowen, Tom Cwik, and Timothy B. Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", General Dynamics Information Systems, Minneapolis, MN, March 22, 2000.
- [S16] Gerhard Klimeck, Chris Bowen, and Tom Cwik, "Simulator Development for Nanoelectronic and Electromagnetic Devices", National Reconnaissance Office, Chantilly, VA, March 31, 1999.
- [S15] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and 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, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", Gerhard Mercator University Duisburg, Nov 25, 1998.
- [S13] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and 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.

INVITED SEMINARS (WORK PERFORMED PRIOR TO JPL)

- [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. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", IMEC, Leuven, Belgium, May 31, 1996.
- [S6] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Ruhr-Universität Bochum, Germany, May 30, 1996.
- [S5] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Universität Duisburg, Germany, May 28, 1996.
- [S4] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Texas Instruments Research Colloquium, Dallas, TX, May 23, 1996.
- [S3] Gerhard Klimeck, Roger Lake, Garnett Bryant, Guanlong Chen, Supriyo Datta, Chris 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, Chris Bowen, William R. Frensley, "Elektronen-Elektronen und Elektronen-Phononen Wechselwirkungen in der Nanotechnologie", Universität Duisburg, Germany, Dec. 15, 1994.

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

PROGRAM REVIEWS

- [R77] Gerhard Klimeck, Mathieu Luisier, "3D Quantum Transport Modeling" NRI Annual Review, MIND, Gaithersburg, Oct 27, 2010.
- [R76] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Rajib Rahman, S.H Park, Neerav Kharche, Z Jiang, Timothy B. Boykin, Lloyd C. L. Hollenberg, Gabri Lansbergen, Sven Rogge, Bent Weber, M 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.
- [R75] Gerhard Klimeck, Mathieu Luisier, "3D Quantum Transport Modeling" MIND - Annual Review Meeting, (Midwest Institute for Nanoelectronics Discovery), Notre Dame, Aug. 10-11, 2010.
- [R74] Gerhard Klimeck, "NCN Director's Overview" NCN annual review, April 28-29, 2010.
- [R73] Gerhard Klimeck, "Quantum Simulation of Advanced Transistors" MSD / FCRP All hands meeting, Stanford University, Pre-review March 1, full review May 5-6, 2010.
- [R72] George B. Adams III, Rick Kennell, Gerhard Klimeck, Michael J. McLennan, Debbie Perouli, Mehdi Salmani, "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
- [R71] George B. Adams III, Rick Kennell, Gerhard Klimeck, Michael J. McLennan, Debbie Perouli, Mehdi Salmani, Strategic Technologies for CyberInfrastructure STCI and Software Development for CI (SDCI) PI Meeting at NSF in Arlington, Virginia, "Instant on Computing", January 28-29, 2010.
- [R70] Gerhard Klimeck, NSF STC proposal site visit, Norfolk State University, "Cyber-Enabled Knowledge Transfer", Oct. 26, 2009.
- [R69] Gerhard Klimeck, "Knowledge Transfer using nanoHUB.org", Norfolk State University, Sept. 21, 2009.
- [R68] Gerhard Klimeck, Hoon Ryu, Sunhee Lee, Rajib Rahman, B Haley, S.H Park, Neerav Kharche, Z Jiang, Timothy B. Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabri Lansbergen, Sven Rogge, Bent Weber, M 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.
- [R67] Gerhard Klimeck and Mathieu Luisier, "3D Quantum Transport Modeling", MIND - Annual Review Meeting, (Midwest Institute for Nanoelectronics Discovery), Notre Dame, Aug. 20, 2009.
- [R66] Gerhard Klimeck, "Full 3-D quantum transport modeling of realistically extended devices ", SRC - Semiconductor Research Corporation, Annual Review Austin, Tx, June 24, 2009.
- [R65] Michael McLennan, Gerhard Klimeck, "nanoHUB and HUBzero overview and demo", NCN annual review, June 17-18, 2009.
- [R64] Gerhard Klimeck, "NCN Director's Overview", NCN annual review, June 17-18, 2009.
- [R63] Gerhard Klimeck, Neerav Kharche, Rajib Rahman, Ben Haley, Timothy B. Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabri 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.
- [R62] Gerhard Klimeck, Michael McLennan, "nanoHUB overview and demo", NCN annual review, June 24-26, 2008.

