Multi-Scale Quantum Transport Modeling of LED

Junzhe Geng
Ph.D. Defense
July 12th, 2017

PURDUE
UNIVERSITY

Nanoscale Optoelectronics Modeling

① III-V Quantum Cascade Laser (~20%)

- Full-scale NEGF simulation
- Model validation of photon absorption
- Device engineering

② GaN-based LED (~80%)

- Developed a new modeling approach
  - ○ Multi-scale NEGF framework
  - ○ Algorithms such as meshing, matrix inversion, nonlinear solver
- New radiative recombination model
- Device modeling

Everything implemented in *NEMO5*
Core features implemented in nanoHUB tool *quantumLED*

NEMO5

LED – Lighting of the 21st Century

- **Energy Efficiency (lm/W)**
  - » LED (300) >> fluorescent (70) & incandescent (16)
- **Durability**
  - » LED Lifetime: 10x florescent, 1000x incandescent;
- **Cost savings:** $150B/year in the U.S. alone
- **Environmental benefits:** 200M tons less carbon emission in the U.S. alone

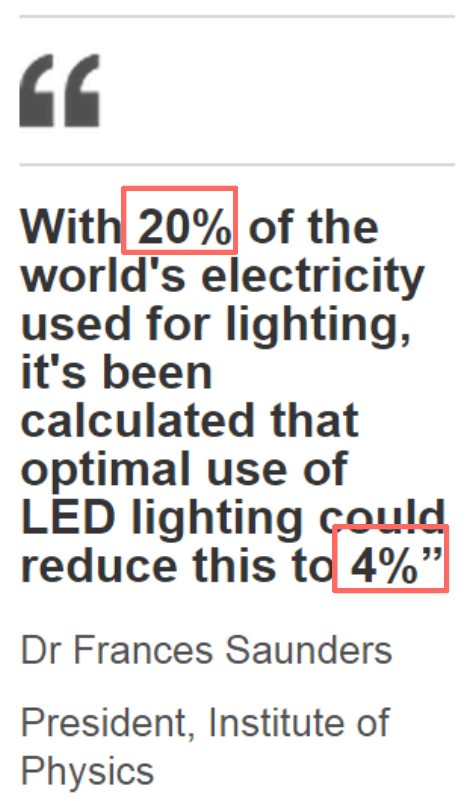
KUNGL.
VETENSKAPS-
AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

THE NOBEL PRIZE IN PHYSICS 2014

POPULAR SCIENCE BACKGROUND

Blue LEDs – Filling the world with new light

***Isamu Akasaki**, **Hiroshi Amano** and **Shuji Nakamura** are rewarded for inventing a new energy-efficient and environment-friendly light source – the blue light-emitting diode (LED). In the spirit of*



> “
>
> **With 20% of the world's electricity used for lighting, it's been calculated that optimal use of LED lighting could reduce this to 4%”**
>
> Dr Frances Saunders
>
> President, Institute of Physics

Outline

Key Challenges in LED Development

Multi-Scale Quantum Transport Model

Modeling Results and Insights into LED Physics

New Radiative Recombination Model

Outline

Key Challenges in LED Development

- Experimental Challenges
- Requirements of Predictive Modeling
- Challenges and Current Approaches to LED Modeling

Multi-Scale Quantum Transport Model

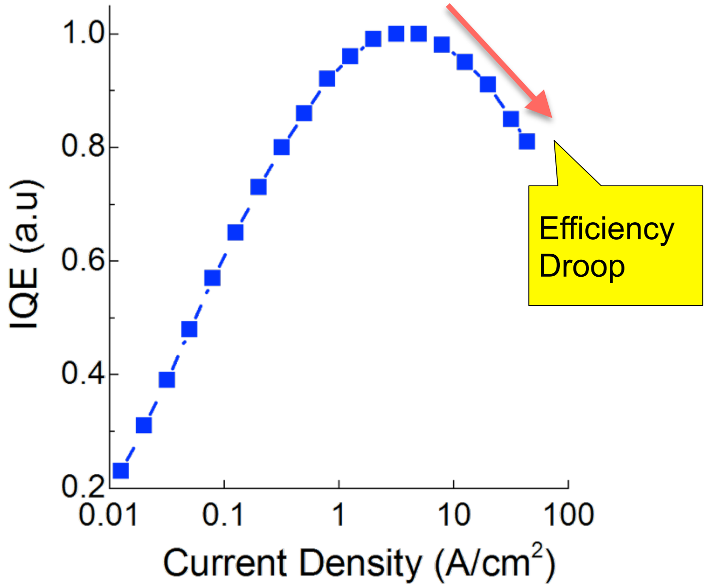
Modeling Results and Insights into LED Physics

New Radiative Recombination Model

Key challenges in LED development
1) Efficiency ‘droop’ 2) Uneven carrier distribution

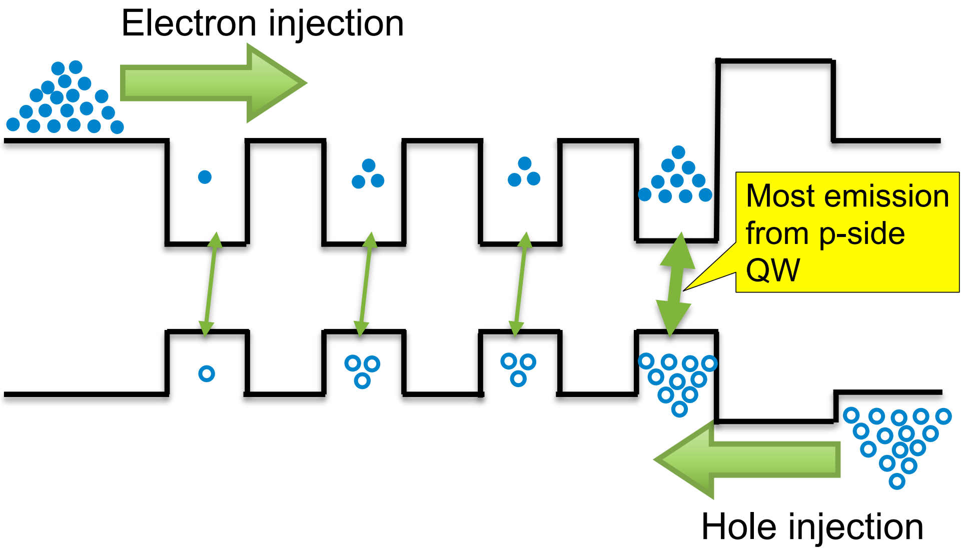
● Efficiency ‘droops’ at high current density

Auger effect at high carrier density believed to be the main cause [1, 2]



● Uneven light emission distribution across MQW [3]

Carrier pile-up worsens ‘droop’



Carrier distribution determined by transport properties

[1] Y.C. Shen, et al, Appl. Phys. Lett. 91, 141101 (2007), [2] J. Iveland, et al, Phys. Rev. Lett. 110, 177406 (2013),
[3] Aurélien David, et al, Appl. Phys. Lett. 92, 053502 (2008)

Key challenges in LED development

3) Completing mechanisms 4) Infeasible 'trial-and-error'

3 Trade off between radiative and Auger recombination

Thin QW:

→ Good e-h overlap

→ Better radiative recomb.

→ **Worse droop**

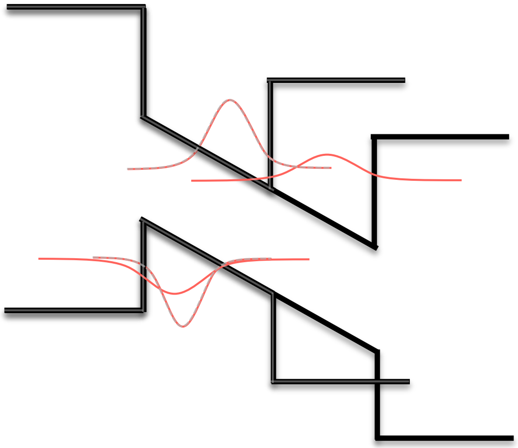
Remedy?

Thick QW:

→ Reduced e-h overlap

→ Smaller peak density

→ **Less radiative recomb.**



Ideal QW-thickness has to consider balance between radiative and Auger recombination

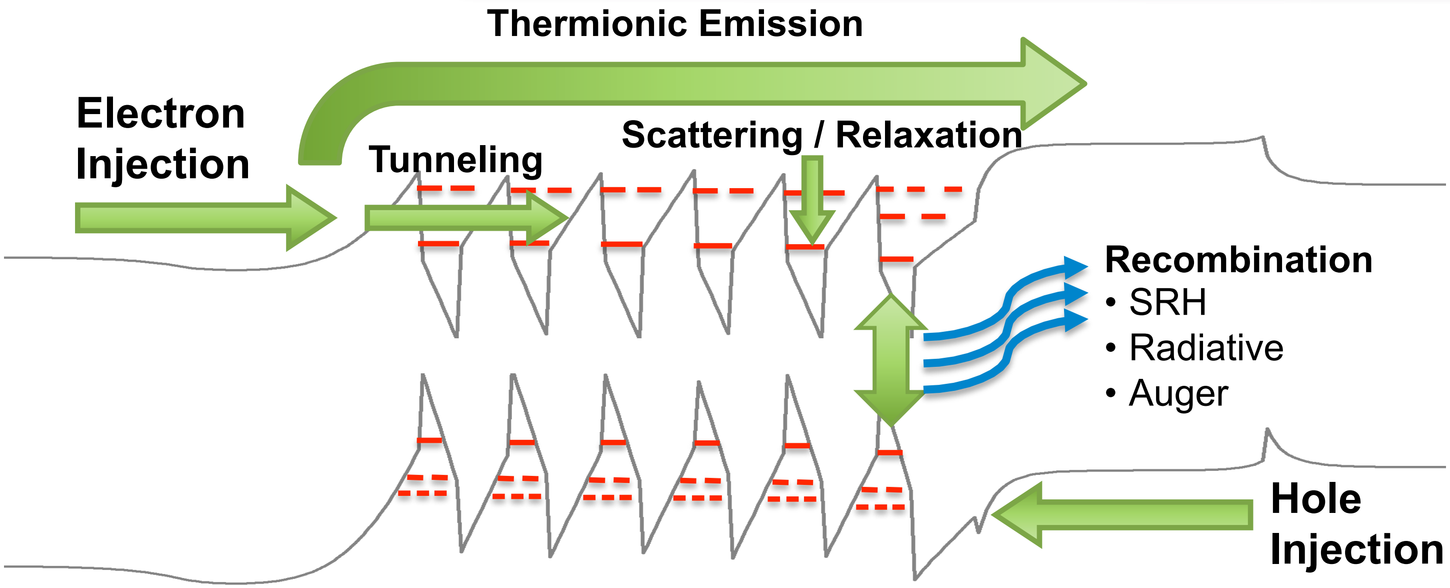
---

4 Not feasible to evaluate every LED design experimentally

- Cost prohibitive
- Interfering effects (e.g. structure changes, crystal growth, electrical and optical response) confuse results interpretation

Theoretical models essential to guide experimental device design

Predictive modeling requires deep understanding of LED transport physics

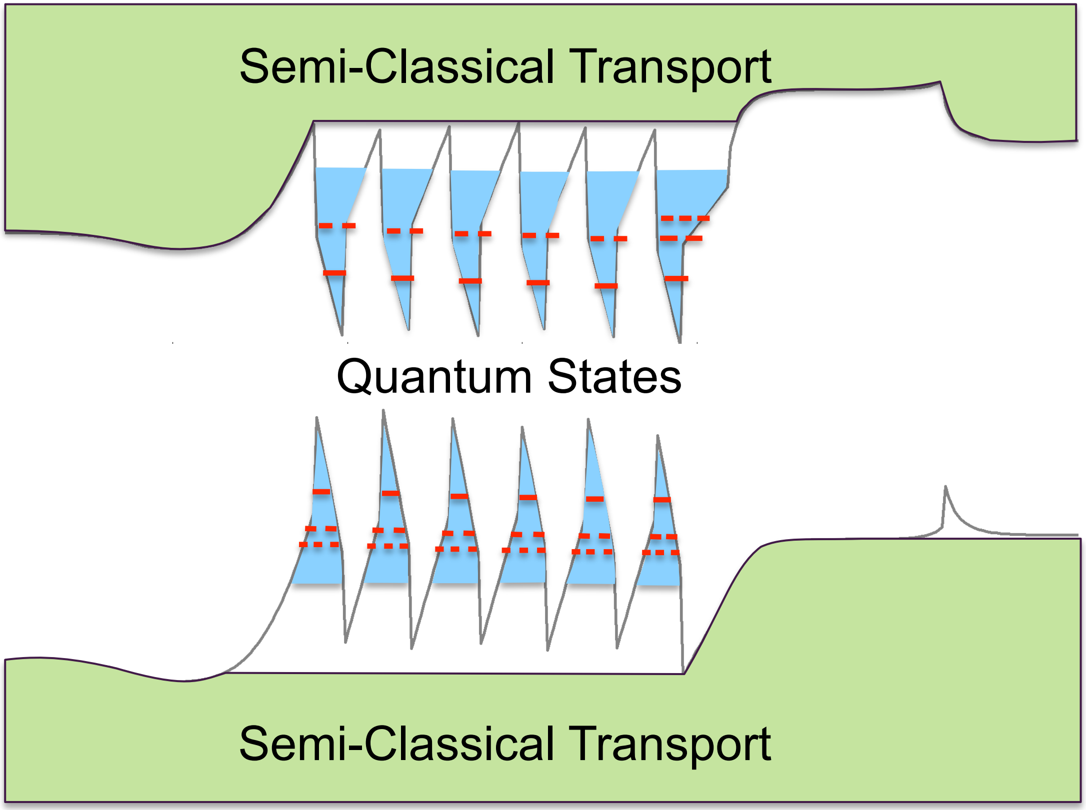


Predictive modeling must provide:

- Correct transport behavior: carrier density and turn-on voltage
- Electron & hole transport through extended structure
- Consistent treatment of tunneling and thermionic emission
- Physical, realistic recombination model
- Numerical efficient, allow rapid engineering

Traditional approaches have severe challenges in accurately modeling nanoscale LED

Modeling challenges
– Classical models missing key information



Semi-classical transport often neglects:

- Bandstructure details
- Quantum effects

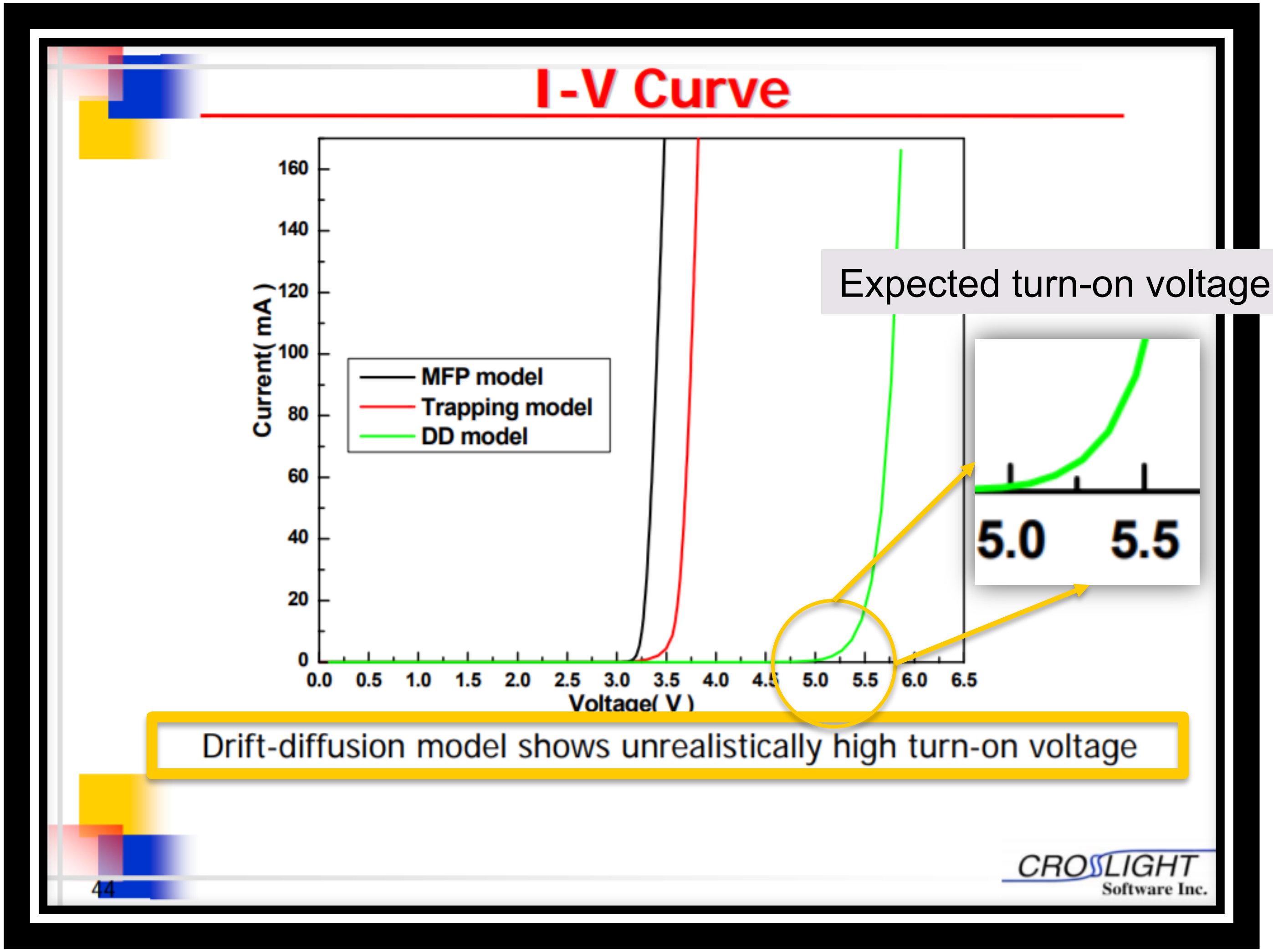
Distinction between continuum and discrete states is required

- Where to draw the boundary?
- How to couple classical to quantum transport?
- Rely on ad-hoc heuristics
- Cannot be truly predictive

Achieving correct transport behavior is challenging

- Inaccurate transport physics → unrealistic turn-on voltage

Classical model's I-V challenge



Expected turn-on voltage ~ 3V

Drift-diffusion model shows unrealistically high turn-on voltage

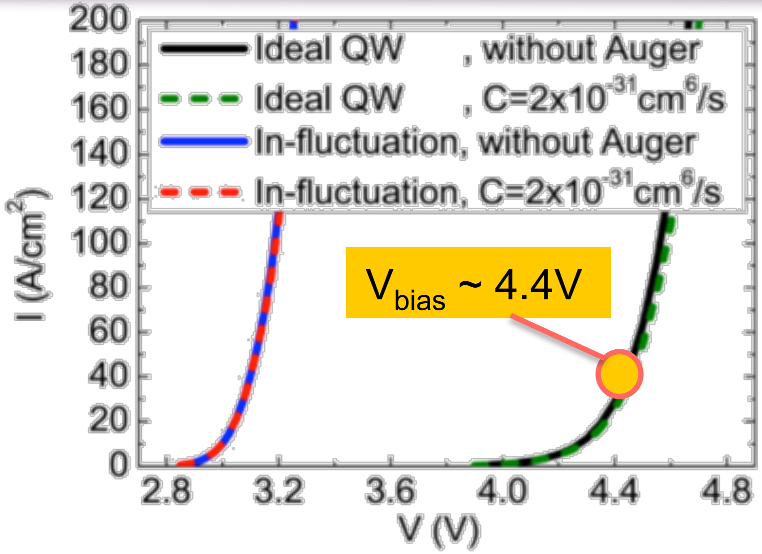
Documentation of *Crosslight* software by ***APSYS*** — A famous commercial LED tool

http://crosslight.com/wp-content/uploads/2013/11/crosslight_led_research2.pdf

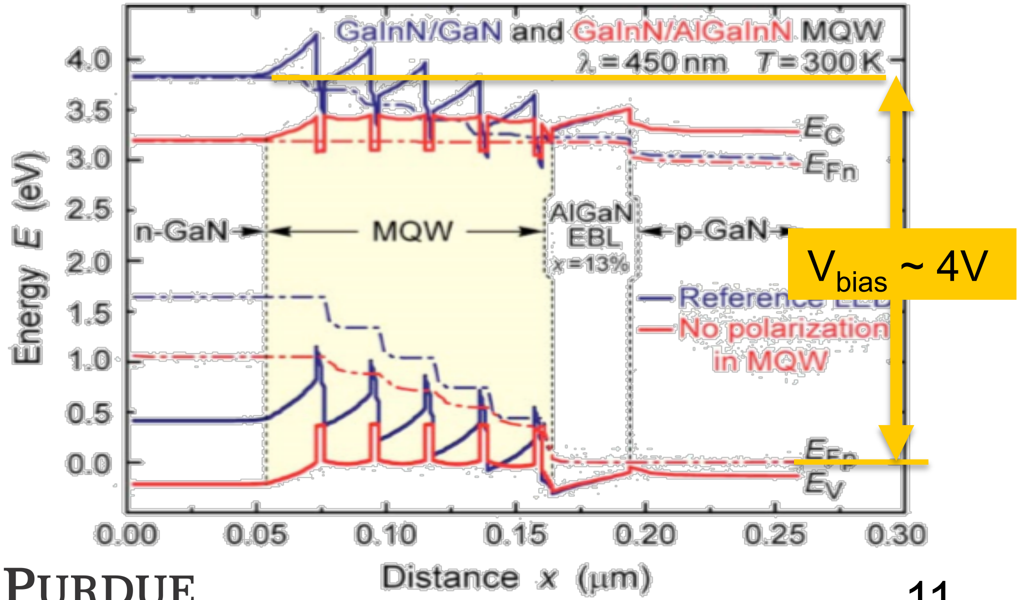
Classical model's I-V challenge

Yang, et al. discussed about the turn-on voltage issue in their paper.
Their claimed solution is to *3D transport simulation with random alloy*

Yang, et al. JAP 116, 113104 (2014)



V_{bias} ~ 4.4V



V_{bias} ~ 4V

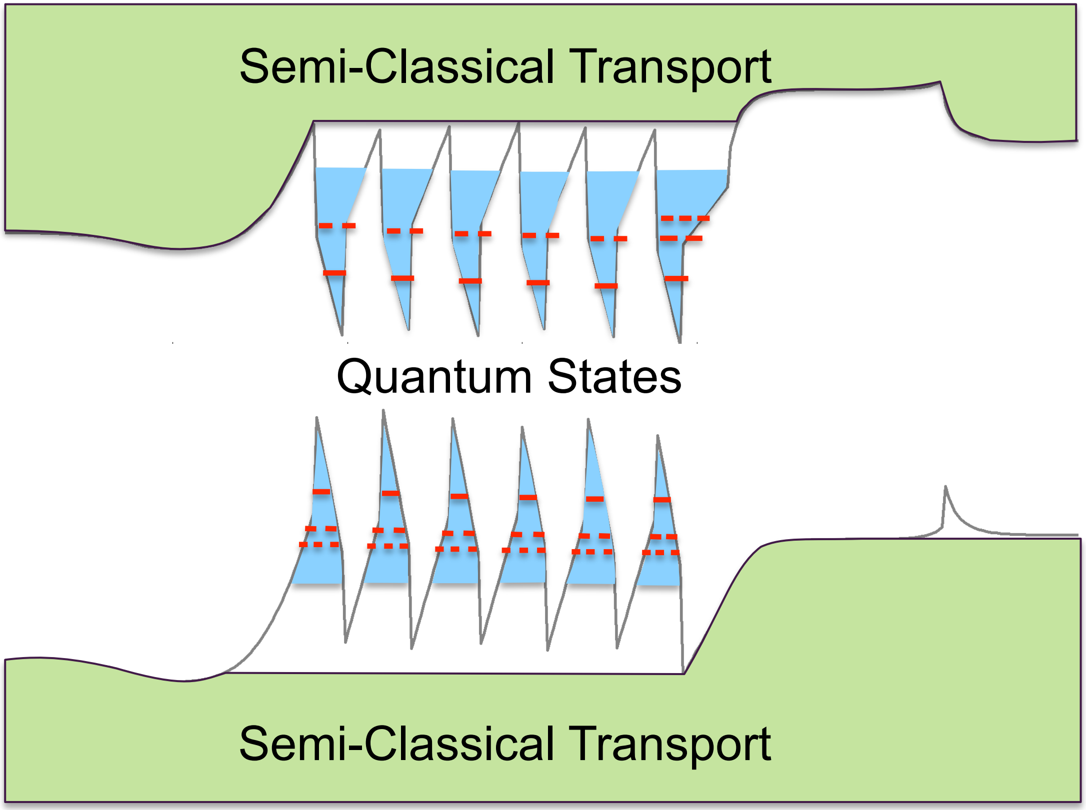
The "Auger vs. Leakage" Debate

A main supporting argument of "leakage causing droop" theory was based on simulation using *APSYS*

Kim, et al. "Origin of efficiency droop in GaN-based light-emitting diodes ", APL (2007)

The biggest debate in the LED community was backed by unrealistic transport result?