- [R61] Gerhard Klimeck, Diane Beaudin, "nanoHUB metrics, statistics, and assessment", NCN annual review, June 26-27, 2007.
- [R60] Gerhard Klimeck, "Full 3-D quantum transport modeling of realistically extended devices", SRC - Semiconductor Research Corporation, Annual Review Austin, TX, June 24, 2008.
- [R59] 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.
- [R58] Gerhard Klimeck, Michael McLennan, George Adams, Mark Lundstrom, "nanoHUB - future cyberinfrastructure serving over 62,000 users today", Birck Nanotechnology Research Review 2008, April 14th, 2008.
- [R57] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN all hands meeting, External Advisory Board meeting, April 2nd and 3rd, 2008.
- [R56] Gerhard Klimeck, "Software Customization and Deployment on the nanoHUB", MSD / FCRP All hands meeting, Stanford University, March 4, 2008.
- [R55] Gerhard Klimeck, Neerav Kharche, Rajib Rahman, Srikant Srinivasan, Leonid Rokhinson, Marta Prada, Ben Haley, Timothy B. Boykin, Cameron Wellard, Jared Cole, Lloyd Hollenberg, Gabri 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.
- [R54] Gerhard Klimeck, "Full 3-D quantum transport modeling of realistically extended devices", SRC - Semiconductor Research Corporation, Annual Review Durham, NC, June 26, 2007.
- [R53] Gerhard Klimeck, Michael McLennan, "nanoHUB overview and demo", NCN annual review, June 19-21, 2007.
- [R52] Gerhard Klimeck, Michael McLennan, "nanoHUB overview, metrics, and plans", NCN all hands meeting, External Advisory Board meeting, April 4th and 5th, 2007.
- [R51] Gerhard Klimeck, Marta Prada, Neerav Kharche, Rajib Rahman, Timothy B. Boykin, Seungwon Lee, Paul von 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.
- [R50] Gerhard Klimeck, Michael McLennan, "nanoHUB overview and Usage Scenarios", Purdue University, Discovery Park Advisory Council Meeting, September 15, 2006.-
- [R49] Gerhard Klimeck, Marta Prada, Neerav Kharche, Rajib Rahman, Timothy B. Boykin, Seungwon Lee, Paul von 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.-
- [R48] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", SRC - Semiconductor Research Corporation, Annual Review Durham, NC, June 26-28, 2006.-
- [R47] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN annual review, June 20-22, 2006.-
- [R46] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN all hands meeting, External Advisory Board meeting, April 3rd and 4th, 2006.-
- [R45] 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.-

- [R44] Gerhard Klimeck, Michael McLennan, "nanoHUB overview", NCN advisory board meeting, Purdue University, Feb 6 and 7th, 2006.
- [R43] 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.
- [R42] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebastien Goasguen, Neerav Kharche, Marek Korkusinski, Jing Wang, Timothy Boykin, Fabiano Oyafuso, Paul von Allmen, and 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.
- [R41] Gerhard Klimeck, Paul von Allmen, Rajib Rahman, Neerav Kharche, Timothy B. Boykin, Seungwon Lee, and 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.
- [R40] 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
- [R39] 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
- [R38] Gerhard Klimeck, "NCN Infrastructure Development", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 21-22, 2005.
- [R37] Gerhard Klimeck, "HPC and Visualization for multimillion atom simulations", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 21-22, 2005.
- [R36] Sebastien Goasguen, Markek Korkusinski, Michael McLennan, Gerhard Klimeck, and Mark S Lundstrom, "The nanoHUB a TeraGrid Science Gateway", TeraGrid Grid Infrastructure Group Review Argonne National Lab, IL, November 17-19, 2004.
- [R35] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul von Allmen, Seungwon Lee, and K. Birgitta 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.
- [R34] 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.
- [R33] Anisur Rahman, Mark Lundstrom, Gerhard Klimeck, "Bandstructure effects in Ultra-thin Body MOSFETs", SRC Research Annual Review, June 30, 2004.
- [R32] Gerhard Klimeck, "NCN Computational Research Overview", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 24-25, 2004.
- [R31] Gerhard Klimeck, "NCN Infrastructure Development", Network for Computational Nanotechnology (NCN), NSF Site visit, Jun 24-25, 2004.
- [R30] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Susan Coppersmith, Mark Friesen "Empirical Atomic Level Simulations for QC Applications", ARDA Kickoff Meeting, Madison, WI, June 3, 2004.

- [R29] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul von Allmen, Seungwon Lee, and K. Birgitta 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.
- [R28] Gerhard Klimeck, Fabiano Oyafuso, Bob Tisdale, Hook Hua, R. Chris Bowen, "Development of a Parallel Eigensystem Solver for Beowulf Clusters", Oct 31 2002, JPL ESTO-CT program review.
- [R27] Gerhard Klimeck, Joey Czikmantory, Hook Hua, "WIGLAF – A Web Interface Generator and Legacy Application Facade", Oct 31 2002, JPL ESTO-CT program review.
- [R26] Gerhard Klimeck, Timothy B. Boykin, Fabiano Oyafuso, and Paul von 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.
- [R25] Nikzad Toomarian, R. Chris 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.
- [R24] R. Chris 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.
- [R23] R. Chris 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.
- [R22] R. Chris 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.

PRESENTATIONS AT PROGRAM REVIEWS (WORK PERFORMED AT TEXAS INSTRUMENTS)

[R1-R21] 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.

- [R21] Gerhard Klimeck, "NanoElectronic MOdeling–Software Development Approach", Dec. 1997.
- [R20] Gerhard Klimeck, "Program Status, Activities Overview", May 19, 1997.
- [R19] Gerhard Klimeck, "Software Development – Theory", May 19, 1997.
- [R18] Gerhard Klimeck, "Software Demo", May 19, 1997.
- [R17] Dan Blanks, Gerhard Klimeck, "Software / Interface Development", Nov. 1996.
- [R16] Gerhard Klimeck, "Test Matrix Results", Nov. 1996.
- [R15] NEMO Phase I Review in Washington DC, "NEMO Software Summary", May 1996.
- [R14] NEMO Phase I Review in Washington DC, "NEMO Software Tutorial" (3 hours), May 1996.
- [R13] Gerhard Klimeck, "NEMO: Software Development", Feb. 7, 1996.
- [R12] Gerhard Klimeck, "NEMO: GUI Development", Feb. 7, 1996.

- [R11] R. Chris Bowen, Gerhard Klimeck, "Multiband Simulations", Feb. 7, 1996.
- [R10] Gerhard Klimeck, "GUI and Theory Interaction - A Dynamic Design", October 11, 1995.
- [R9] Gerhard Klimeck, "NEGF Code Development", October 11, 1995.
- [R8] R. Chris Bowen, Gerhard Klimeck, "Multiband Simulation Results", October 11, 1995.
- [R7] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach – Software Development", June 27, 1995.
- [R6] R. Chris Bowen, Gerhard Klimeck, William R. Frensley, "Multiband Simulations", June 27, 1995.
- [R5] Chenjing L. Fernando, Gerhard Klimeck, William R. Frensley, "Polar Optical Phonon Scattering Simulations", June 27, 1995.
- [R4] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach – Software Development", Feb. 23, 1995.
- [R3] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach – Software Development", Feb. 23, 1995.
- [R2] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach – Software Development", fall 1994.
- [R1] William R. Frensley, Gerhard Klimeck, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach – Software Development", summer 1994.