Modeling challenges
– Classical models missing key information



Need a physically consistent model to address these challenges

Semi-classical transport often neglects:

- Bandstructure details
- Quantum effects

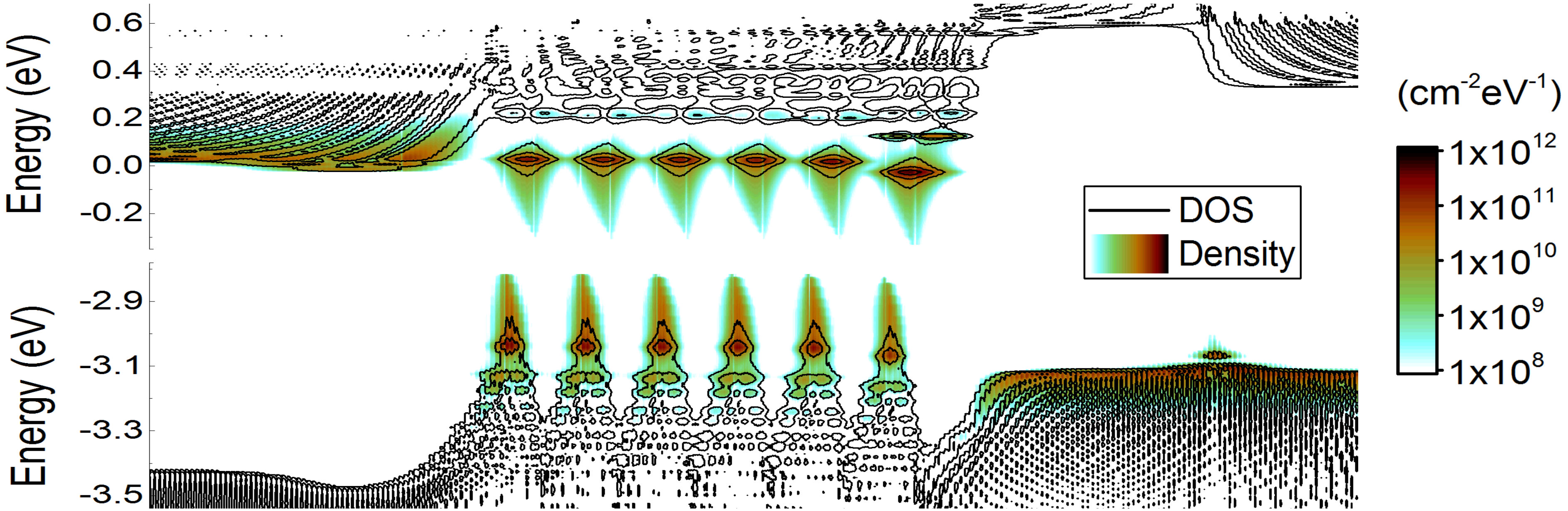
Distinction between continuum and discrete states is required

- Where to draw the boundary?
- How to couple classical to quantum transport?
- Rely on ad-hoc heuristics
- Cannot be truly predictive

Achieving correct transport behavior is challenging

- Inaccurate transport physics → unrealistic turn-on voltage
- Impacts carrier density, recombination and calculated efficiency

Modeling challenges – Quantum model too expensive



The 'Quantum' Reality

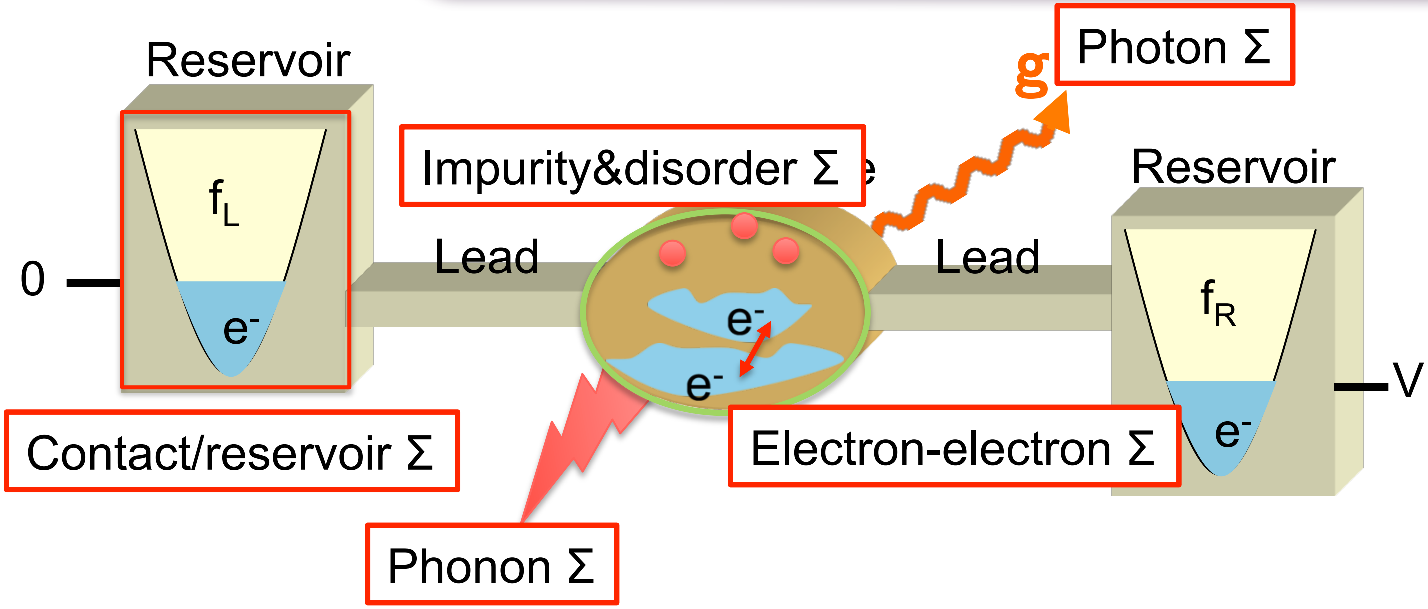
- Quantum interference everywhere, no distinct classical and quantum regions
- Coupling between continuum and discrete states occurs naturally
- States are distributed and broadened
- Transport through a complex, extended structure

Computation Challenges

- Very large structure
- Scattering rate expensive to solve
- No 'good' e-e scattering model

No quantum transport tool available for LED industry

Nonequilibrium Green's functions (NEGF) Overview

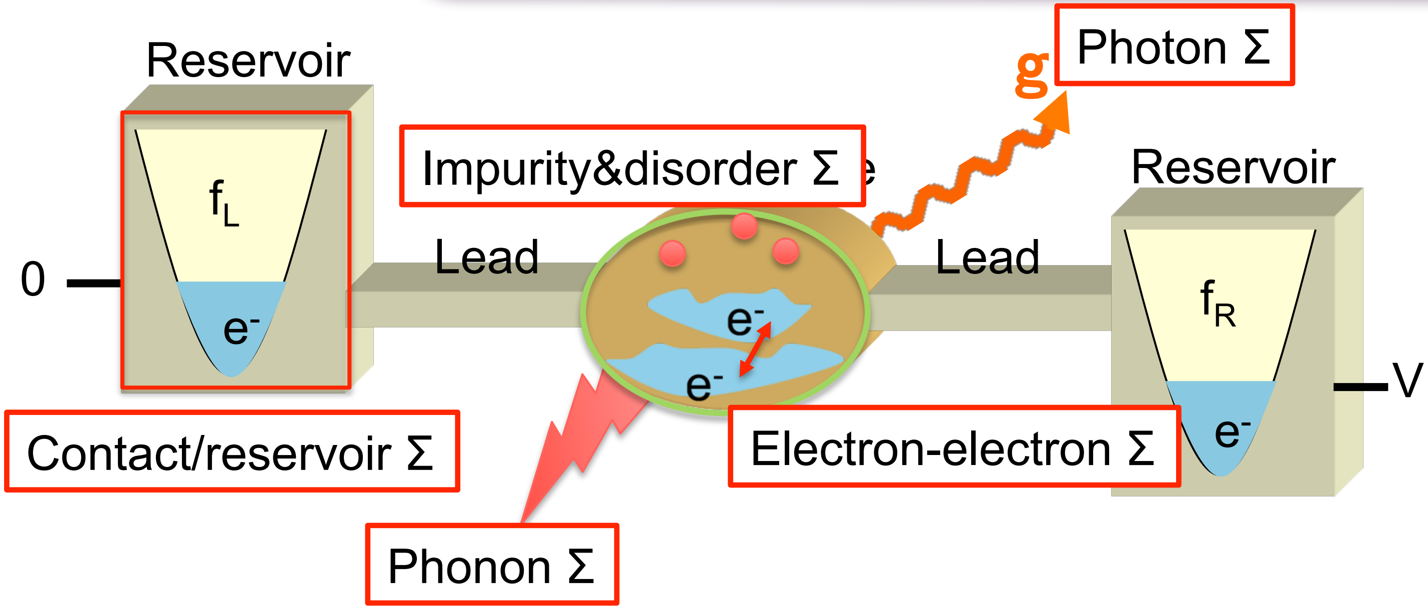


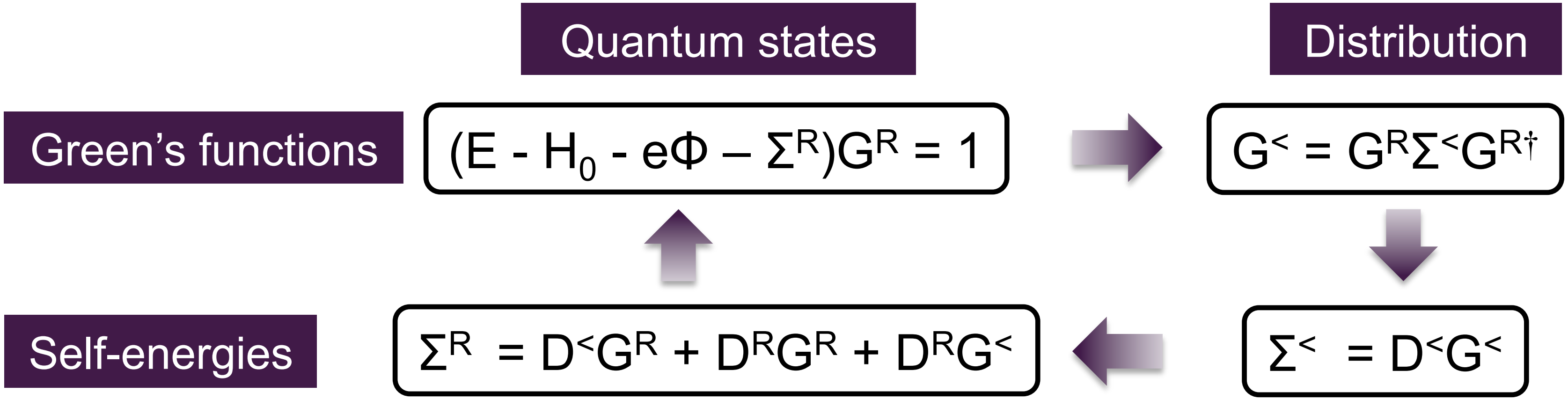
NEGF Overview

- Separation of active device and reservoirs
- Reservoirs treated as thermal equilibrium
- Interaction with reservoirs described by self-energies Σ
- All other interactions (phonon, e-e, etc.) described by self-energies

Provides consistent description of coherent quantum effects and incoherent scattering

Nonequilibrium Green's functions (NEGF) Overview





$(E - H_0 - e\Phi - \Sigma^R)G^R = 1$

$G^< = G^R \Sigma^< G^{R\dagger}$

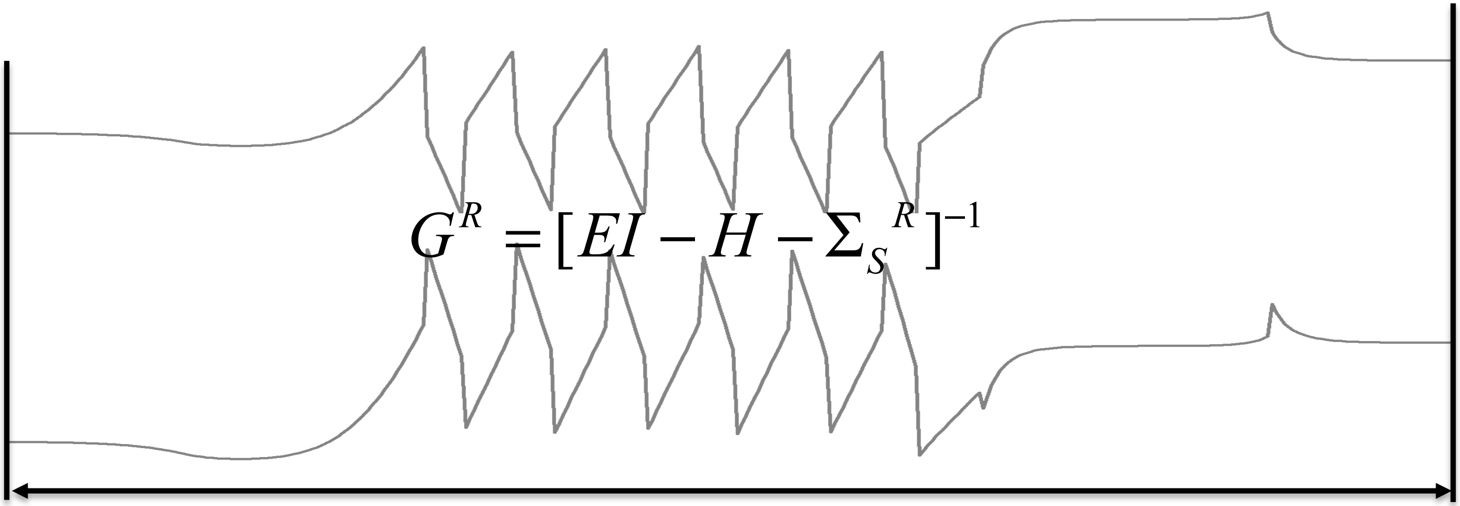
$\Sigma^< = D^< G^<$

$\Sigma^R = D^< G^R + D^R G^R + D^R G^<$

Incoherent scattering requires self-consistent solution between Green's function and self-energies

The Challenges to Quantum Modeling

Matrix Inversion in Large Structrue



~130 nm, or 1000 atoms long

Matrix size for this device: $20{,}000^2$
Storing the full matrix requires:

6 GB

Matrix inversion (Tri-diagonal LU ~ $O(n^2)$)
To invert a full matrix of 20,000 x 20,000

4 x 10^8 operations

x

Typical simulation: 2000 energy, 50 k, 10 iterations:

one million

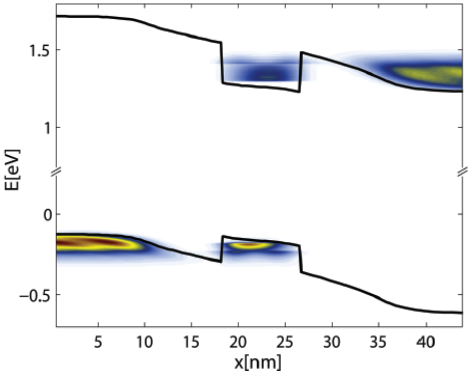
LED structure is very large, matrix inversion expensive

The Challenges to Quantum Modeling
Existing Work

Electroluminescence from a Quantum-Well LED using NEGF

Sebastian Steiger† and Ratko G. Veprek
Integrated Systems Laboratory
ETH Zurich

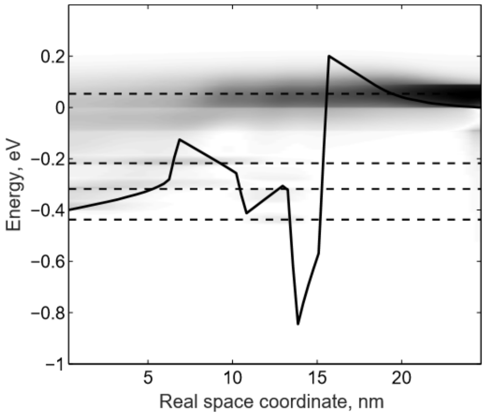
Bernd Witzigmann
Computational Electronics and Photonics Group
University of Kassel
mshöher Allee 71, D-34121 Kassel, Germany
Email: bernd.witzigmann@uni-kassel.de



Single band,
Single QW
No e-e
No Auger

Challenges towards the simulation of GaN-based LEDs beyond the semiclassical framework

Michele Goano[a,b], Francesco Bertazzi[a,b], Xiangyu Zhou[a], Marco Mandurrino[a], Stefano Dominici[a],
co Calciati[b], Pierluigi Debernardi[b],
o Meneghini[e], Nicola Trivellin[e], Carlo
ico Bellotti[f]



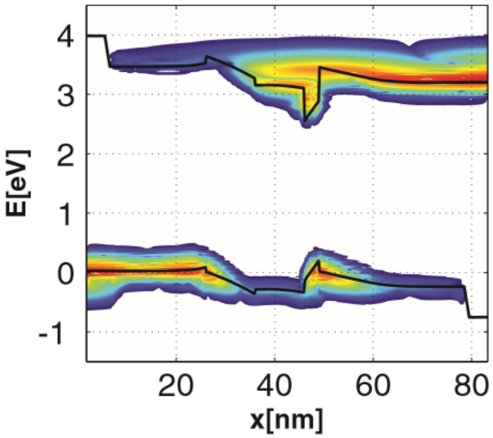
Phys. Status Solidi B 253, No. 1, 158–163 (2016) / DOI 10.1002/pssb.201552276

Part of Topical Section on
Polarization-field control in nitride light emitters

physica status solidi b
www.pss-b.com
basic solid state physics

Simulation of an indium gallium nitride quantum well light-emitting diode with the non-equilibrium Green's function method

Akshay Shedbalkar*,1, Zhelio Andreev2, and Bernd Witzigmann1



No good NEGF model for e-e scattering & Auger recombination, both are very important

[Conclusion] Key Challenges in LED Development

- Need transport modeling to guide experimental design
- Semiclassical-based transport lacks coherent treatment for quantum phenomenon, problem manifested in unrealistic I-V
- Quantum transport model too expensive — can’t handle realistic device

Multi-Scale Quantum Transport Model

Modeling Results and Insights into LED Physics

New Radiative Recombination Model

Outline

Key Challenges in LED Development

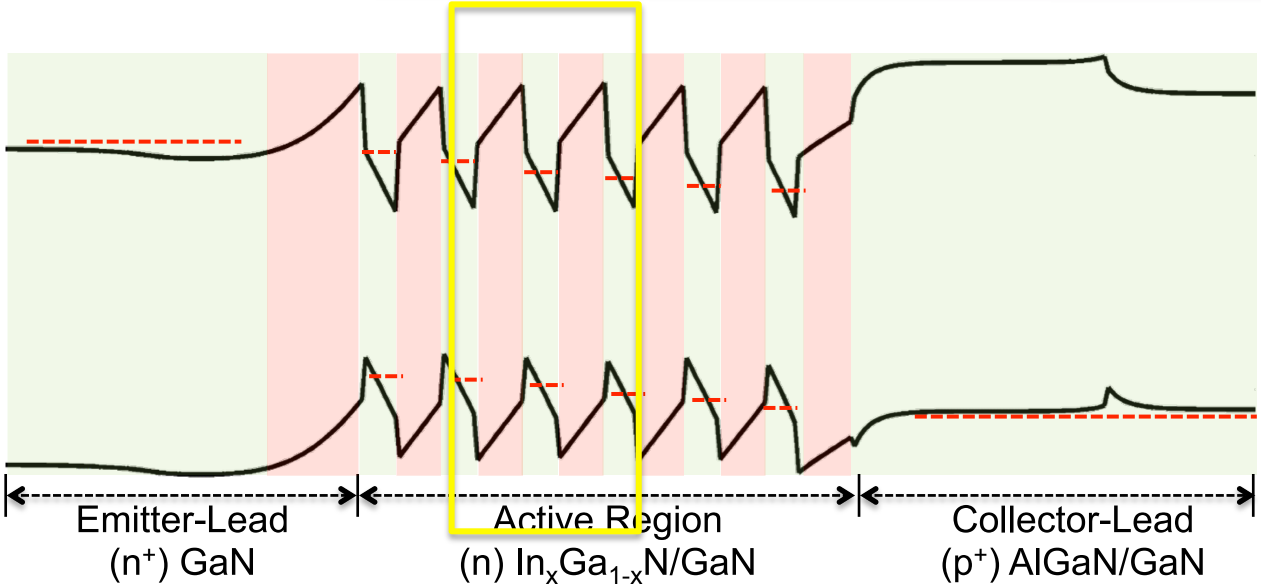
Multi-Scale Quantum Transport Model

Modeling Results and Insights into LED Physics

New Radiative Recombination Model

Multi-domain, multi-physics model

Exact QM, approximate occupancy, strong scattering



Multiple Domains / Physics:

Emitter / Collector contacts + QWs:

- High carrier density, strong scattering
- Charge reservoir, thermal equilibrium
- Include scattering rate as “known”

→ Assume equilibrium occupancy

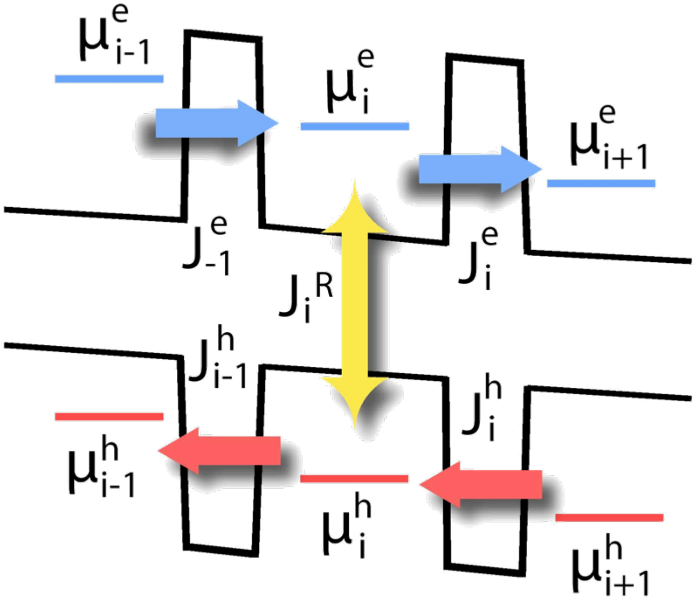
Barriers:

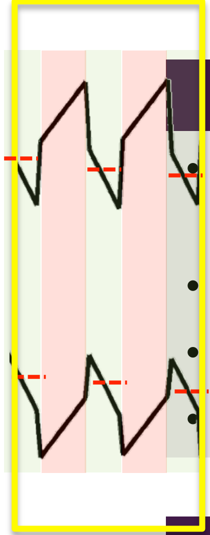
- Coherent quantum transport (automatically include thermionic emission and tunneling)
- Scattering can be included

NEGF throughout device — quantum mechanics are “exact” everywhere

Detailed balance:

1) ensure current conservation 2) separate recomb. from QT





Essential Physical Quantities

- **J^e / J^h** : coherent current (thermionic + tunneling) across each barrier
- **μ^e / μ^h** : equilibrium Fermi levels
- **n / p** : electron / hole density
- **J^R** : Recombination rates.

Recombination Model

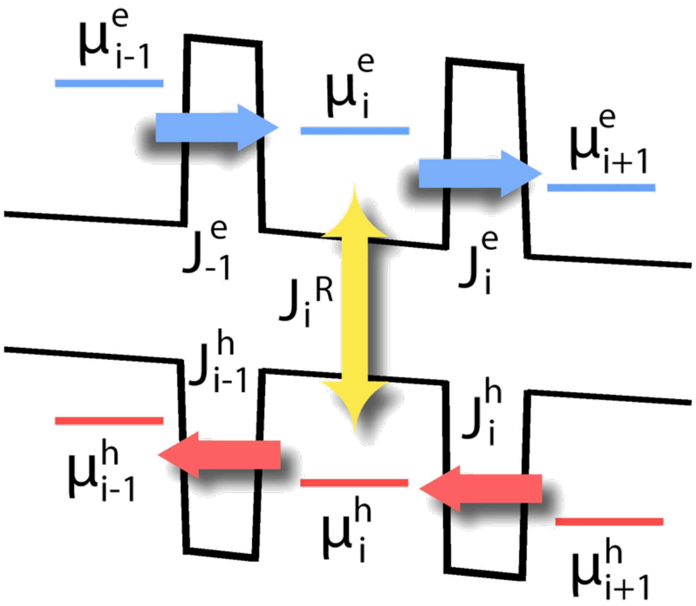
- SRH, Auger— ‘ABC’ model*
- Radiative — ‘ABC’ model and quantum-based model (will be discussed later)

Current conservation ensured with detailed balance between coherent current, thermalization and recombination

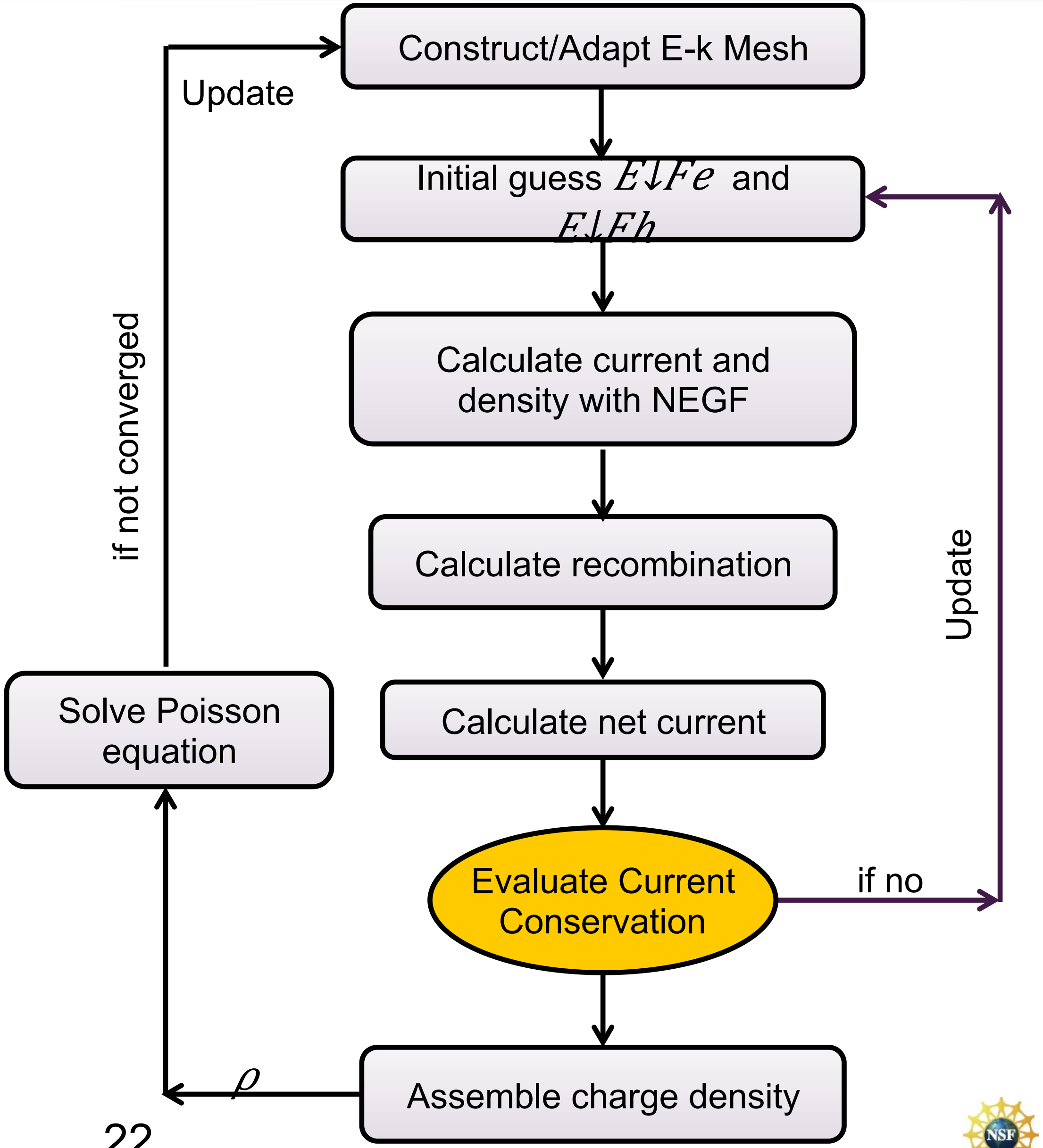
*ABC model described in backup slides

Multi-Scale, Multi-Physics Approach:

Charge self-consistent + quantum transport + detailed balance



Current conservation ensured with detailed balance between coherent current, thermalization and recombination



Construct/Adapt E-k Mesh

Initial guess E_{Fe} and E_{Fh}

Calculate current and density with NEGF

Calculate recombination

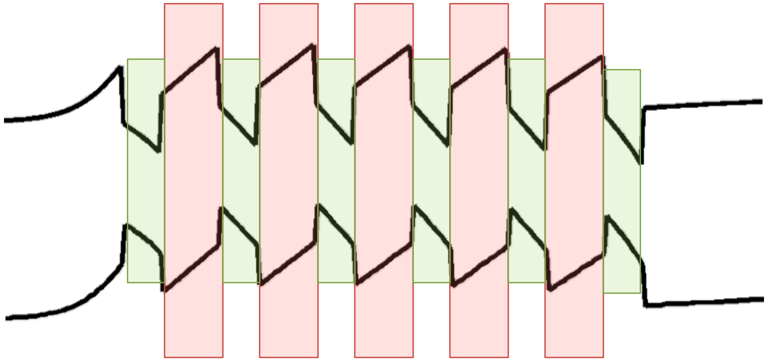
Calculate net current

Evaluate Current Conservation

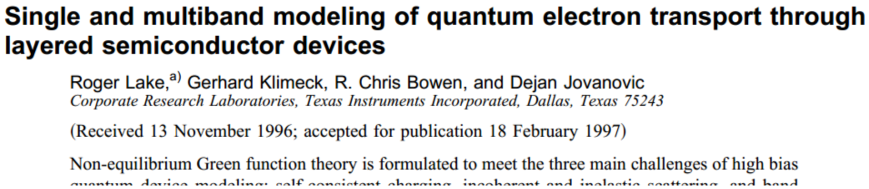
Assemble charge density

Solve Poisson equation

Multi-Scale, Multi-Physics Modeling
Inversion Algorithm



The RGF Algorithm

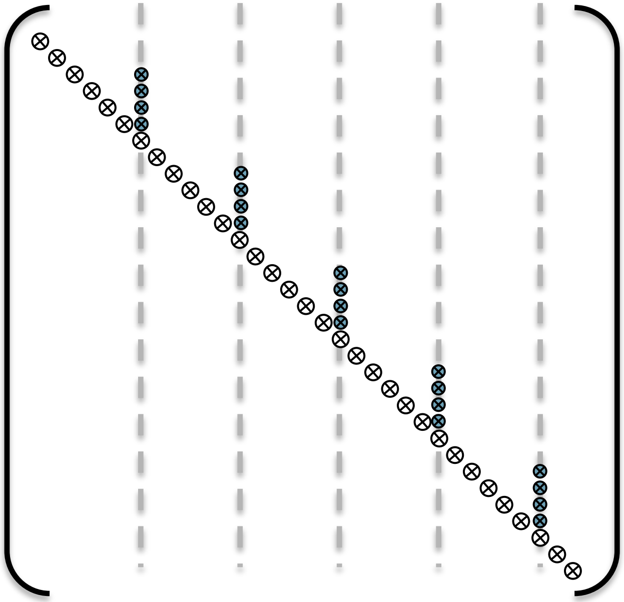


Single and multiband modeling of quantum electron transport through layered semiconductor devices

Roger Lake,[a] Gerhard Klimeck, R. Chris Bowen, and Dejan Jovanovic
Corporate Research Laboratories, Texas Instruments Incorporated, Dallas, Texas 75243

(Received 13 November 1996; accepted for publication 18 February 1997)

Non-equilibrium Green function theory is formulated to meet the three main challenges of high bias

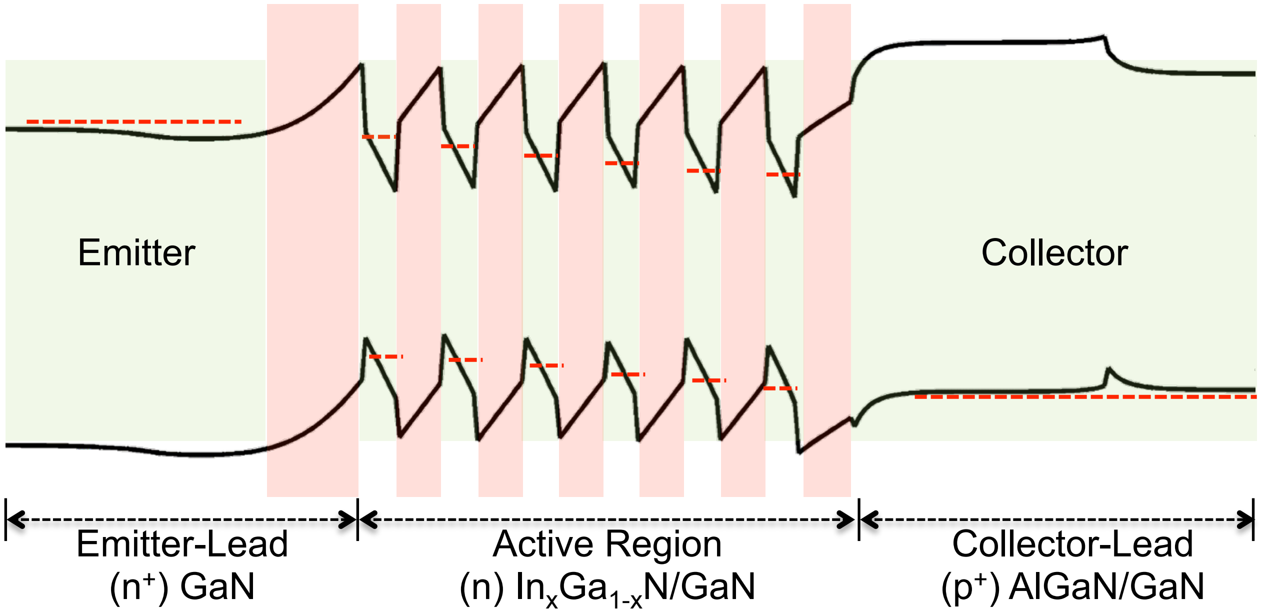


With the RGF algorithm, only the diagonal and some off-diagonals are needed

- Matrix inversion time & memory complexity both reduced O(n^2) to O(n)

Developed an extension of the RGF algorithm to include multiple equilibrium regions

Model Summary



Model Summary

- QW treated as thermal equilibrium, scattering is assumed rather than solved.
- Recombination are solved separately.
- Quantum transport is limited to only small domain, the rest of structure treated as boundary conditions.

Key Challenges Addressed

- ✓ Scattering Σ too expensive, no good e-e model
- ✓ No SRH and Auger model available
- ✓ Structure is large, matrix inversion expensive

Outline

Key Challenges in LED Development

Multi-Scale Quantum Transport Model

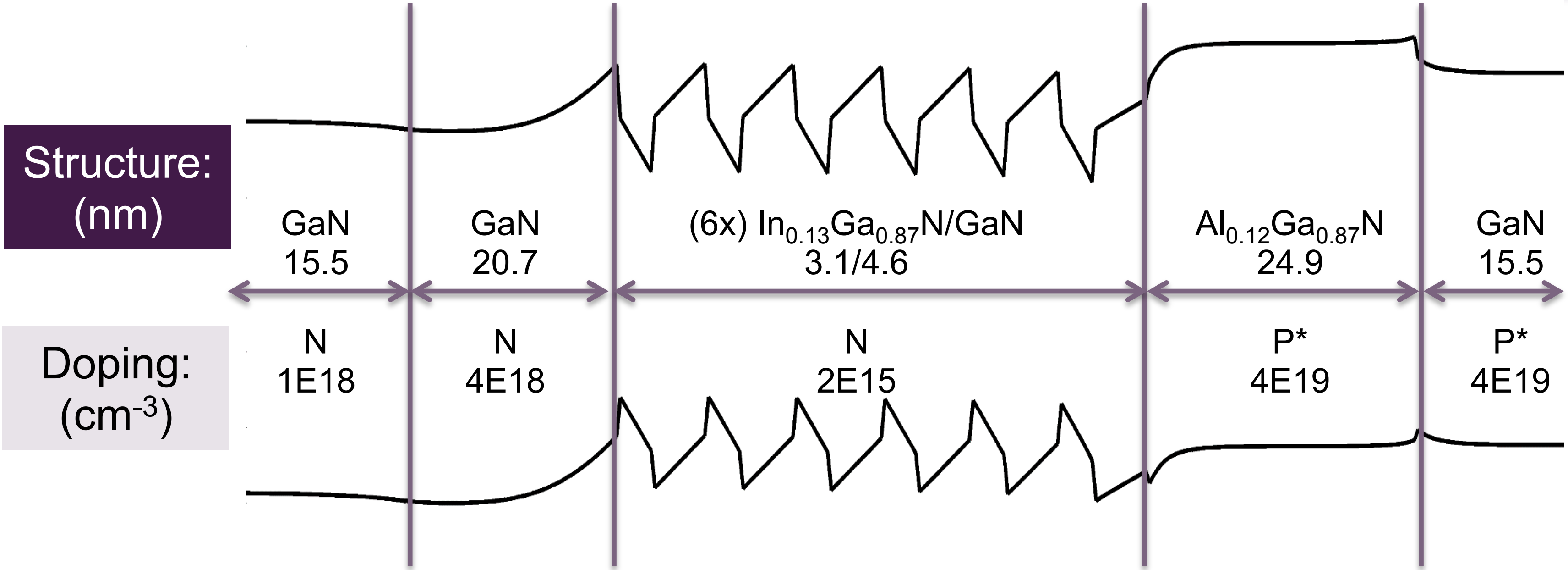
Modeling Results and Insights into LED Physics

- **Simulation of a prototypical LED and comparison with experiment**
- **Impact of scattering strength**
- **Impact of hot carriers**
- **Trend analysis w.r.t barrier thickness and Al%**

New Radiative Recombination Model

Simulation on a realistic LED

Atomic resolution with sophisticated bandstructure

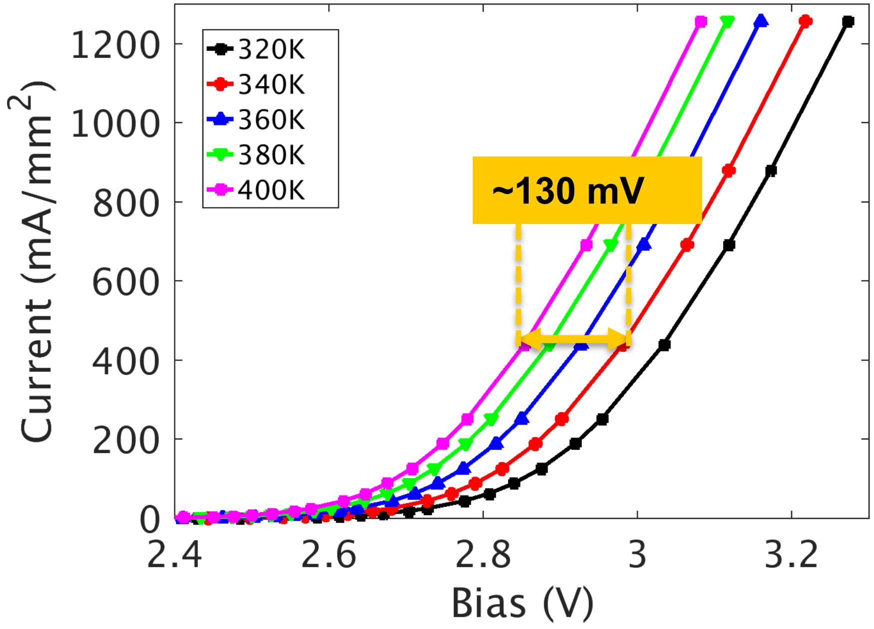


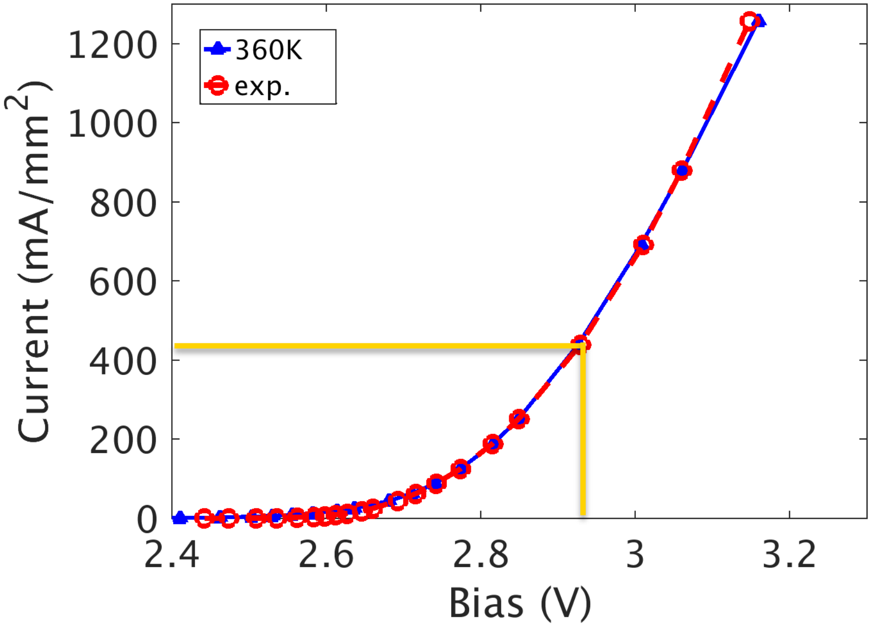
Structure: (nm)	GaN 15.5	GaN 20.7	(6x) $In_{0.13}Ga_{0.87}N$/GaN 3.1/4.6	$Al_{0.12}Ga_{0.87}N$ 24.9	GaN 15.5
Doping: (cm^{-3})	N 1E18	N 4E18	N 2E15	P* 4E19	P* 4E19

- MQW: GaN/$In_{0.13}Ga_{0.87}N$; EBL: $Al_{0.12}Ga_{0.87}N$
- Atomistic 20 band tight-binding ($sp^3d^5s^*$ with spin-obit coupling)
- A = 2.9 x 10^6 (s^{-1}), B = 1.5 x10^{-11} (cm^3 s^{-1}), C = 1.6 x10^{-30} (cm^6 s^{-1}) values extracted from experimental measurement
- Scattering rate: ~3 x 10^{14}/s, corresponding to 100 meV emission broadening width
- Included a known contact resistance: 2.0 mΩ·cm^2 in the I-V comparison

* Incomplete ionization with ionization energy = 0.16eV

Results:
I-V agrees quantitatively with experiment



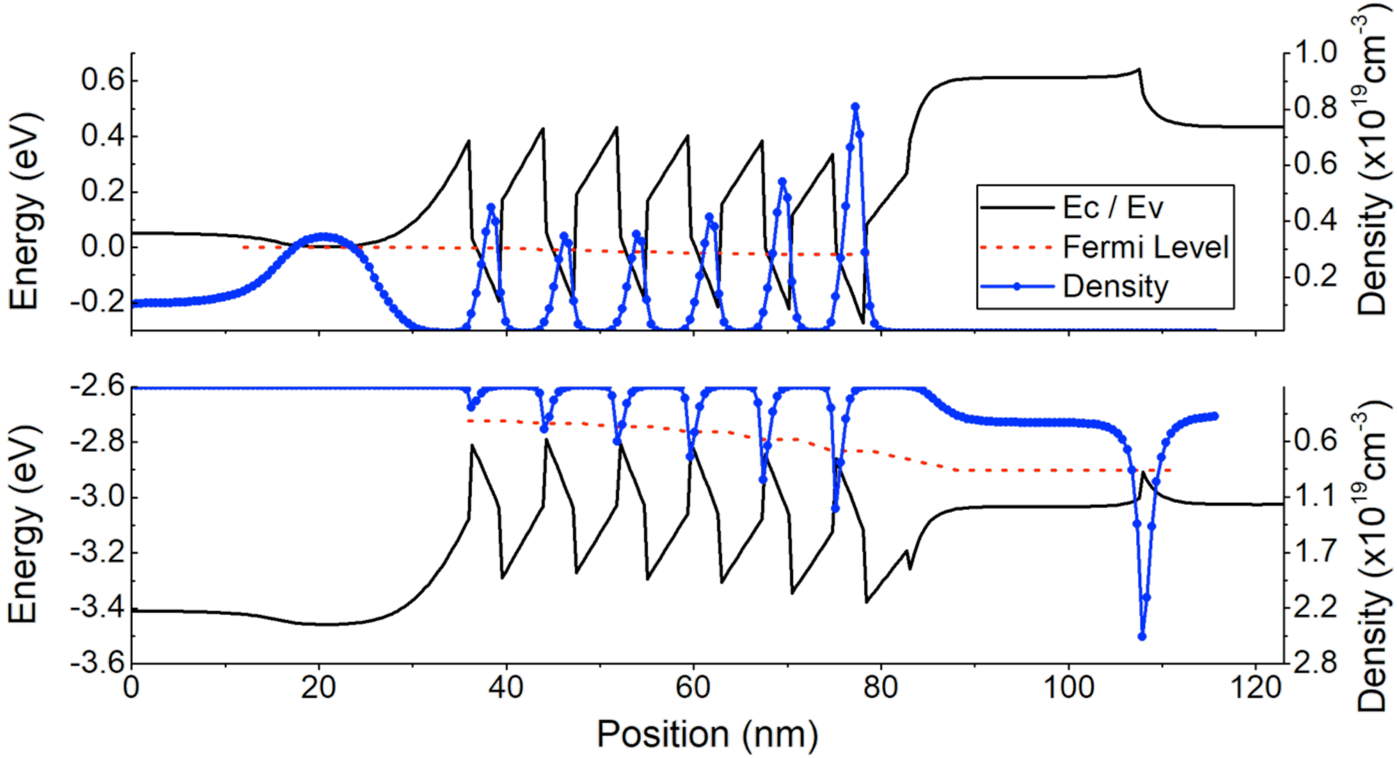


- At LED operating current 440 mA /mm^2, temperature swing of 60K leads to forward voltage shift by ~130mV; exp. value: ~100meV
- Electron temperature @ 360K (~85 ℃) gives **quantitative agreement with experiment**, forward voltage (V_F) ~ 2.9V @ 440 mA /mm^2
- Agree with experimental evidence: **electron temperature well-above room temperature** [1]

---

[1] Christophe A. Hurni, et al, Applied Physics Letters 106, 031101 (2015)

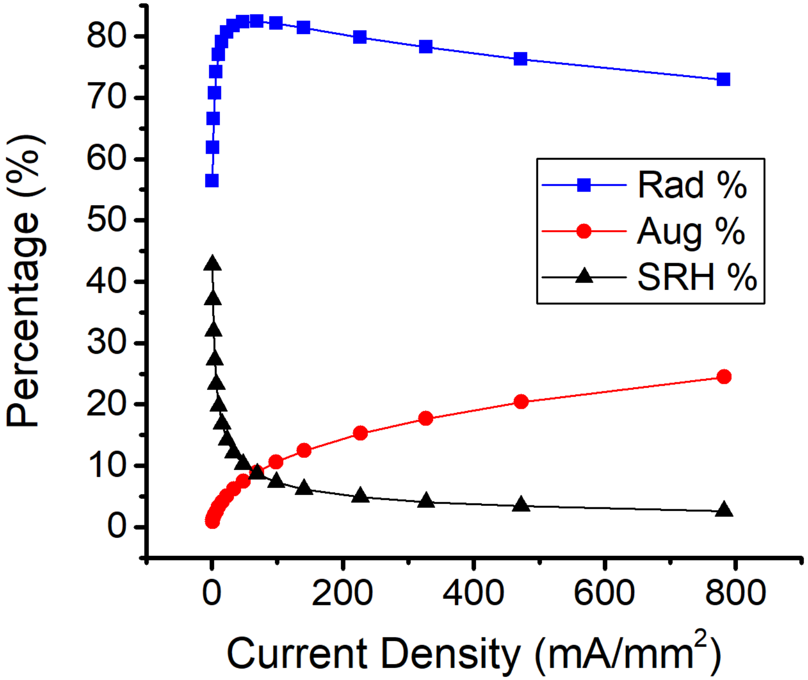
Results: Charge accumulation on p-side



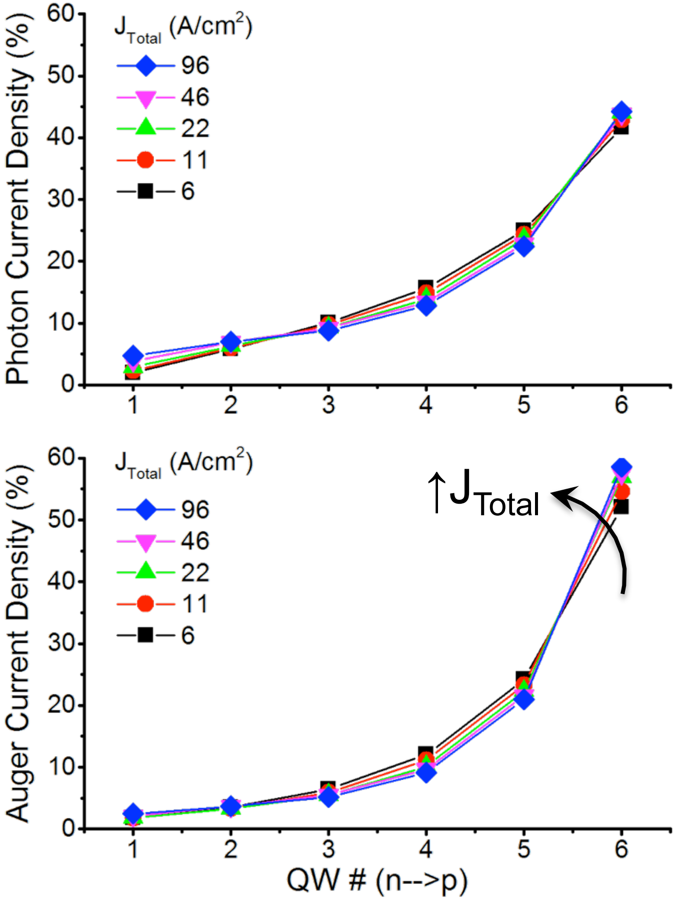
- Uneven density distribution — **charge accumulation at p-side**
- Fermi level drop: Hole (176meV) >> Electron (25meV)
- Hole transport is much more difficult compared to electron

Results:

IQE, QW emission matches experimental observations



- Efficiency droop qualitatively captured
- Simulation indicates droop contribution: **Auger recombination >> carrier leakage** — matches with experimental observation [1]