TECHNICAL BRIEFINGS SINCE DEC. 2003

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.

- [B49] 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.
- [B48] Gerhard Klimeck, "nanoHUB.org overview", NCN Workshop on Simulation-Based Learning, Nov. 5-6, Big Ten Conference Center, Chicago.
- [B47] 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.
- [B46] Gerhard Klimeck, "nanoHUB.org Demo and Content Development Options", Briefing to Dr. Deb. Newberry, Dakota County Technical College, Feb. 23, 2009, Purdue University.
- [B45] 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.
- [B44] 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.
- [B43] 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.
- [B42] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 85,000 users today", Briefing to the NCN Education Advisory Board, November 20, 2008, Purdue University.

- [B41] 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.
- [B40] 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.
- [B39] Gerhard Klimeck, "nanoHUB.org: Future Cyberinfrastructure serving over 58,000 users today", Briefing to Purdue IGERT proposal team, Feb. 14, 2008.
- [B38] 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.
- [B37] 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.
- [B36] Gerhard Klimeck, "nanoHUB.org opportunities", Briefing Purdue ECE untenured faculty, Host: Head of ECE, Prof. Mark Smith, Friday, Nov. 16, 2007.
- [B35] Gerhard Klimeck, "nanoHUB.org", Briefing to IEEE Spectrum Editor Glen Zorpette, Host: Purdue CIO Gerry McCartney, Friday, Nov. 7, 2007.
- [B34] Gerhard Klimeck, "Blue Ocean Opportunity", Briefing Purdue ECE external Advisory board, Host: Head of ECE, Prof. Mark Smith, Friday, Nov. 1, 2007.
- [B33] Gerhard Klimeck, "nanoHUB.org demo", Briefing Purdue ECE Industrial Advisory Board, Host: Head of ECE, Prof. Mark Smith, Sept. 10, 2007.
- [B32] 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.
- [B31] Gerhard Klimeck and 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.
- [B30] Gerhard Klimeck and Michael McLennan, "nanoHUB.org demo", Briefing to Steven Kahn, Stanford University, Host: Prof. Chris Hoffmann, Purdue Rosen Center for Advanced Computing. April 19, 2007.
- [B29] Gerhard Klimeck, "nanoHUB.org demo", Briefing to Brian R. Wilson, Distinguished Director, CTO, SUN micorsystems, Host: Ahmed Elmargamid, Purdue Cyber Center. April 2, 2007.
- [B28] Gerhard Klimeck, "nanoHUB.org demo", Briefing to Winslow Sargeat, Venture Investors LLC, Host: Barbara Fossum, Purdue Cyber Center. April 2, 2007.
- [B27] 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.
- [B26] Gerhard Klimeck, "The nanoHUB: a demo", Argonne National Lab, October 30, 2006.
- [B25] Gerhard Klimeck, Mark Lundstrom, Michael McLennan, Sebsten Goasguen, Krishna Madhavan, "The nanoHUB: a demo", NCN Purdue University Advisory Board, Purdue University, Jan 5, 2006.
- [B24] 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.