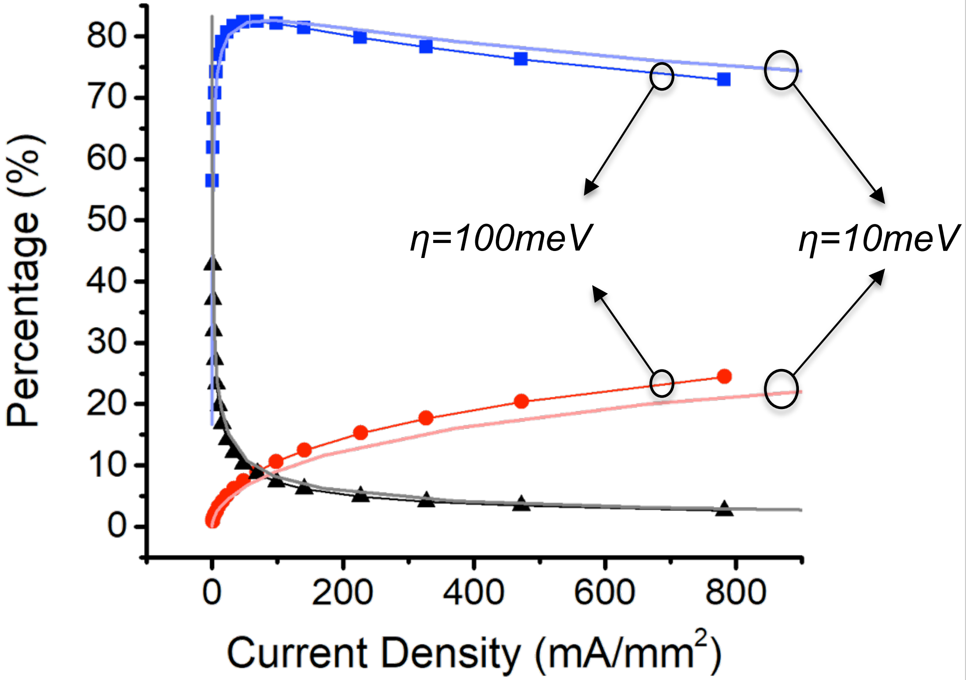
- Carrier pileup led to p-side emission, matching experimental observations [2]
- Also led to stronger Auger recombination at p-side, worsens droop

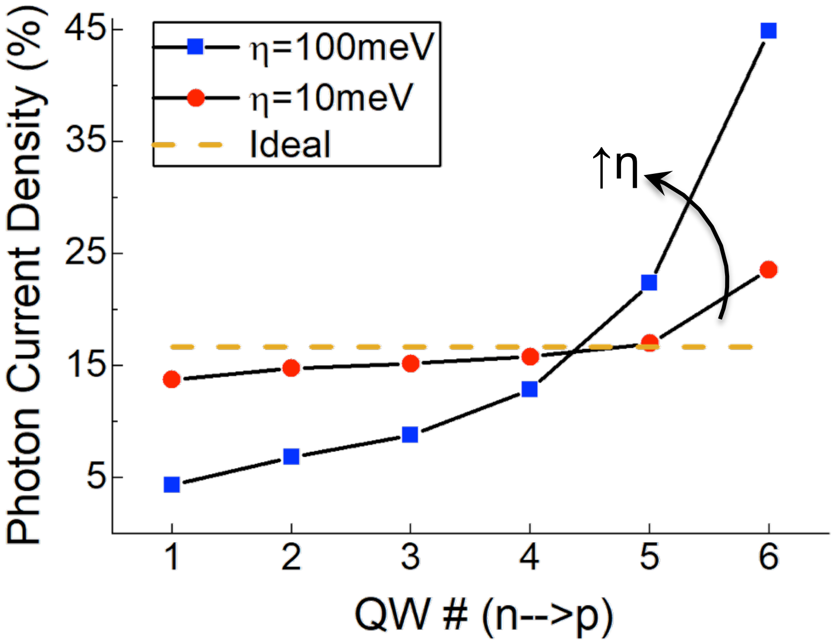
---

[1] J. Iveland, et al, Phys. Rev. Lett. 110, 177406 (2013) → Auger emission spectroscopy

[2] Aurélien David, et al, Appl. Phys. Lett. 92, 053502 (2008)

Results: Weak vs. Strong Scattering

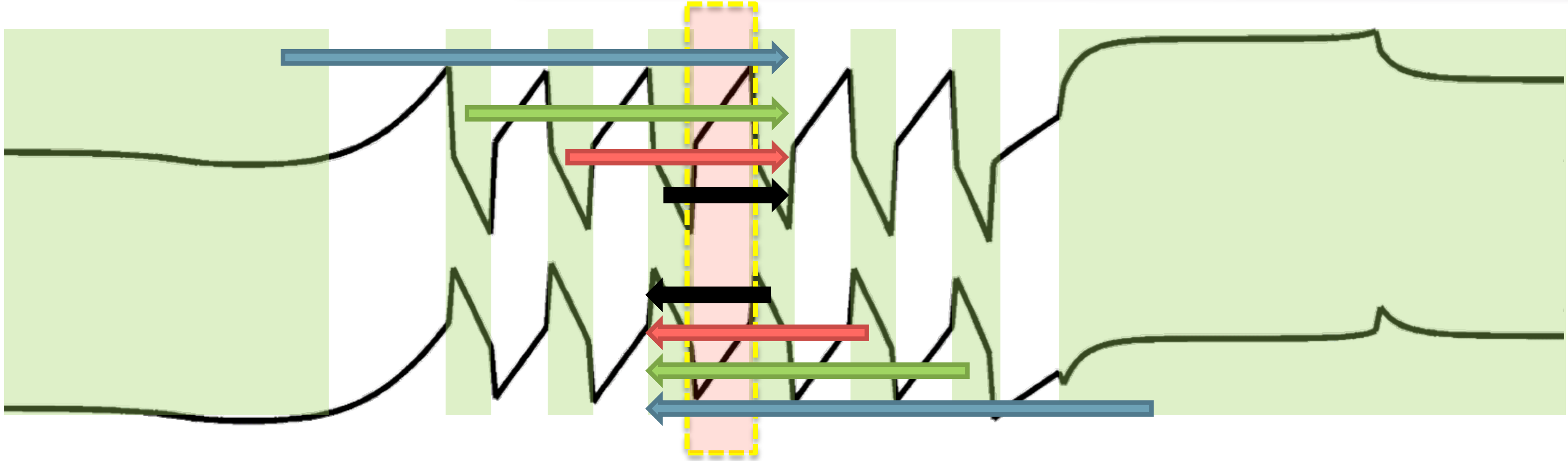




- Same device under less scattering (η=10meV) has better performance
- Weaker scattering in QW → better carrier spreading → better photon distribution
- Given non-uniform light emission is commonly observed in LED. We deduce the scattering in the QWs are strong (η closer to 100meV than 10meV)

Reducing scattering may lead to better light distribution and better device performance

Model Expansion—Long Range Tunneling

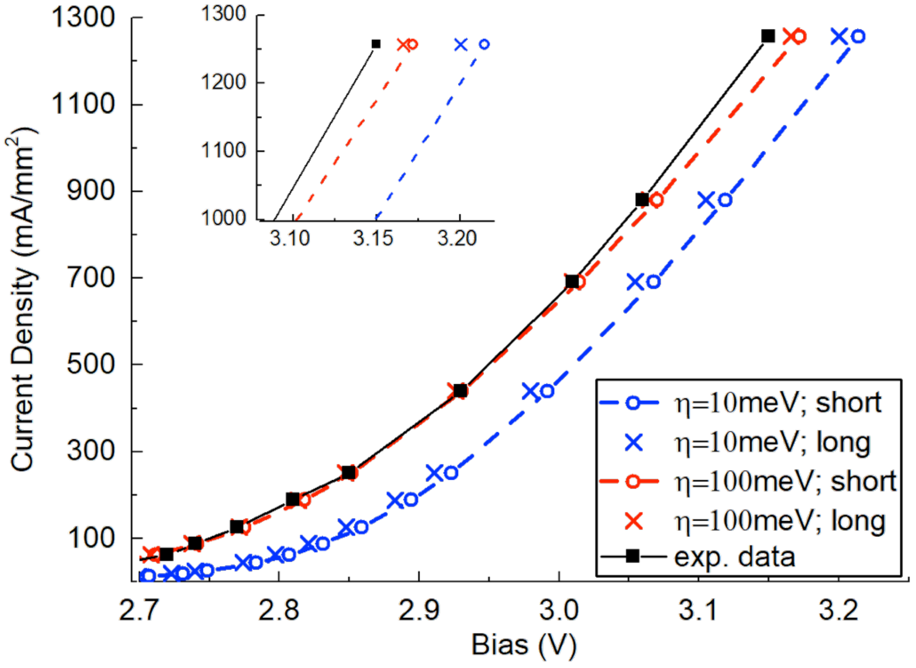


- In the equilibrium region (QWs + leads), we assume complete thermalization
- Only allow transport between nearest-neighbor QWs (➡ & ⬅)
- In reality some electrons may accumulate energy and “hop over” 2+ QWs (hot electrons)
- How important are these “**hot electrons**”?

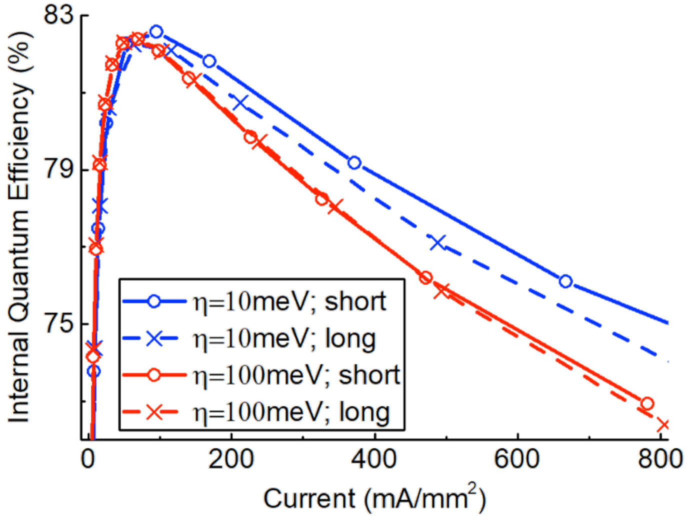
Model can be expanded to include long range components → Gives good estimation of the impact of hot electrons

Results:
Impact of long range coupling

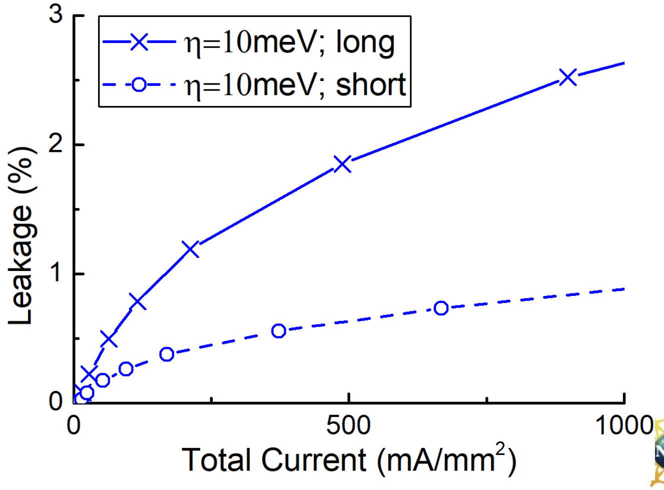
Stronger thermalization shifts IV to higher voltages



"Hot" carriers leads to slight IQE degradation



Worse case leakage current **< 3%**



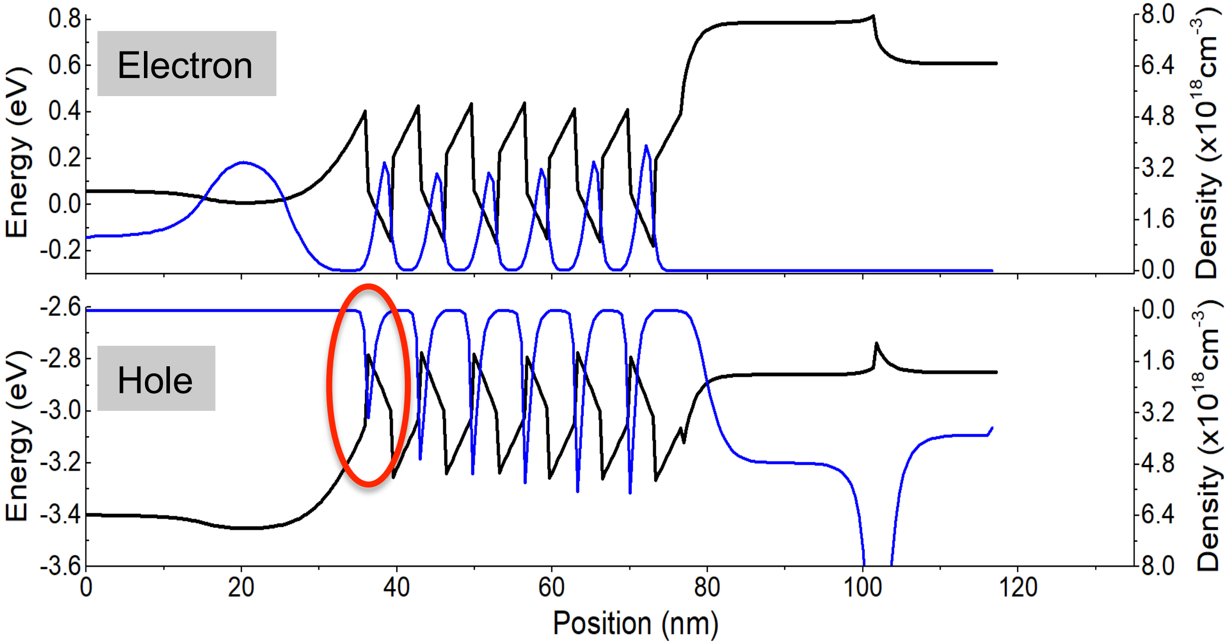
Long range tunneling relevant only for weak scattering

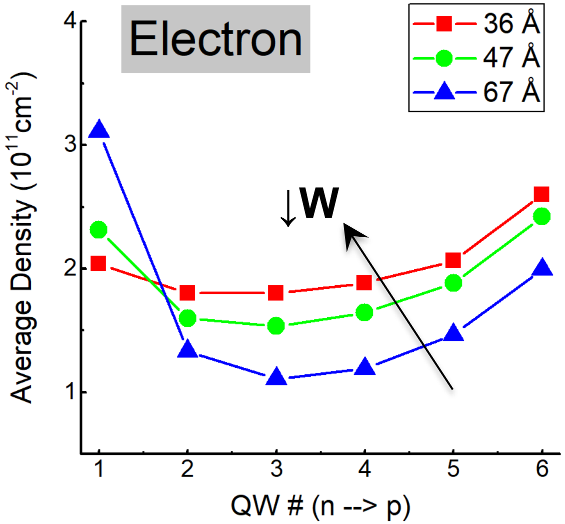
Hot electrons have small impact I-V and efficiency

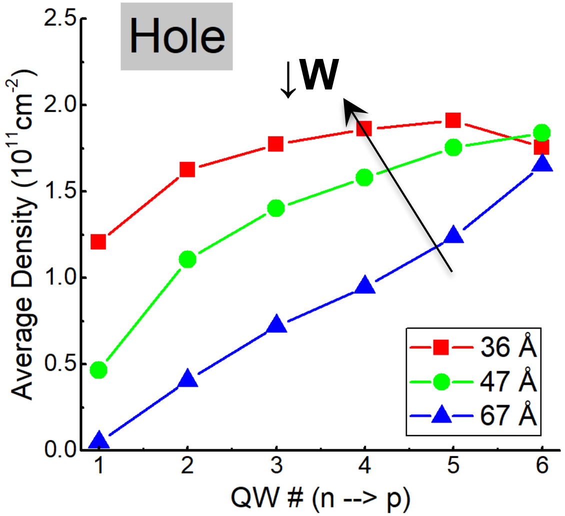
In this device, leakage plays very small role in droop

Exploring LED design trends

Reducing barr. thick.→ Improving hole transport





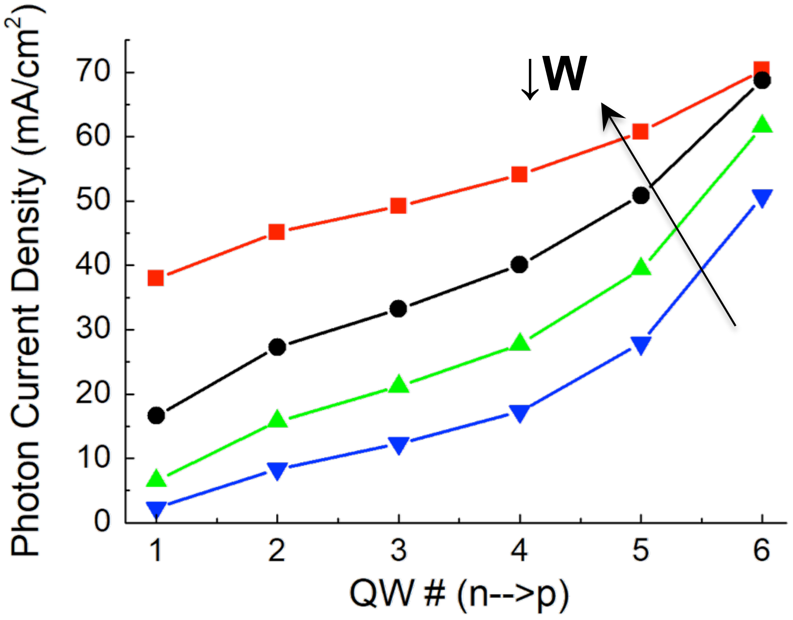


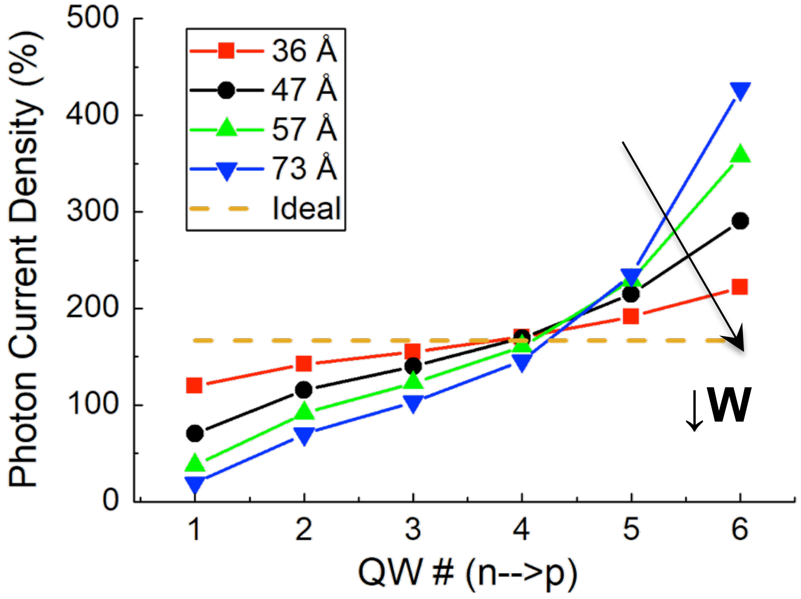
Reducing Barrier Thickness:

- Improves transport, especially for holes
- Carrier density distribution became more uniform
- Holes more effectively fill the left (n-side) QWs

Reducing barrier thickness can significantly improve **hole transport**

Thin barriers led to uniform emission

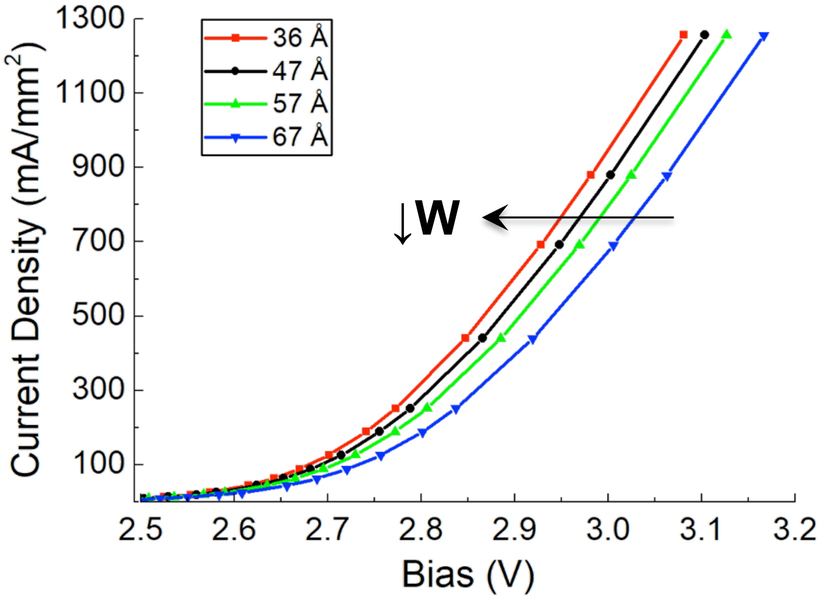


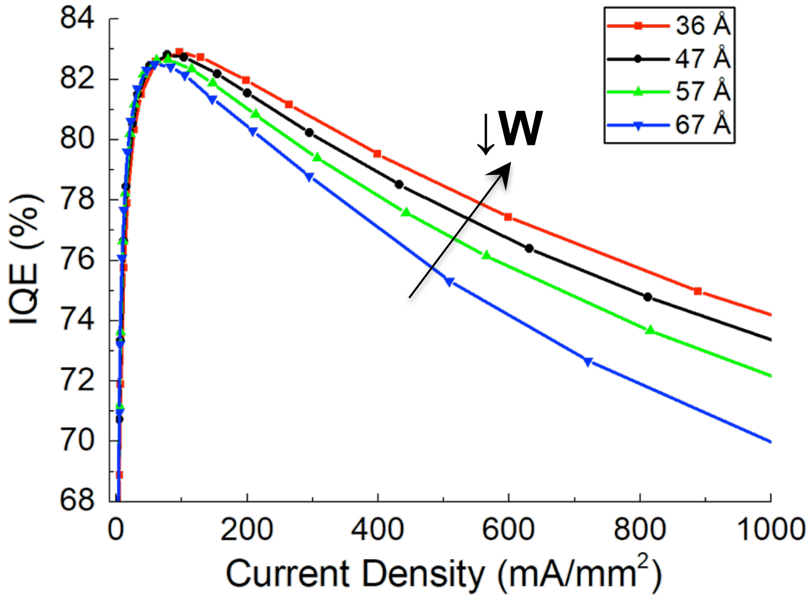


Reducing Barrier Thickness:

- Increases overall light emission
- Light emission distribution becomes more uniform

Barrier thickness affects I-V and IQE





Thinner barriers at given bias

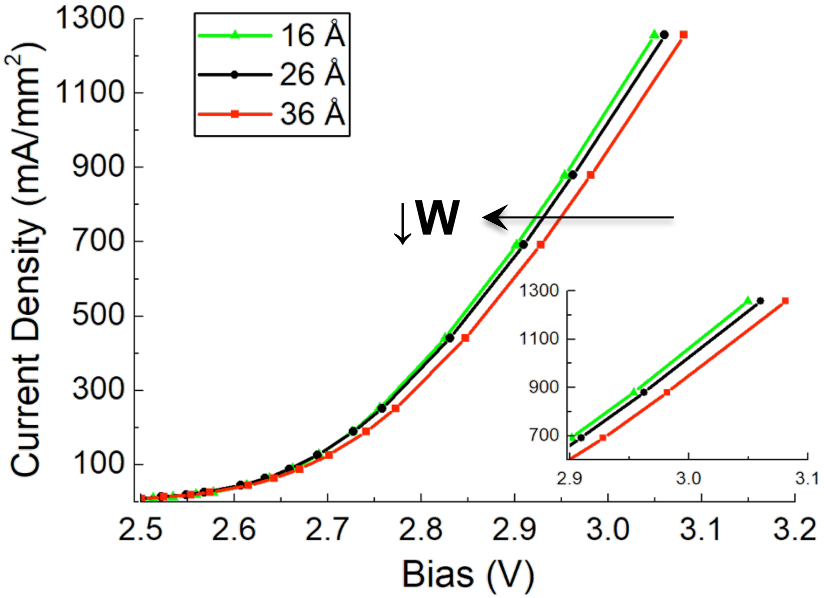
- Improves **hole** transport
- Increases carrier recombination
- Leads to more uniform emission

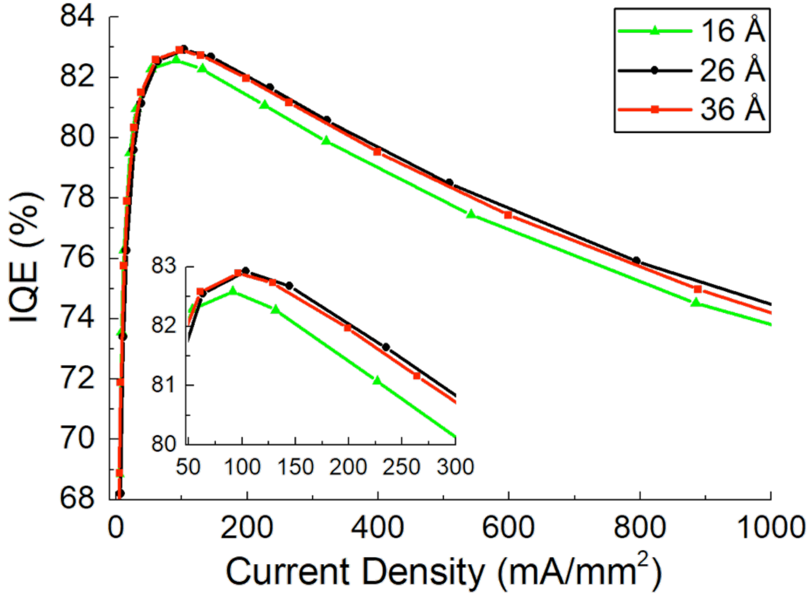
Overall trend

- I-V shifts towards lower bias (left)
- Improves IQE — Less droop

Reducing barrier thickness improves overall quantum efficiency.
Barrier thickness of 36Å is close to optimum

Optimal barrier thickness ≈ 36Å



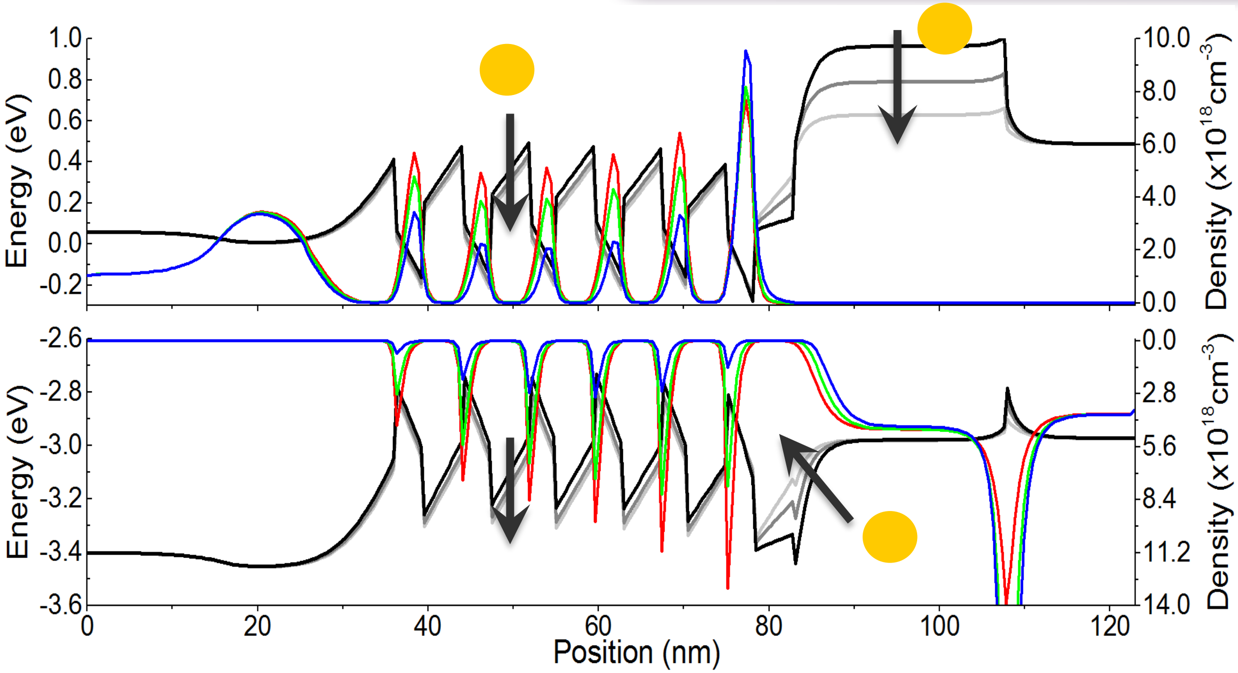


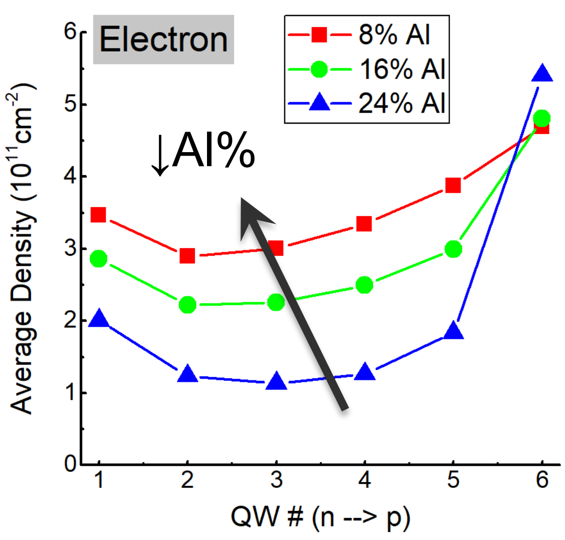
Further thinning barriers below 36Å continues the I-V trend. However, IQE can improve no further.

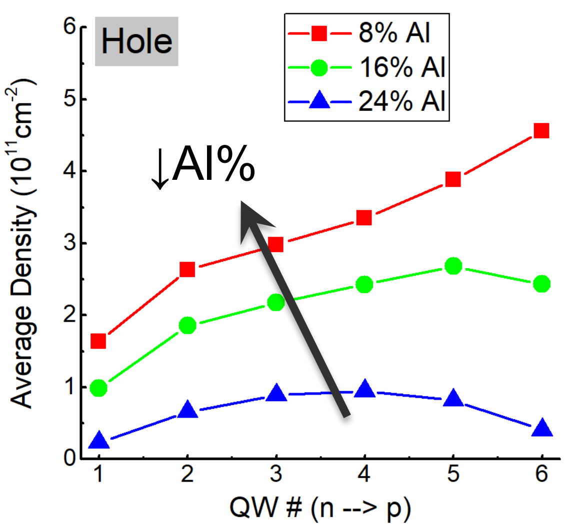
Based on simulation results, the optimal barrier thickness is around 36Å

Exploring LED Design Trends

Reducing Al% → Improving hole injection





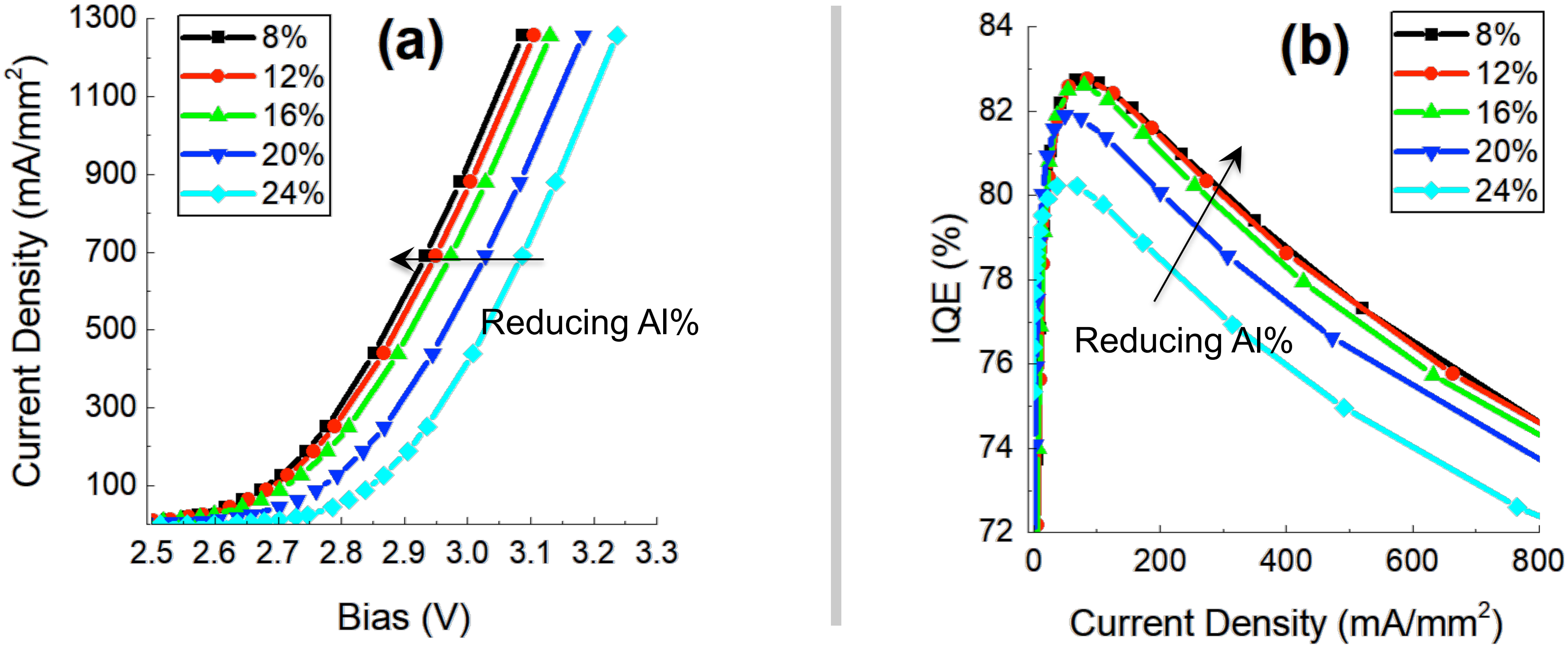


Reducing Al%

- Reduces p-side barrier for holes → improve **hole injection** → increase hole density
- Hole 'replenishing' → pushes entire band profile downwards → increases electron density

Reducing Al% improves hole injection; increases hole and electron density

Al% affects I-V and IQE



Lowering Al% at given bias

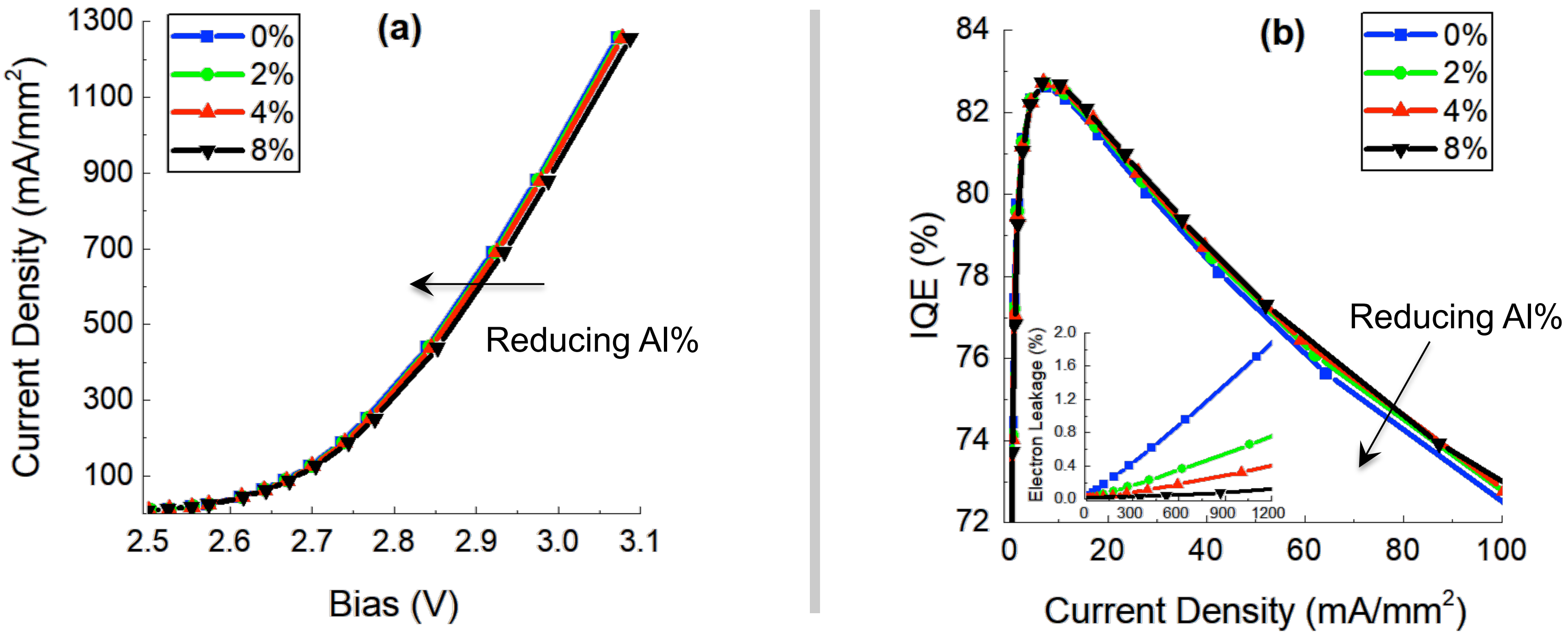
- Increases charge density
- Increases recombination current

Overall trend

- I-V shifts towards lower bias (left)
- Overall efficiency improves

Reducing Al% in EBL improves quantum efficiency
Simulation results indicate EBL with 8% Al is optimum

Al% affects I-V and IQE

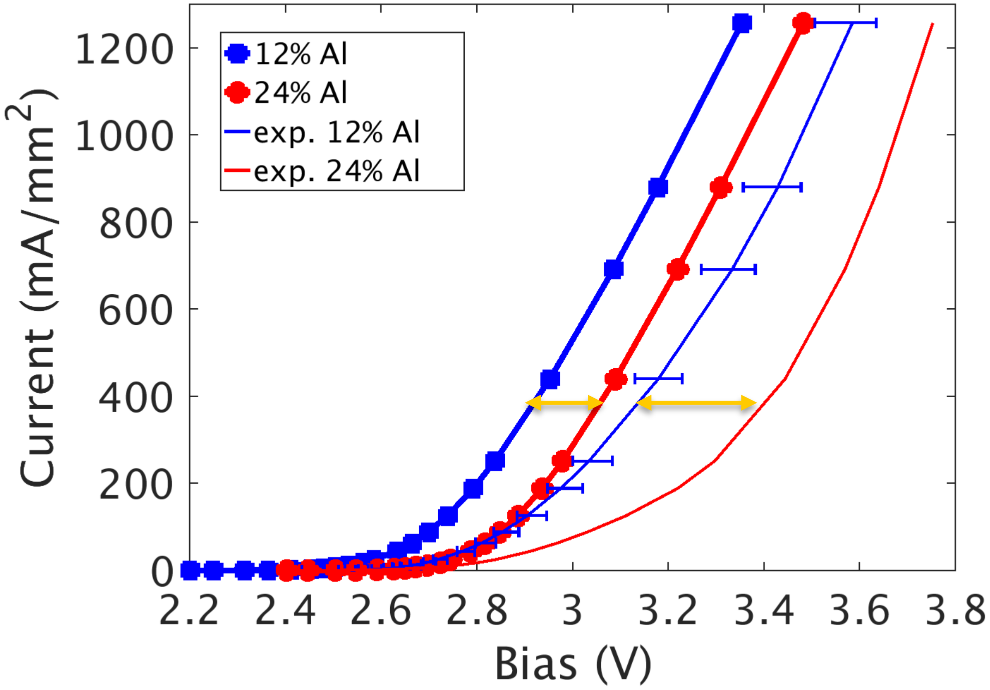


Further reducing Al% below 8% continues the I-V trend. However, IQE can improve no further, due to increased leakage.

Since our model does not account for hot carrier generation due to Auger, leakage (and extent of IQE degradation) might be underestimated.

Based on simulation results, the optimal Al% is around 8%

Simulation matches experimental trend



- The experimental result is on a similar device with different (proprietary) design parameters
- The I-V shift trend is reproduced by simulation: @ I_F = 350mA: 0.14V (sim.) vs. 0.26±0.05V (exp.)

Model successfully reproduces experimental trend

Key Challenges in LED Development

Multi-Scale Quantum Transport Model

[Conclusion] Modeling Results and Insights into LED Physics

- I-V matches quantitatively with experiment
- Hole transport is a critical bottleneck
- Leakage plays very little role in droop
- Hot carriers only relevant under weak scattering, not in real devices
- Device engineering tips: reduce scattering, keep barriers thin, keep EBL’s Al% low

New Radiative Recombination Model

Outline

Key Challenges in LED Development

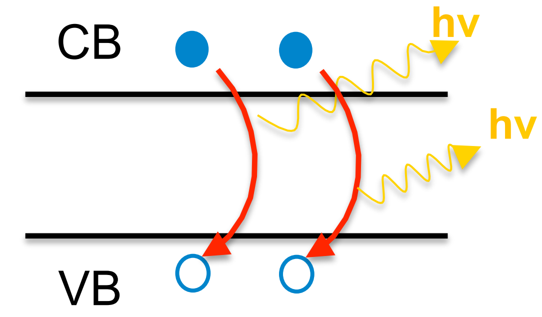
Multi-Scale Quantum Transport Model

Modeling Results and Insights into LED Physics

New Radiative Recombination Model

- Why we need a better model than ‘ABC’?
- Comparison of existing models
- Introduce new model
- Compare results with previous simulation

Why We Need A Better Recombination Model?



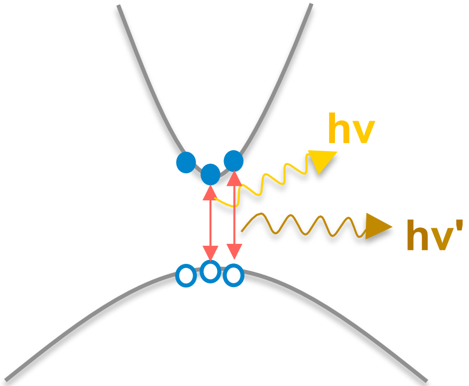
$R{\downarrow}rad = B \cdot n \cdot p$

The "ABC" Model

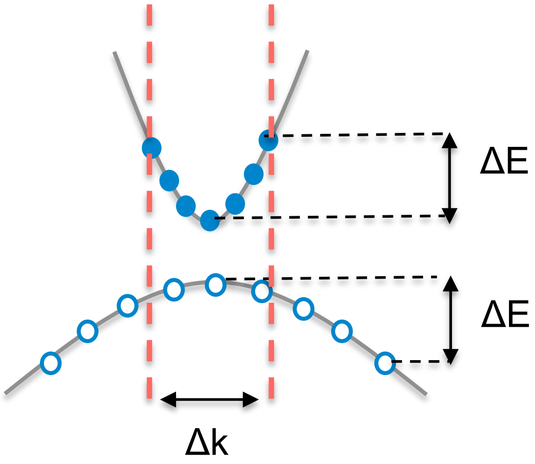
- Based on simple heuristics
- Works reasonably well at producing trends (e.g. I-V, IQE) efficiently

Missing several key physics

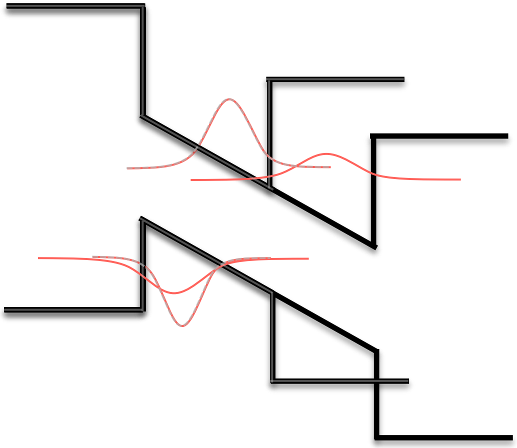
● Photon Frequency



● Momentum Selection



● Spatial Distribution

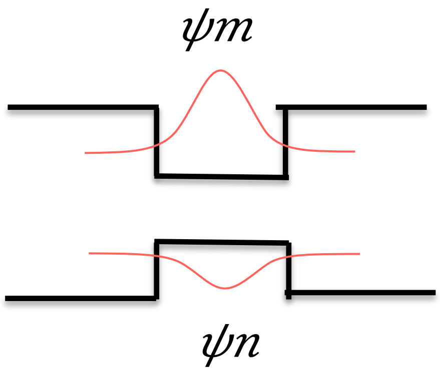


Status Quo Approaches

1 Fermi's Golden Rule

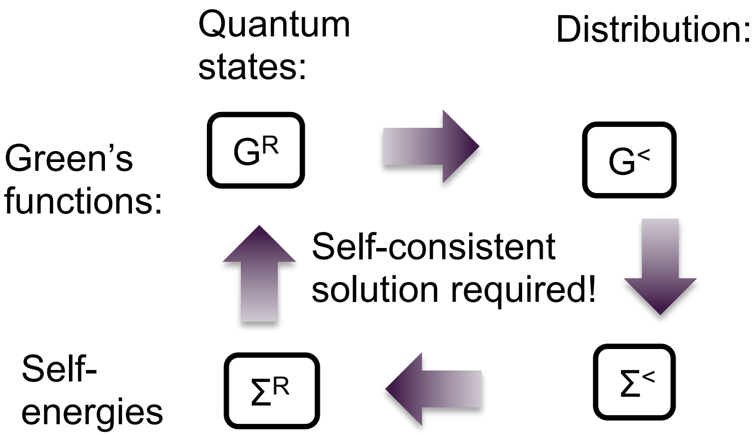
$$R_{rad} \sim \sum_{m,n} \sum_{K} |\langle \psi_m | r | \psi_n \rangle|^2 \delta(E_{m,\mathbf{k}} - E_{n,\mathbf{k}} - \hbar\omega)(f_V - f_C)$$

- Linear response: transitions don't affect states' occupancy
- Only apply to closed system where ψ, ψ* can be determined.



2 NEGF

- Photon emission treated as a scattering process
- Non-local
- Self-consistent solution required



Quantum states:

Distribution:

Green's functions:

G^R

$G^<$

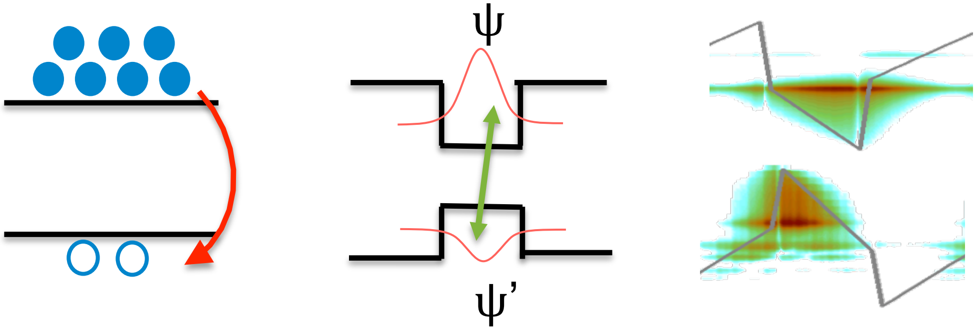
Self-consistent solution required!

Self-energies

Σ^R

$\Sigma^<$

Summary of Various Approaches



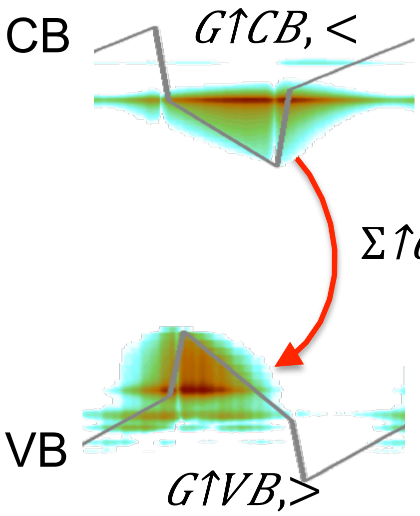
Status-Quo		ABC Model	Fermi's Golden Rule	NEGF
	Computation	Very light ✓	Medium ✗	Very high ✗
	Physics	Lacking ✗	Good ✓	Best ✓
	Open System?		No ✗	Yes ✓
	Compatibility	Yes ✓	No ✗	No ✗

Can we bridge the gap?

Ideal

- Include essential physics
- Computationally light
- Fit into quantum transport
- Compatible with Multi-Eq-Neq

New Approach:
Deriving the B-coefficient



Start with NEGF, derive the radiative recombination rate assuming linear response*

Photon Self-Energy

$$\Sigma^{CB,>}(k,E)|_{\hbar\omega} \sim M(k)\cdot G^{VB,>}(k,E-\hbar\omega)\cdot M(k)$$

Transition Rate

$$R(\hbar\omega) \sim \int dk \int dE\, G^{CB,<}(k,E)\cdot\Sigma^{CB,>}(k,E-\hbar\omega)$$

Model Assumptions:
Wide Eg → inter-band only
No absorption → emission only

$$R(\hbar\omega) \approx 1/\omega \int dk\, M'(k)^2 \int dE\, G^{VB,>}(k,E-\hbar\omega)\cdot G^{CB,<}(k,E)$$

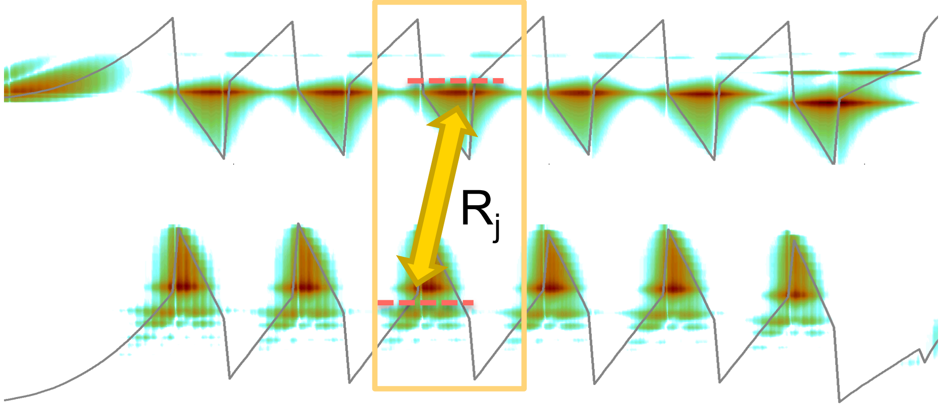
'β' — no charge dependence

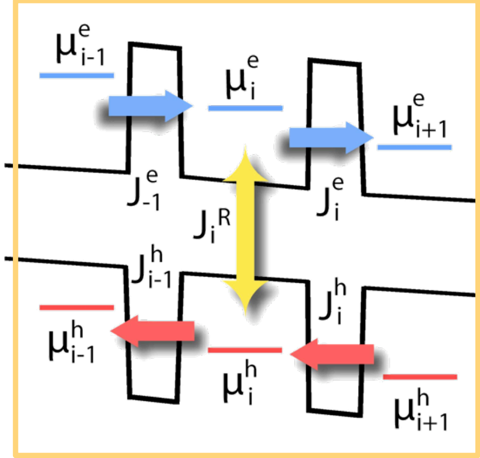
Charge dependent term ~ 'p·n'

The new rate equation resembles the old 'B·n·p' model
But now it is non-heuristic, physics-based

*Derivation see backup slide

New Approach: Procedure Summary





Step 1*: Evaluate the integral K for individual QW

$$R_{j} = \sum_{\omega} R_{j}(\hbar\omega) = \underbrace{\beta_{j} \cdot \sum_{\omega} 1/\omega \int kdk \int dE\, G^{CB,<}(k,E) \cdot G^{VB,>}(k,E-}_{K}$$

Step 2: Calibrate the β_j

$$\beta_{j} = \boxed{B \cdot n_{j} \cdot} p_{j} / K$$

This is just “ABC” model

Covers material, structural dependence. Once calibrated, doesn’t change from iter.-to-iter.