- [B23] 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.
- [B22] Gerhard Klimeck and Mark Lundstrom, "The Network For Computational Nanotechnology", Briefing to Dennis Buss, Chris Bowen, Ramesh Venugopal, Texas Instruments, Purdue University, Nov 10, 2005.
- [B21] Gerhard Klimeck, "The Network For Computational Nanotechnology", Briefing to Ralph Roskies, Pittsburgh Supercomputing Center, Purdue University, Nov 4, 2005.
- [B20] 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.
- [B19] Gerhard Klimeck, "Nanowire Simulations and The Network For Computational Nanotechnology", Briefing to Alan Seabaugh (Notre Dame) and Lars-Erik Wernersson (Lund). Sept. 14, 2005.
- [B18] Gerhard Klimeck, Mark Lundstrom, Mike McLennan, Sebastien Goasguen, "The Network For Computational Nanotechnology", Briefing to Oak Ridge National Laboratory, Dr. John Cobb, May. 19th, 2005.
- [B17] Marek Korkusinski, Gerhard Klimeck¹, Haiying Xu, Seungwon Lee, Sebastien Goasguen, and Faisal Saied, "Atomistic simulations in nanostructures composed of tens of millions of atoms", Briefing to Intel, Dr. Robert Chau, March 31st, 2005.
- [B16] Gerhard Klimeck, Mark Lundstrom, Mike McLennan, Sebastien Goasguen, "The Network For Computational Nanotechnology", Briefing to Lockheed Martin, Sharon L. Smith, Raj. K. Jain, Feb. 11th, 2005.
- [B15] Gerhard Klimeck, "The Network For Computational Nanotechnology", Briefing to Raytheon, Jill Pate and Dr. Zaher Bardai, Feb. 3rd, 2005.
- [B14] 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.
- [B13] Gerhard Klimeck, "nanoHUB infratructure for NCLT simulations", Briefing to Bob Chang, NCLT, Northwestern University, Dec. 8, 2004.
- [B12] Gerhard Klimeck, "NEGF details in NEMO 1-D and Multimillion atom simulations", Briefing to Intel, Mark Stettler, and Borna Obradovic, Oct. 28, 2004.-
- [B11] Gerhard Klimeck and Michael McLennan, "Computing, Software, and Cyberinfrastructure, Briefing to Intel, Mark Stettler, Martin Giles, and Borna Obradovic, Oct. 28, 2004.
- [B10] 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.
- [B9] Mark Lundstrom and Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN)", Briefing to Intel, JoZell Johnsson, Sept. 21, 2004.
- [B8] Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN)", Briefing to EMC, Deborah Snow and Gael Keough, Sept. 21, 2004.
- [B7] Anisur Rahman, Jing Wang, Ali Yannik, Gerhard Klimeck, "Bandstructure and Spintronics Research", Briefing to Intel Corp., Dimitry Nikonov, Sept. 21, 2004.

- [B6] Mark Lundstrom, Gerhard Klimeck, "The Network for Computational Nanotechnology (NCN) and Intel", Briefing to Intel Corp., Kevin Kahn, Sept. 10, 2004.
- [B5] 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 Ventine, Neil Peterson, at Purdue University, July 27, 2004.
- [B4] 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.
- [B3] 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.
- [B2] Gerhard Klimeck, "Development of the Nanoelectronic Modeling tool (NEMO)", Briefing to ARO, Barry Perlman, May 3, 2004.
- [B1] 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.

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," Fac-ets, International Union of Materials Research Societies, 2005.

PANEL PARTICIPATION

- [Pa 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
- [Pa 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.
- [Pa 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
- [Pa 6] Nano Frontiers Workshop, by invitation only, Meeting sponsored by NSF, NIH, Pew Charitable Trust, Wilson Center for International Scholars, Feb. 9-10, 2006.
- [Pa 5] "Panel Discussion: Nanotechnology in the Americas", GNN 2005, 3rd International Workshop to Develop a Global Nanotechnology Network, May 25-27, 2005, Saarbrücken, Germany.
- [Pa 4] "Panel discussion: Interaction with Industry", 2004 NSF Nanoscale Science and Engineering Grantees Conference, Washington, DC, Dec. 15, 2004.
- [Pa 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).
- [Pa 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).

- [Pa 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?", International Workshop on Computational Electronics, Glasgow, Scotland, UK, May 22-25, 2000, Moderator: Prof. John Barker (U. of Glasgow).