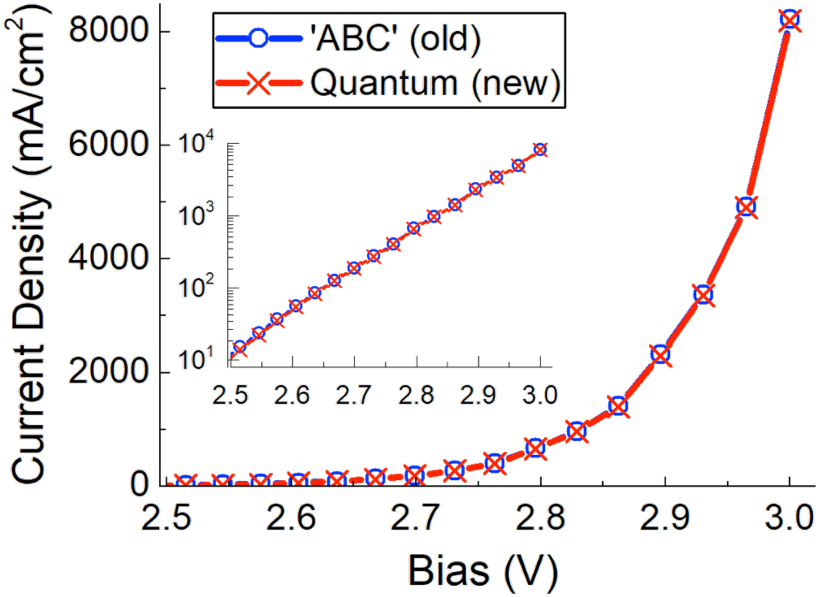
Step 3: Feed β_j back to step 1

Fix β_j for all successive calculations. Update Fermi levels

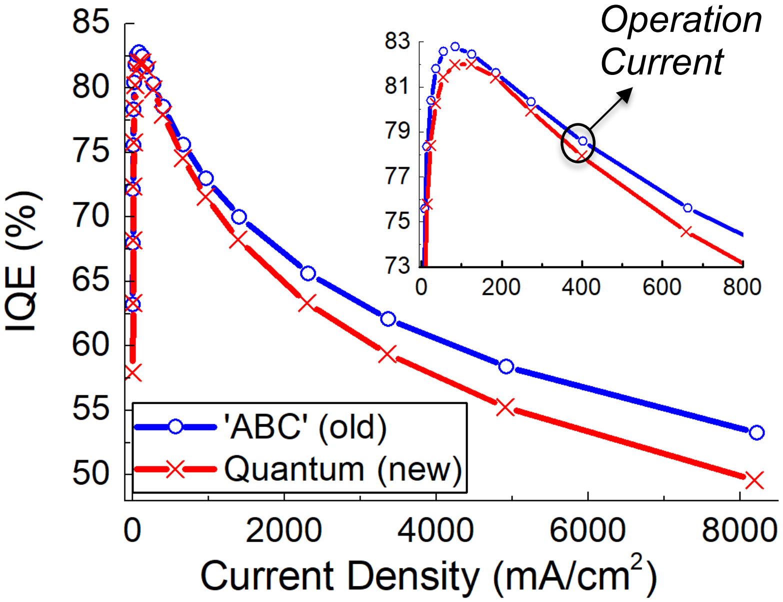
Repeat until current conserved

*Derivation see backup slide

Results:
I-V, IQE comparison with old model



- I-V identical between old and new recombination model
- Validates previous results and choice of ABC model



- Efficiency differ at high current density
- The old model slightly underestimates droop (~5%), since it assumes 'complete' recombination

The new model corrects the overestimation of radiative emission.
Only affecting regions of very high density.

Summary

	ABC Model	Fermi's Golden Rule	NEGF	New
Computation	Very light ✓	Medium ✗	Very high ✗	Light ✓
Physics	Lacking ✗	Good ✓	Best ✓	Good ✓
Open System?		No ✗	Yes ✓	Yes ✓
Compatibility	Yes ✓	No ✗	No ✗	Yes ✓

[Summary] New Radiative Recombination Model

- **New radiative recombination model developed and validated**
- **β coefficient covers material and geometry dependent properties**
- **Energy, momentum, spatial dependence covered**

Overall Summary

Developed an efficient quantitative model for LED

- NEGF-based — includes coherent quantum effects and relaxation
- Multi-scale — numerically efficient, solves transport in critical regions only
- Efficient inclusion of recombination, both in heuristic and QM (radiative only) form
- Capable of handling real-scale LED devices with realistic bandstructure effect

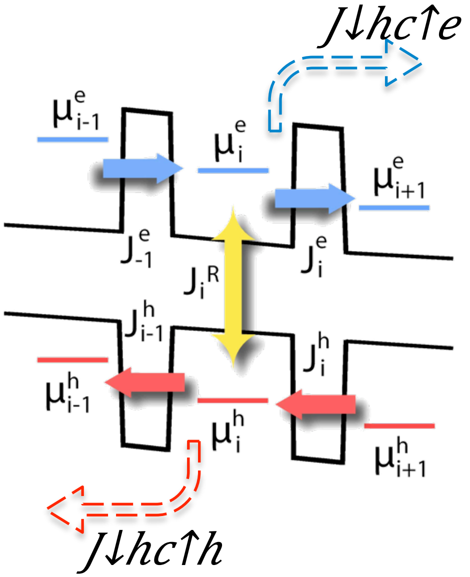
Successfully simulated an commercial LED device

- Quantitatively matched I-V with experiment
- Deduced carrier temperature from simulation; reproduced p-sided emission pattern; validated Auger as the dominant contributor to droop
- Advised engineering for better hole transport, suggested optimal choices of barrier thickness and EBL Al%

Future Work #1

Include hot carrier contribution due to Auger

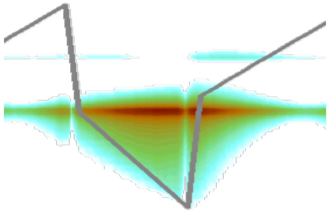
- Auger recombination generates excess carriers with high energy, these “hot carriers” lead to increased leakage current
- Our simulation result suggesting EBL not needed (leakage is too low) is indication that we are underestimating the leakage current
- A simple way to include it is to add hot carrier current terms $J{\downarrow}hc{\uparrow}h$ and $J{\downarrow}hc{\uparrow}e$ in the current balance equation (see right figure)
- Build physical connection between J_{hc} and the Auger current



Future Work #2

Improve the "η" model

- Our current Ση is constant value defined by the band edges, which are parameterized for bulk materials
- This leads to DOS in the equilibrium region following the bulk band edges, rather than the shape of quantum states
- Also, our Ση is pure imaginary, in reality it has real-part too, which causes the resonance states to shift in energy
- The alternative approach is use Ση that is function of G^R



Density should not follow the band edge, but rather the shape of quantum states

Future Work #3

Improved QW distribution

- Fermi distribution is currently assumed in each QW
- In reality, the carrier distribution could be skewed towards higher energy, due to hot electrons
- A proposed solution is to perform a full NEGF simulation on a single QW, including all relevant scattering mechanisms (POP, impurity, e-e, etc.), extract the 'real' carrier distribution under real conditions, and use them in our model (eq regions)

Future Work #4

Scattering in the barriers

- Only coherent transport is currently allowed in the non-eq. regions
- Scattering could have impact on tunneling current (e.g. via traps) and thermionic emission
- The non-eq. regions could be expanded to solve incoherent transport with the self-consistent Born, with neighboring eq. regions as boundary conditions
- Additional simulation flow need to be added, namely iterating SC-born with multi-eq-neq. Significant increase in computational load expected. See backup slides for details.

Future Work #5

Improve the Auger model

- Auger recombination is still calculated with the ‘ABC’ approach in the current model
- Similar enhancement on the radiative recombination could be applied to Auger
- However, the Auger mechanism is much more involved compared to radiative recombination. Instead of interaction between an e-h pair, it involves two more elements: another electron (or hole), an empty electronic (hole) states in higher (lower) energy. This significantly complicates the matter.
- Two types of Auger processes: e-e-h and h-h-e needs to be considered.
- Direct Auger recombination could be much less important compared to phonon-assisted Auger recombination[1]

[1] Kioupakis E, Rinke P, Delaney K and Van de Walle C, Applied Physics Letters 98, 161107 2011

Acknowledgement

This research was supported in part by Lumileds.

nanoHUB.org computational resources have been used.

Purdue research computing (RCAC), Blue Waters (part of National Science Foundation ACI 1238993) computational resources have been used.

The model, along with all related algorithms have been implemented in NEMO5[1] (available academic open source).

---

[1] Jim Fonseca, et al., "Efficient and realistic device modeling from atomic detail to the nanoscale," Journal of Computational Electronics December 2013, Vol. 12, Issue 4, pp 592-600.

SUMMARY: Quantum Simulation & Design Optimization of THz-QCL

I PROBLEM

- Tera-Hertz gap: no high power and reliable THz-source at room temperature
- Quantum cascade laser (QCL), a promising candidate, suffers reliability issues such as NDR (negative differential resistance)

II APPROACH

- Full-scale NEGF simulation, include impurity, acoustic, optical, e-e scattering and optical absorption in III-V QCL
- Utilize in-direct (phonon-assisted) pumping scheme
- Structure, doping design, fine-tuning quantum confined states alignment

III IMPACT

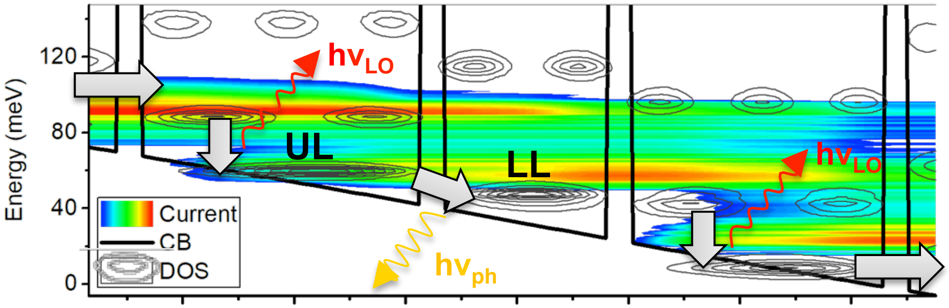
- Improved QCL design with higher output power and 52% Reduction in NDR

Improved Device Structure:

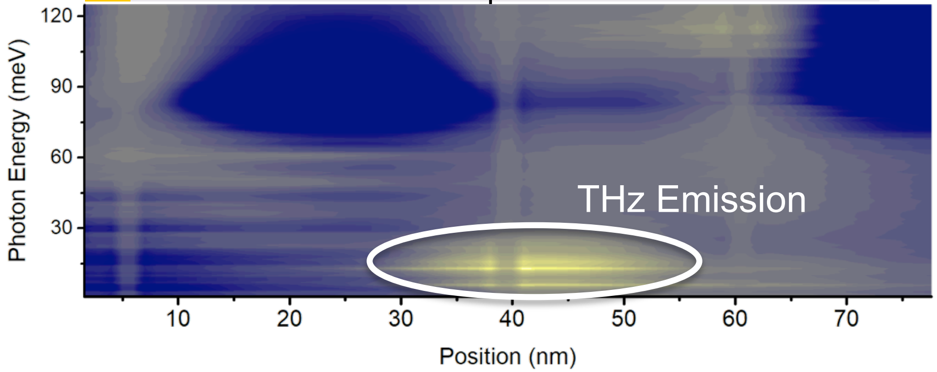
Barrier: $Al_{0.48}In_{0.52}As$; QW: $Ga_{0.47}In_{0.53}As$

Dimension **B**/W (Å): **8**/264/**8**/160/**8**/240

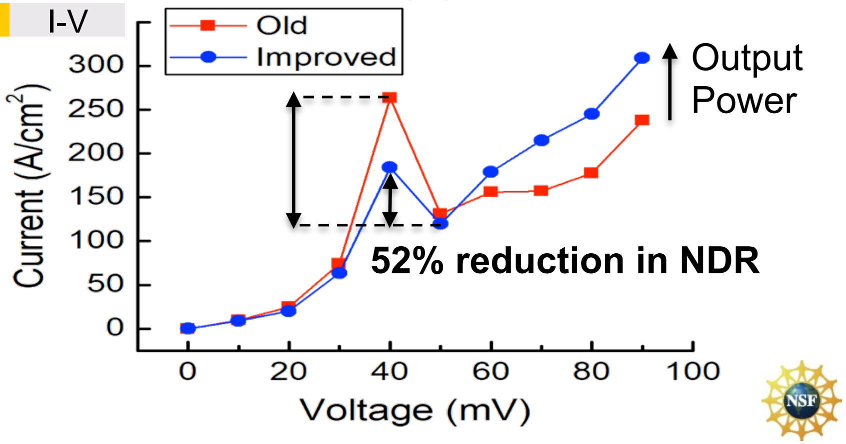
1 Conduction Band, DOS, Energy-Resolved Current



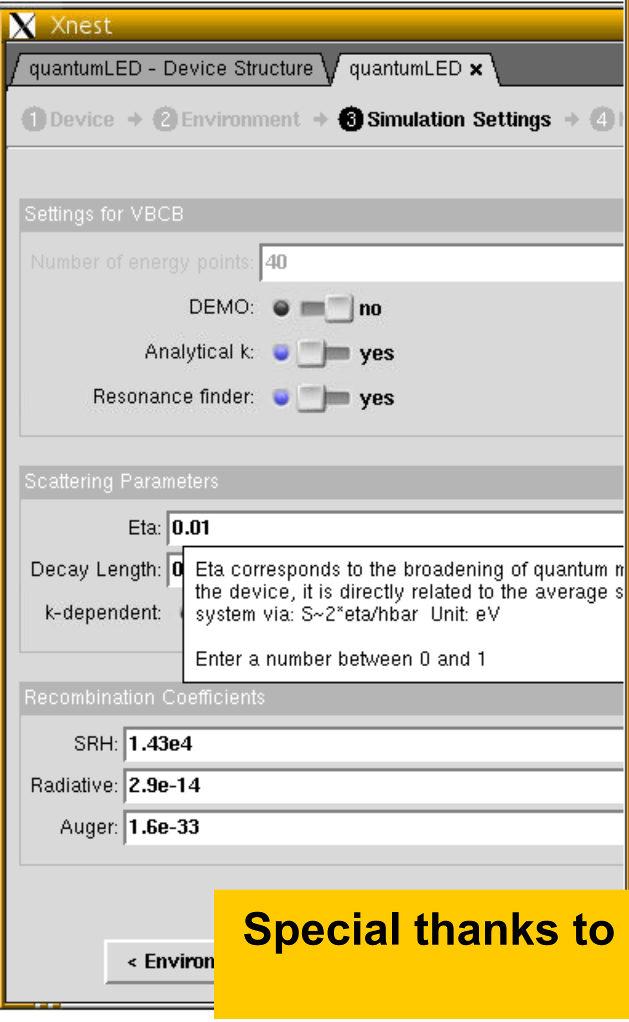
2 Photon Absorption Coefficient



3 I-V



LEDs on nanoHUB.org



Settings for VBCB

Number of energy points: 40

DEMO: no

Analytical k: yes

Resonance finder: yes

Scattering Parameters

Eta: 0.01

Decay Length: 0

k-dependent:

Eta corresponds to the broadening of quantum m
the device, it is directly related to the average s
system via: S~2*eta/hbar Unit: eV

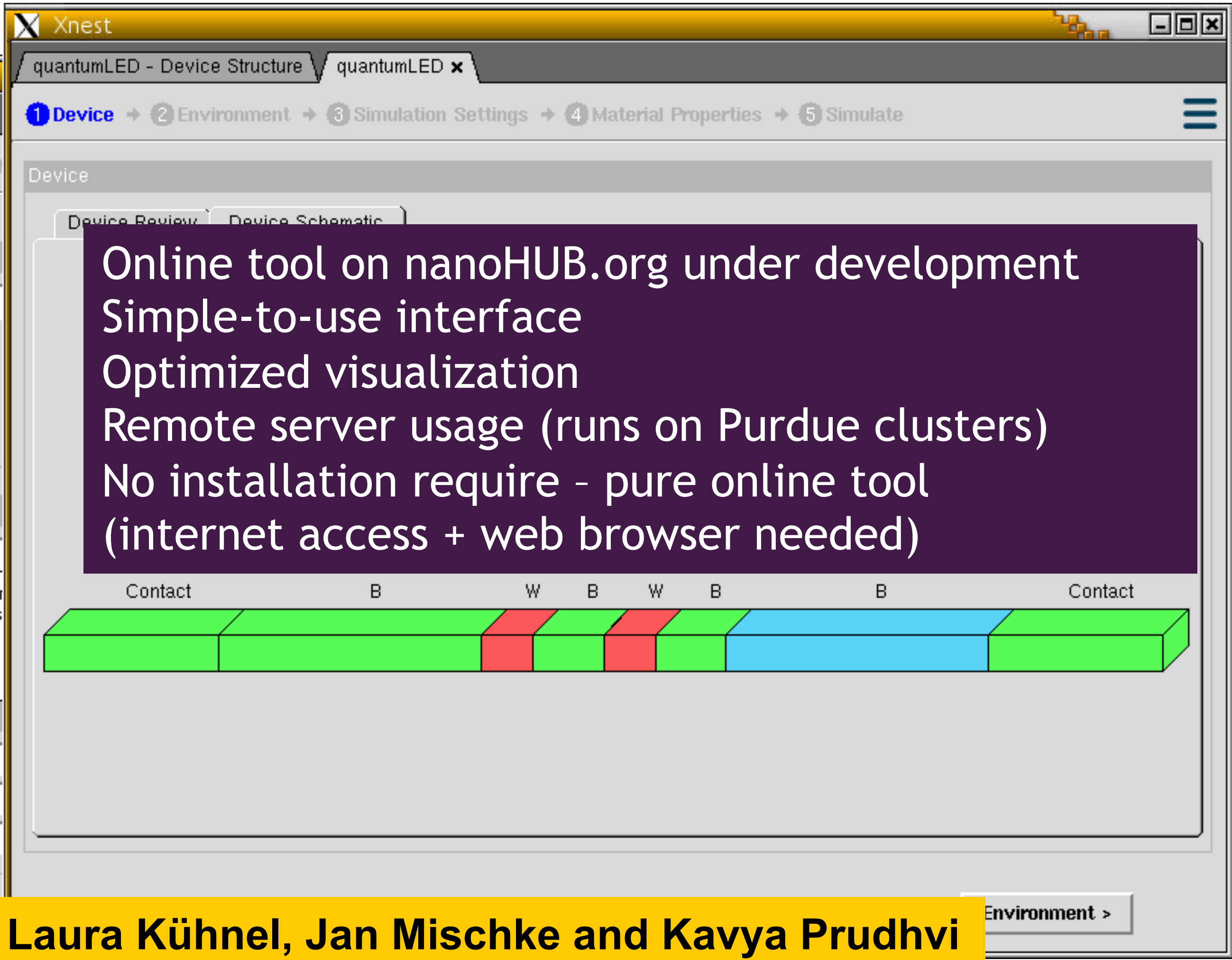
Enter a number between 0 and 1

Recombination Coefficients

SRH: 1.43e4

Radiative: 2.9e-14

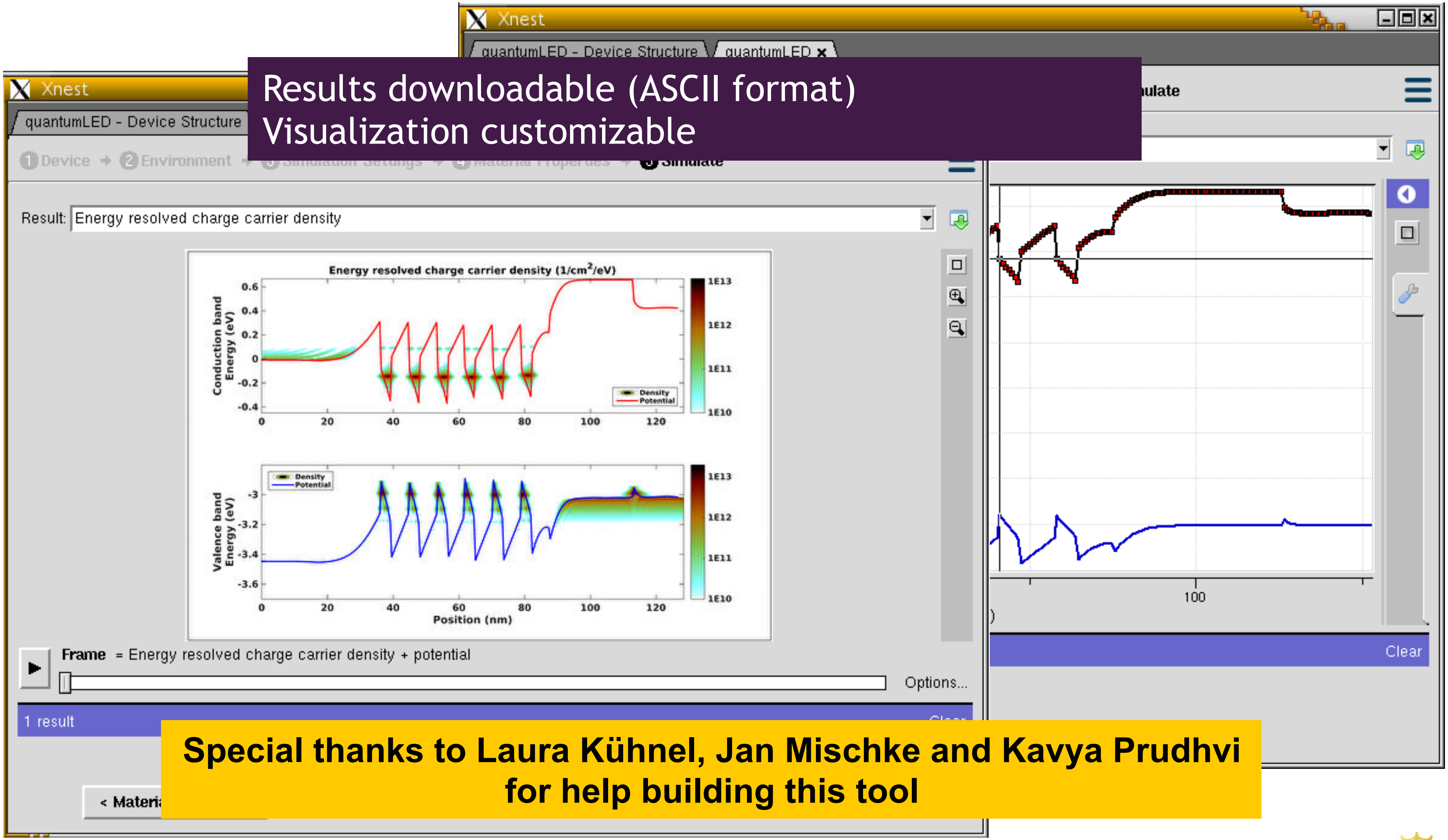
Auger: 1.6e-33



Online tool on nanoHUB.org under development
Simple-to-use interface
Optimized visualization
Remote server usage (runs on Purdue clusters)
No installation require – pure online tool
(internet access + web browser needed)

Special thanks to Laura Kühnel, Jan Mischke and Kavya Prudhvi for help building this tool

LEDs on nanoHUB.org



Result: Energy resolved charge carrier density

Frame = Energy resolved charge carrier density + potential

1 result

Results downloadable (ASCII format)
Visualization customizable

Special thanks to Laura Kühnel, Jan Mischke and Kavya Prudhvi for help building this tool

Acknowledgements

Major Professors


Gerhard Klimeck


Tillmann Kubis

Committee Members


Oana Malis


Michael Manfra


Erik Nelson

NCN Stuff

Vicki Johnson, Ashley Byrne, Leslie Schumacher, Lynn Zentner, Cheryl Haines, Amanda Buckles

Lumileds

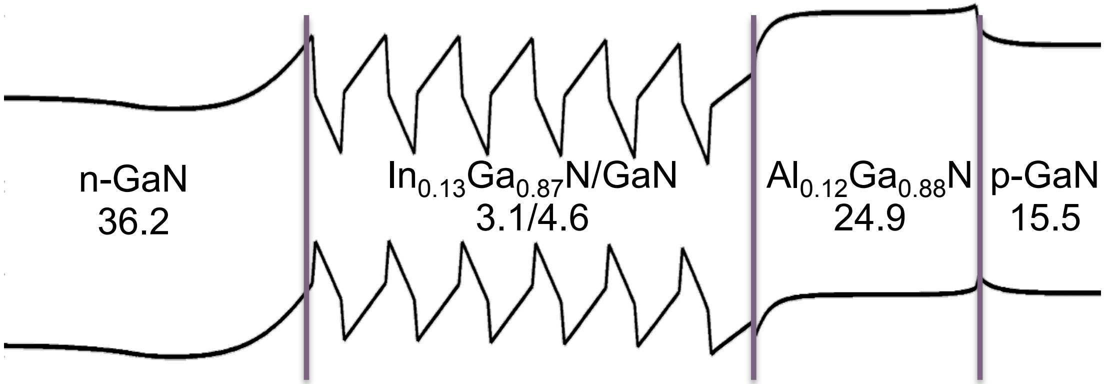
Carl Wordelman, Ben Browne, Rob Armitage, Isaac Wildeson, Parijat Deb

Thank you!

- LED Computation Requirements

Simulation Load: Single I-V

Typical Device Structure (Units in nm)



Simulation load:

- Simulation domain size: 123 nm (952 atoms)
- Using $sp^3d^5s^*$ with SO, G^R matrix size: $\sim 19000^2$
- K-mesh and energy mesh both adaptive; energy mesh is adaptive to each k point; meshing is independent for electron and holes
- No. K at final iteration: 12 for electrons, 24 for holes
- Total no. (E,k): ~36000 (8000 for electrons, 28000 for holes)

Computation details:

- Each I-V, take 10 bias points
- Each bias point uses 3200 cpu cores in Bluewater (100 nodes with 32 cores/node)
- On average takes ~0.5 hr
- Total simulation time for single I-V (10 points): 16000 cpu·hour

Simulation Load: A,B,C fitting

Two-Step Approach:

Step 1: Fix one parameter (A), vary the other two (B, C) by ± 1 order of magnitude, 10 points each, get the general trend, decide which directions to move

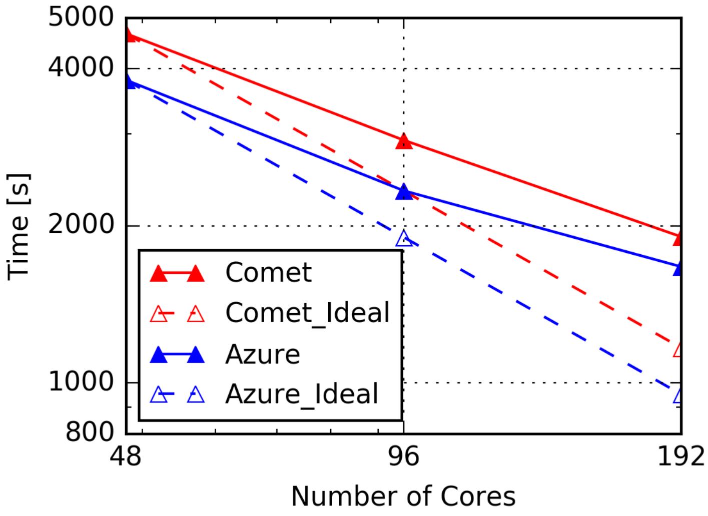
Step 2: Vary A,B,C all at the same time by 1 order of magnitude in one direction (determined in step 1), 6 points each.

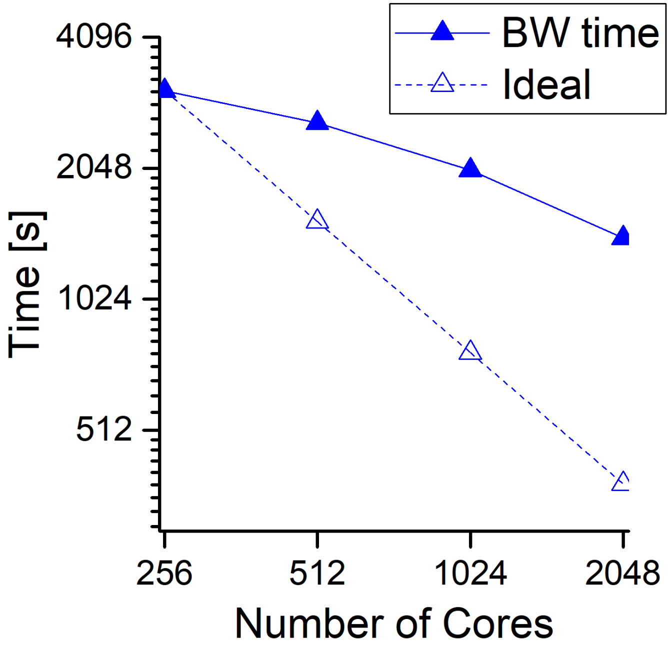
Simulation Summary:

- Total no. I-V runs: 316
- Total no. simulations: 3160 (10 bias each)
- <u>Total cpu hours: ~5,000,000</u>

- LED Simulation Scaling results

Scaling Chart





The parallel efficiency is 61% on Comet and 57% on Azure.

The parallel efficiency is 27%. On Bluewaters with 2048 cores

Scaling Data

Azure		
cores	time [s]	parallel efficiency
24	6965.96	1
48	3953.58	0.8809686411
96	2789.22	0.6243645177
192	2212.95	0.3934770329

Azure	12 nodes NUM_THREADS=1	
cores	time [s]	parallel efficiency
24		
48	3804.32	1
96	2335.63	0.8144098166
192	1669.81	0.5695737838

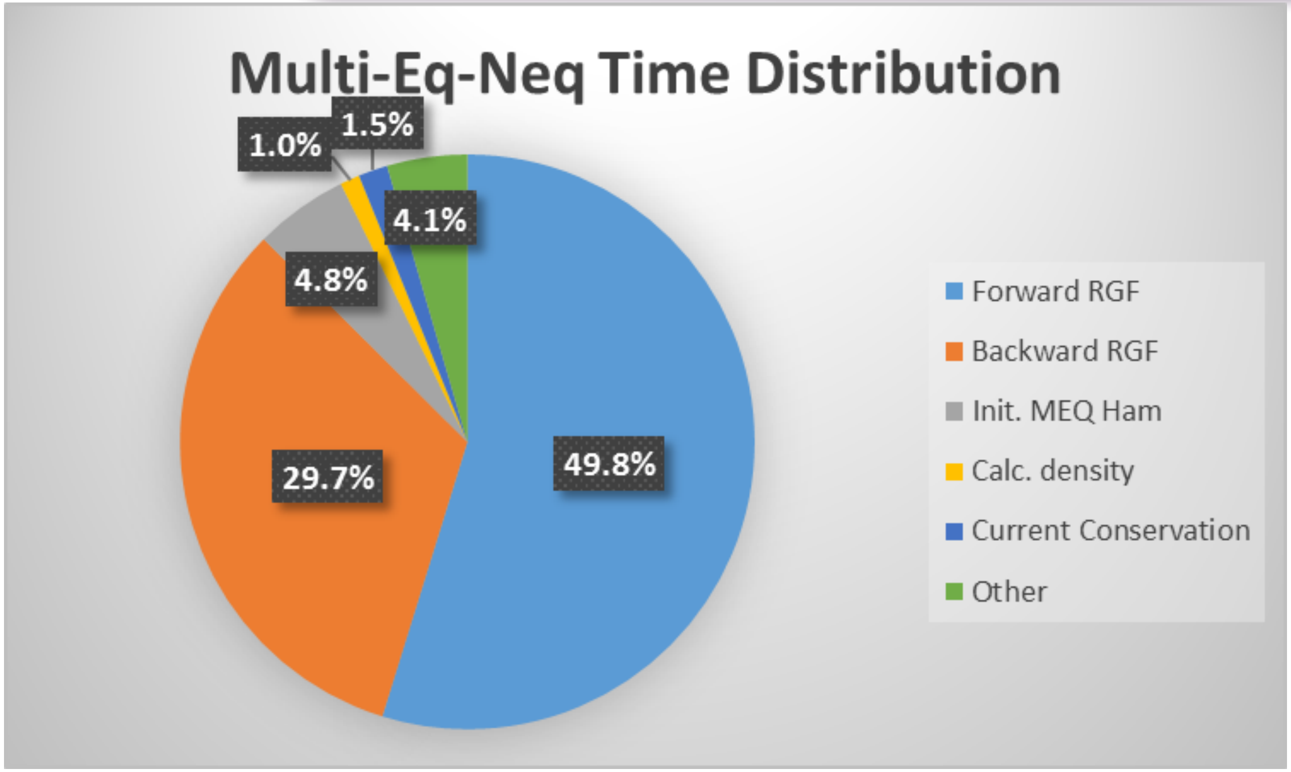
Comet		
cores	time [s]	parallel efficiency
192	1907.62	1
384	1429.94	0.6670279872
768	1176.5	0.405359116
1536	674.477	0.3535368886

Comet	keep 8 nodes all time	
cores	time [s]	parallel efficiency
24	11873.8	
48	4669.07	1
96	2918.44	0.7999256452
192	1905.4	0.6126102131

Bluewaters	1 int core per float core	
cores	time [s]	parallel efficiency
256	3087.03	1
512	2605.73	0.592354158
1024	2029.2	0.3803259905
2048	1417.16	0.2722901789

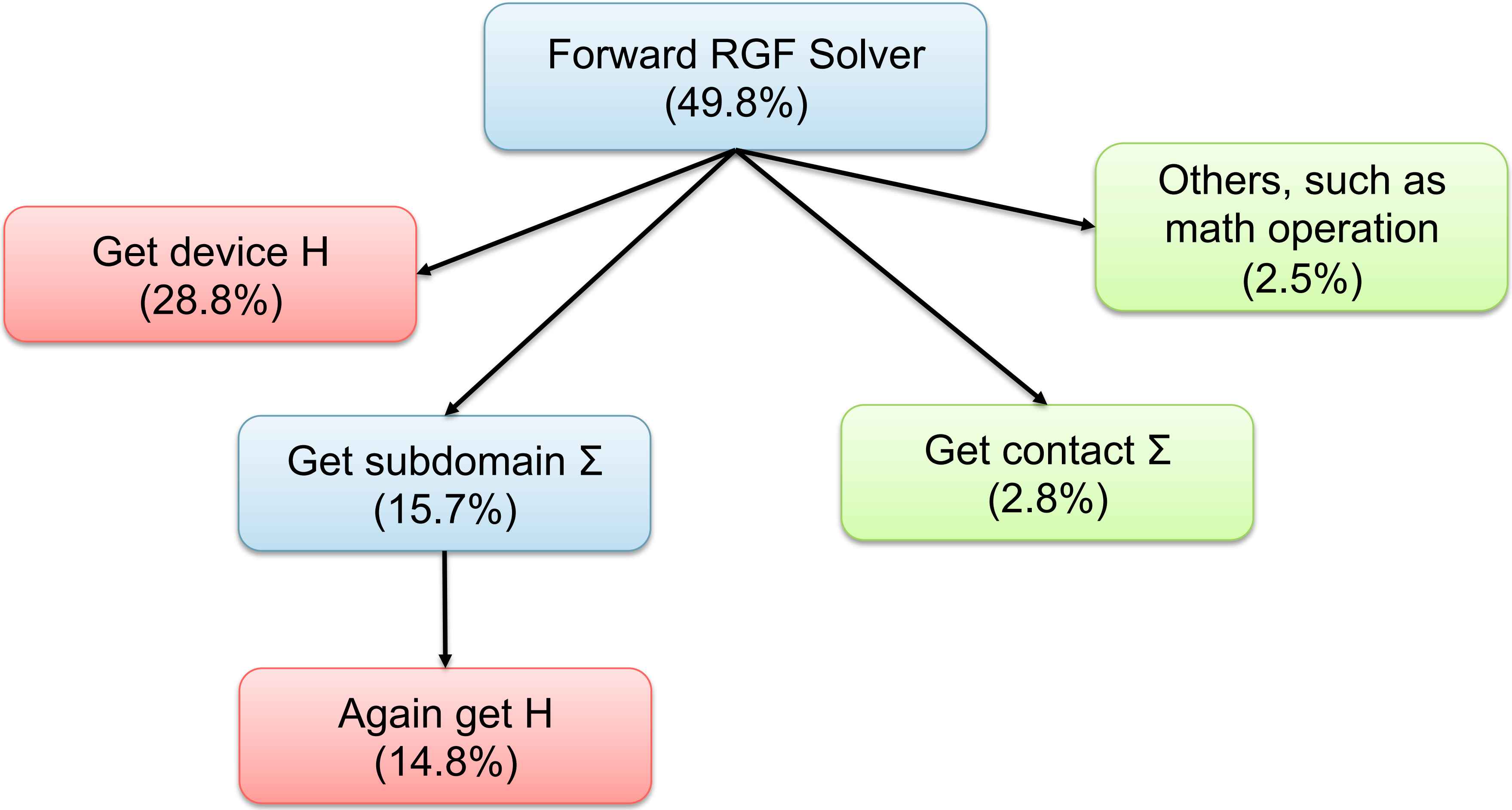
- Multi-Eq-Neq Timing Breakdown

MultiEqNeq Timing Overview



- MultiEqNeq Module takes 90.9% of entire CPU time of a LED simulation, rest is NEMO5 overhead (e.g setting up simulation environment) and Poisson
- Forward RGF > Backward RGF (contrary to expectation)
- Multi-Eq-Neq H-construction (big domain + eq-neq domains) takes 4.1%, a whooping number considering the entire current conservation (13 iterations) only takes 1.5%

Forward RGF



Forward RGF Solver (49.8%)

Get device H (28.8%)

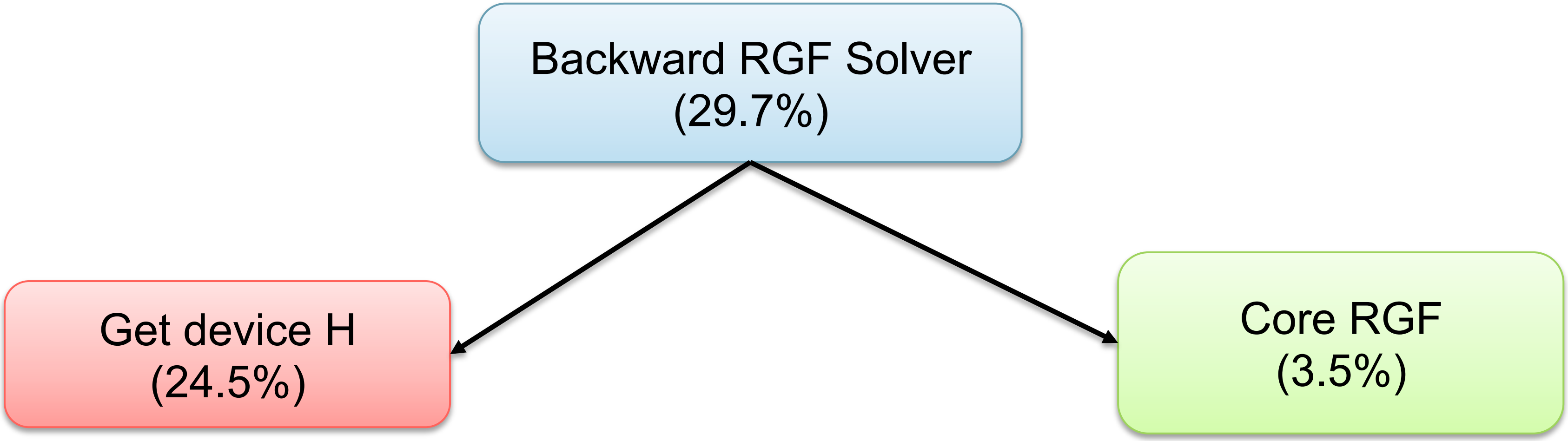
Others, such as math operation (2.5%)

Get subdomain Σ (15.7%)

Get contact Σ (2.8%)

Again get H (14.8%)

Majority of forward RGF is spent on Hamiltonian-related work (43.6/49.8)



Backward RGF Solver (29.7%)

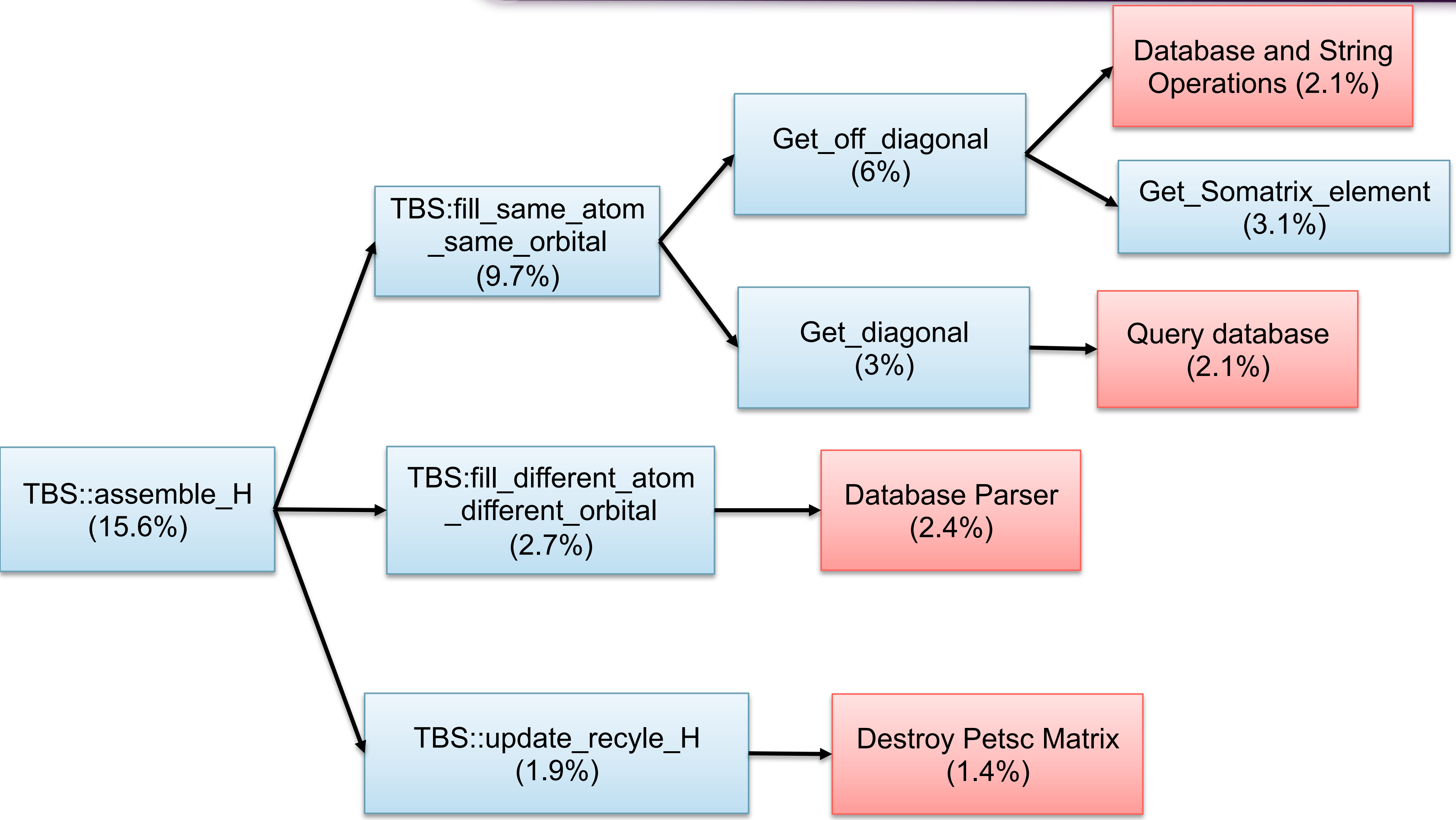
Get device H (24.5%)

Core RGF (3.5%)

Majority of backward RGF too is spent on Hamiltonian-related work (24.5/29.7)

Assemble Hamiltonian

- Forward RGF takes 49.8% total time, 43.6% is spent constructing Hamiltonian.
- Here I pick one instance of assembling Hamiltonian (15.6%) in forward RGF and try to further break down its timing consumption.



TBS::assemble_H (15.6%)

TBS:fill_same_atom_same_orbital (9.7%)

Get_off_diagonal (6%)

Database and String Operations (2.1%)

Get_Somatrix_element (3.1%)

Get_diagonal (3%)

Query database (2.1%)

TBS:fill_different_atom_different_orbital (2.7%)

Database Parser (2.4%)

TBS::update_recyle_H (1.9%)

Destroy Petsc Matrix (1.4%)

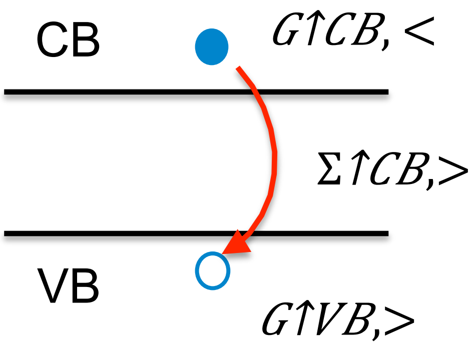
Conclusion:

- Vast majority (72%) of cpu time is spent on Hamiltonian-related functions (mostly Schroedinger solvers)
- Half of Hamiltonian operations are overhead due to material database (6.6% out of 15.6% one representative instance)

Experiment:

- Replace all alloys in the device (InGaN & AlGaN) with GaN
- This way, alloy parameters interpolation (such as VCA) is eliminated.
- This resulted in 10% reduction in total simulation time!
- **Alloy related database parsing = 10% total computation**

Deriving the B-coefficient



Assuming bandgap is wide, and no absorption → $\Sigma^{CB,>}$ is the only interaction that needs to be considered:

$$\Sigma^{CB,>}(k,E)\big|_{\hbar\omega} = i\hbar M(k)\cdot G^{VB,>}(k,E-\hbar\omega)\cdot M(k)$$

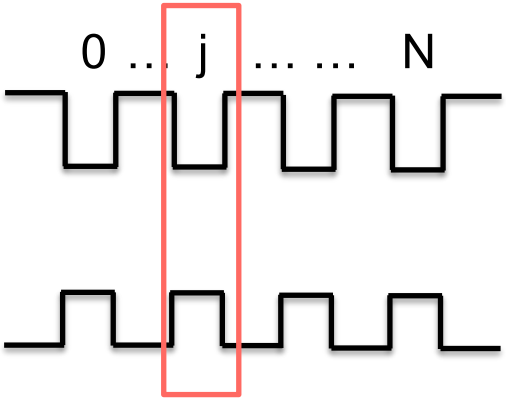
$$R(\hbar\omega)=\frac{1}{V}\int\frac{dk}{2\pi}\int\frac{dE}{2\pi\hbar}\,G^{CB,<}(k,E)\cdot\Sigma^{CB,>}(k,E)\big|_{\hbar\omega}$$

$$R(\hbar\omega)\approx C\cdot\int dk\,M(k)^{2}\int dE\,G^{VB,>}(k,E-\hbar\omega)\cdot G^{CB,<}(k,E)$$

where $M_{\alpha,L;\alpha',L'}(\mathbf{k})=\frac{e}{m_0}A_0\langle\alpha,L,\mathbf{k}|p|\alpha',L',\mathbf{k}\rangle$ and $A_0=\sqrt{\frac{\hbar}{2\epsilon_0 V\omega}}$

$$R(\hbar\omega)\approx C\cdot\underbrace{\frac{1}{\omega}\int dk\,M'(k)^{2}}_{\text{No charge dependence}}\underbrace{\int dE\,G^{VB,>}(k,E-\hbar\omega)\cdot G^{CB,<}(k,E)}_{\text{Charge dependent}}$$

Model Strategy



①. Decouple the radiative equation into a constant and (E, k)-dependent part. Initially, β is an arbitrary constant.

$$R_j(\hbar\omega) = \beta_j \cdot 1/\omega \int dk^2 \int dE\, G^{CB,<}(k,E) \cdot G^{VB,>}($$

②. Perform integration over all photon energy, equate the result to "ABC" model

$$R_j = \int d\omega\, R_j(\hbar\omega) = \beta_j K = B \cdot n_j \cdot p_j$$

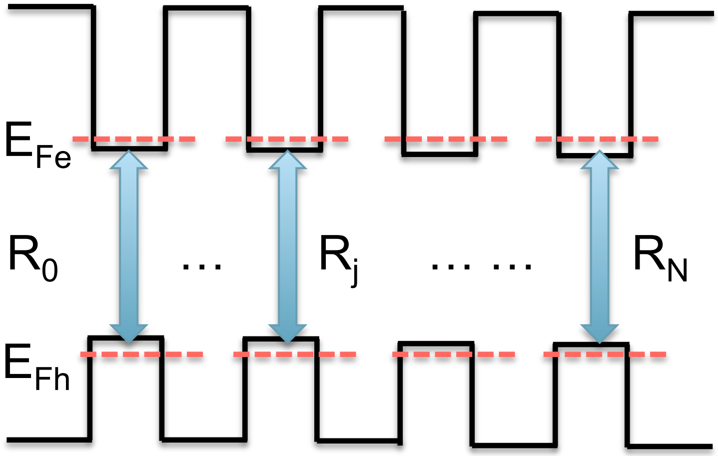
This is just the "ABC" model

③. Calibrate the β coefficient, use it to calculate $R_j(\hbar\omega)$ from step ①

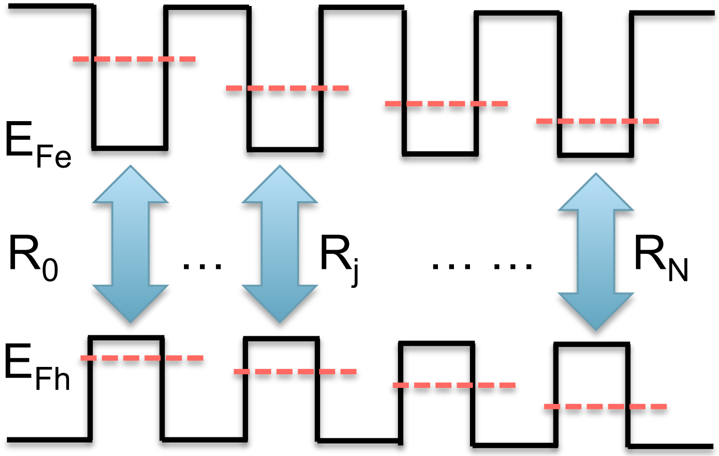
$$\beta_j = B \cdot n_j \cdot p_j / K$$

Process

Start:



End:



Initially set both E_{Fe} , E_{Fh} low, so that B·n·p gives reasonable result

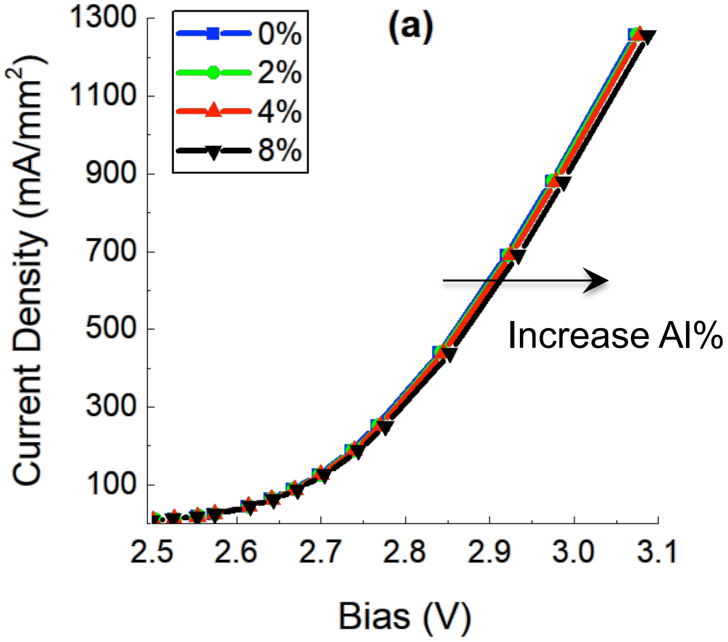
Derive β for each QW from $\beta_j = B\cdot n_j \cdot p_j /K$

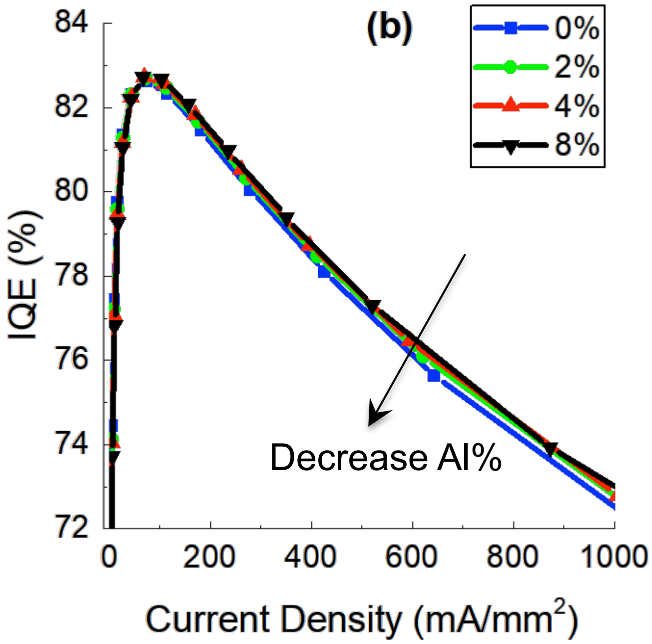
Fix the β values and for successive R_j $(\hbar\omega)$

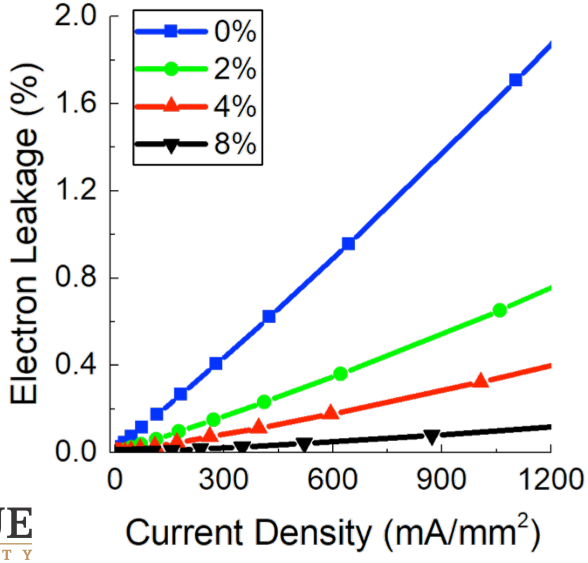
We have a model that is more adaptable than B·n·p model:

- β coefficient is material and geometry dependent
- R dependence on photon energy, charge density covered
- Formula can be extended to calculate β more rigorously

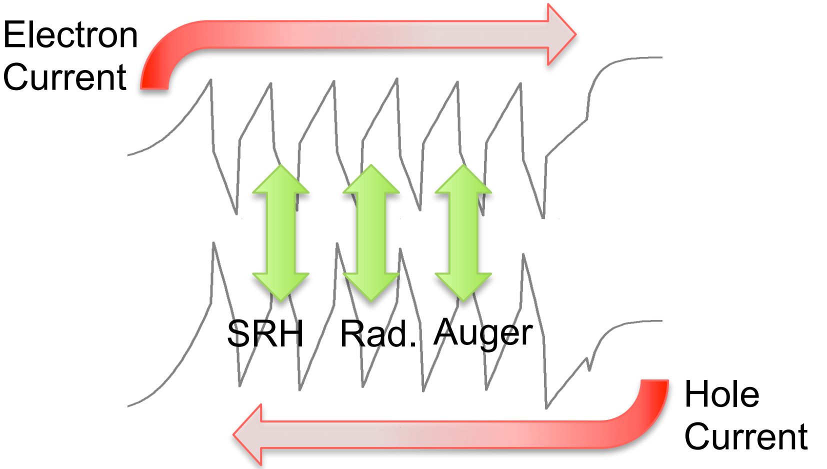
Device trend vs Al% (0-8%)



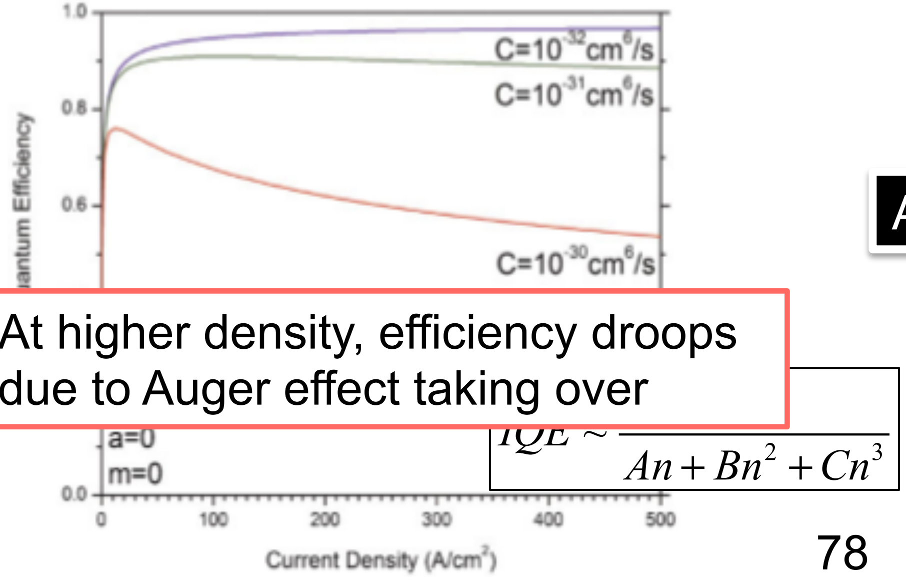




Internal Quantum Efficiency (IQE)

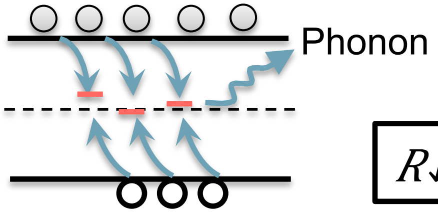


IQE = Radiative current / total current



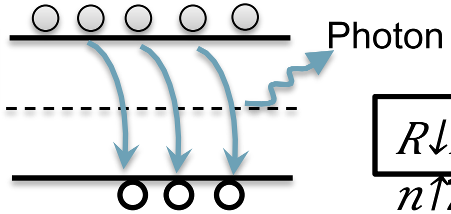
At higher density, efficiency droops due to Auger effect taking over

SRH



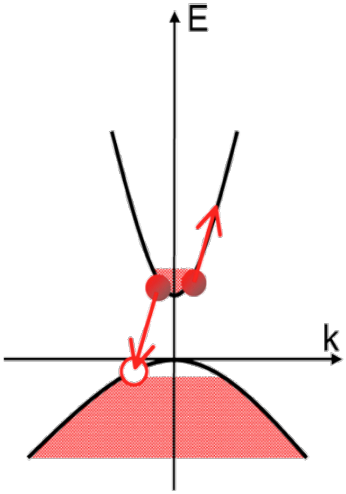
$R_{SRH} \sim n$

Radiative

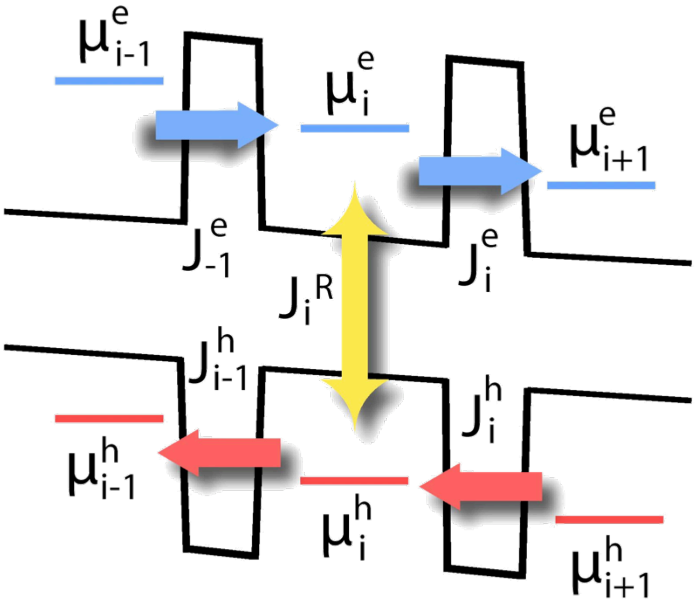


$R_{Rad} \sim n^2$

Auger



$R_{Rad} \sim n^3$



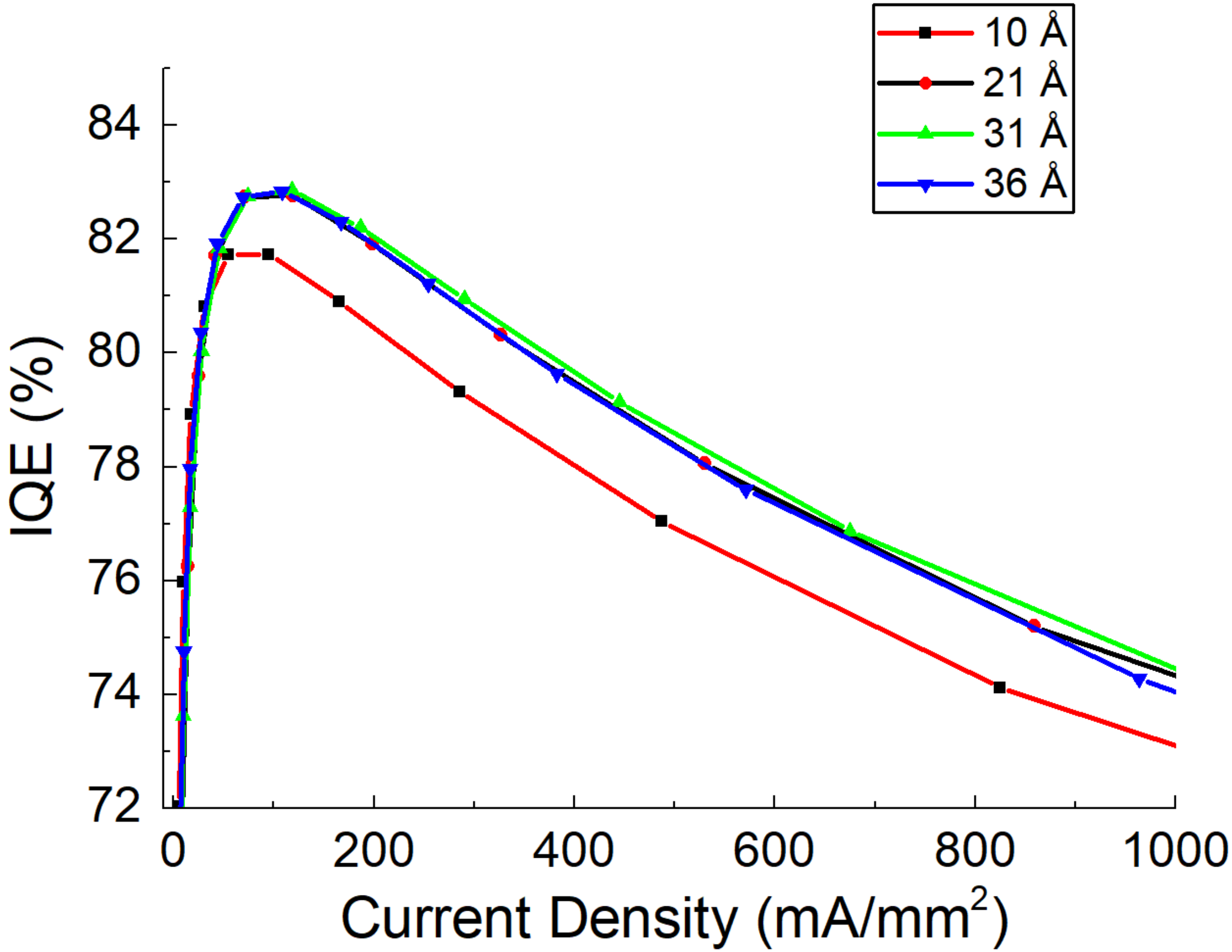
$$J_{j,A} = A_j \cdot \frac{n_j p_j - n_{intri}^2}{\tau_N(p_j + p_1) + \tau_P(n_j + n_1)}$$

$$J_{j,B} = B_j \cdot n_j p_j$$

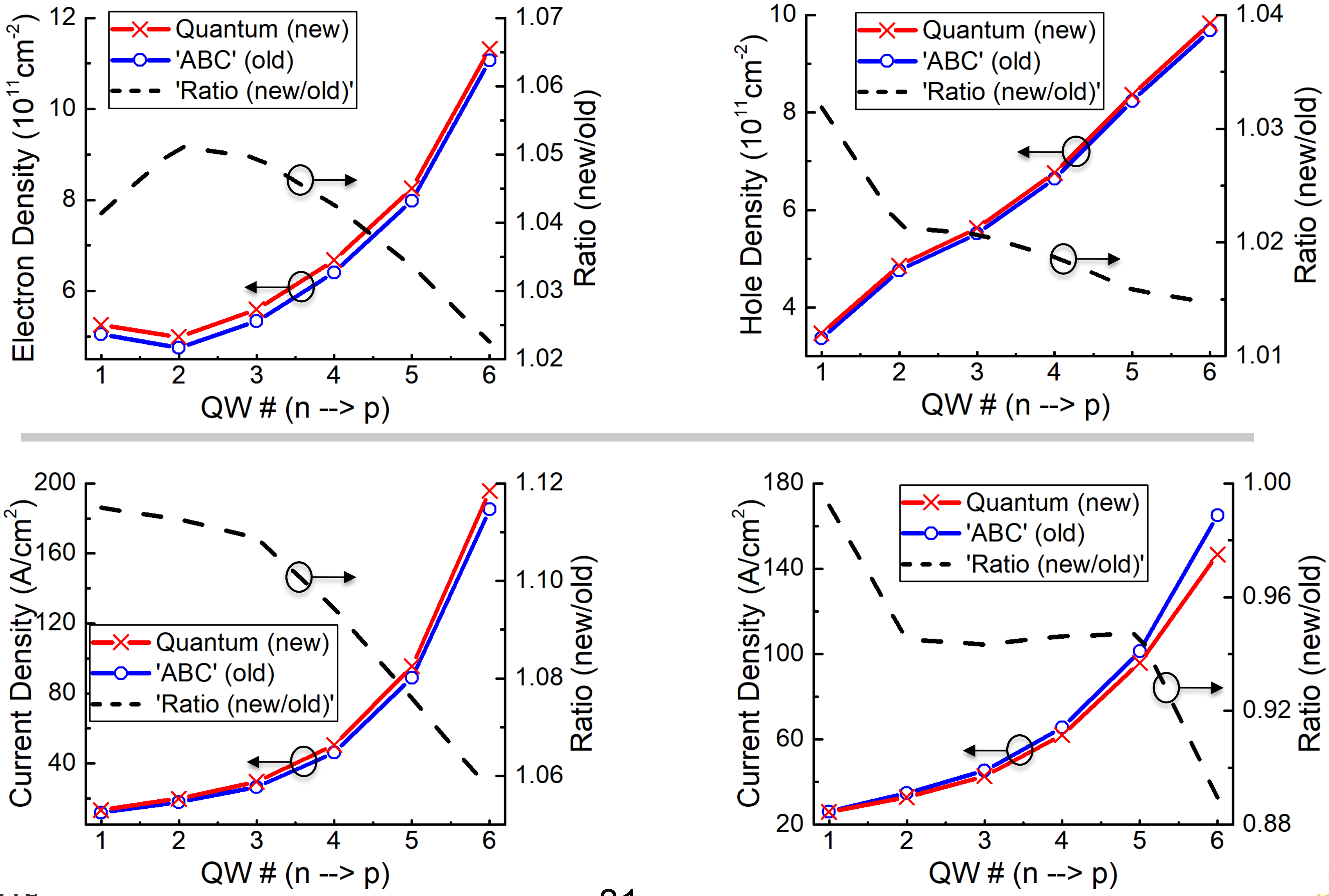
$$J_{j,C} = C_j \cdot (n_j^2 p_j + p_j^2 n_j)$$

$$J^R_{j,total} = J_{j,A} + J_{j,B} + J_{j,C}$$

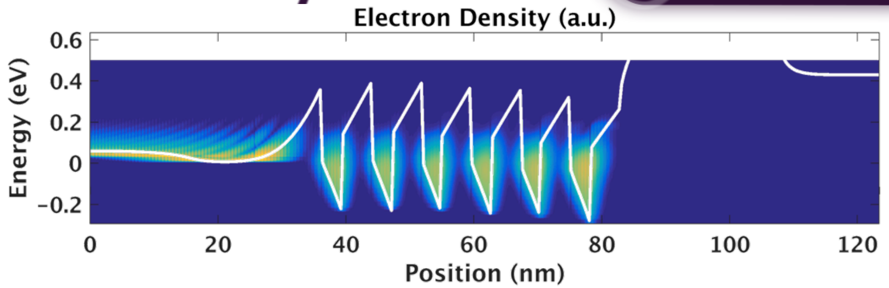
IV for W from 2 to 7uc

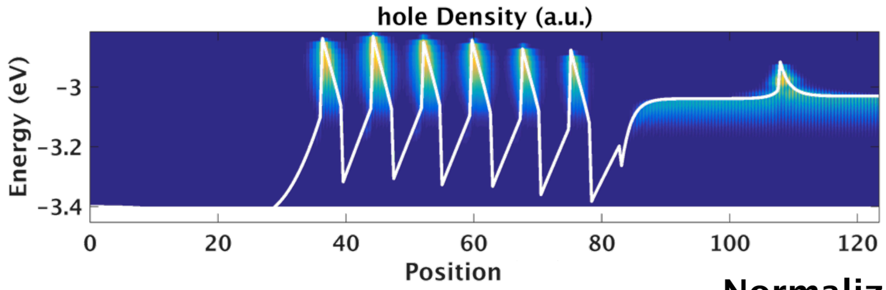


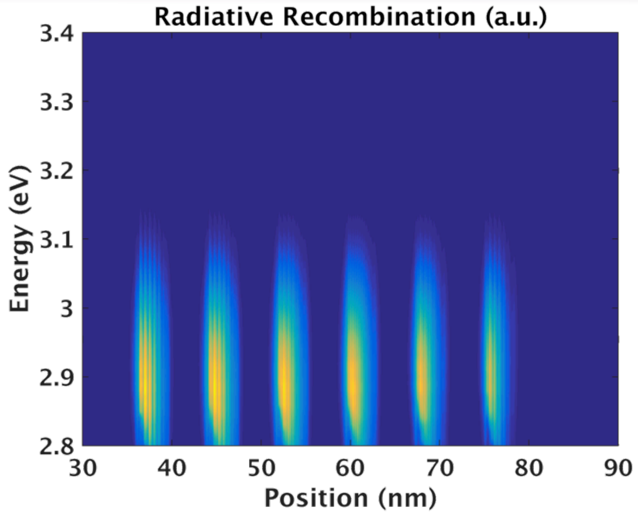
Radiative model comparison: QW-resolved

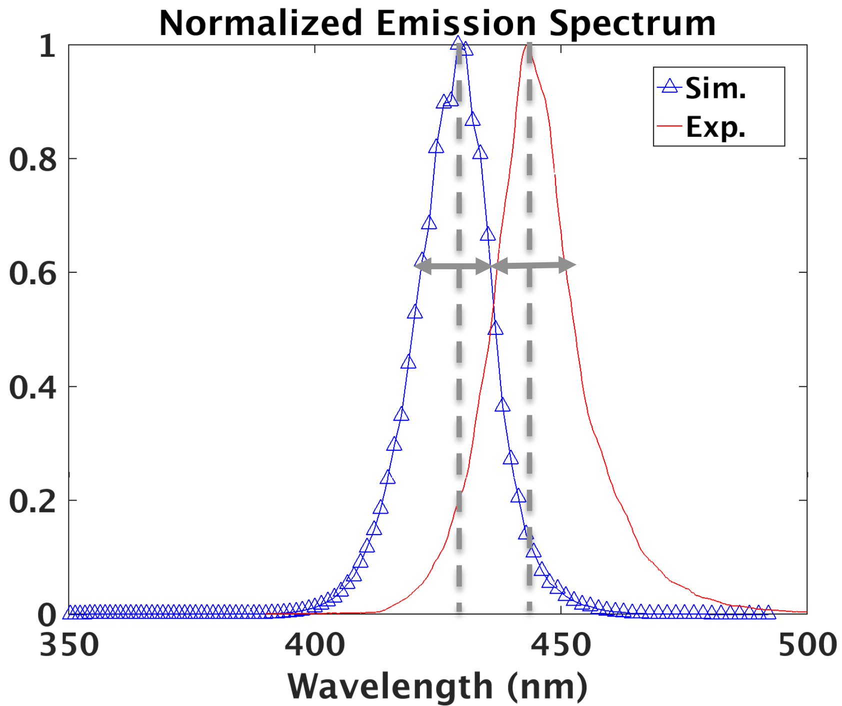


Emission spectrum

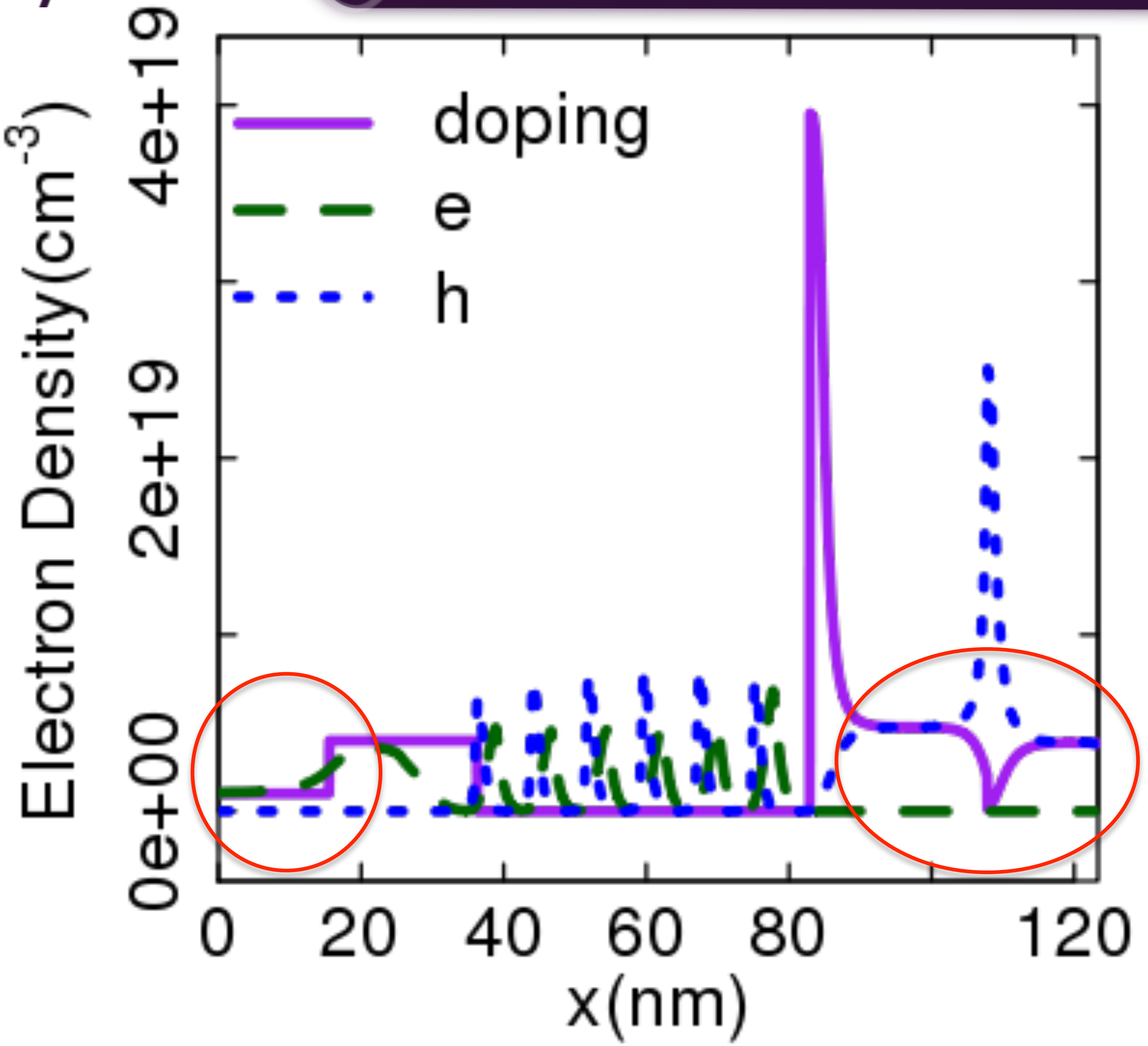

Electron Density (a.u.)


hole Density (a.u.)


Radiative Recombination (a.u.)

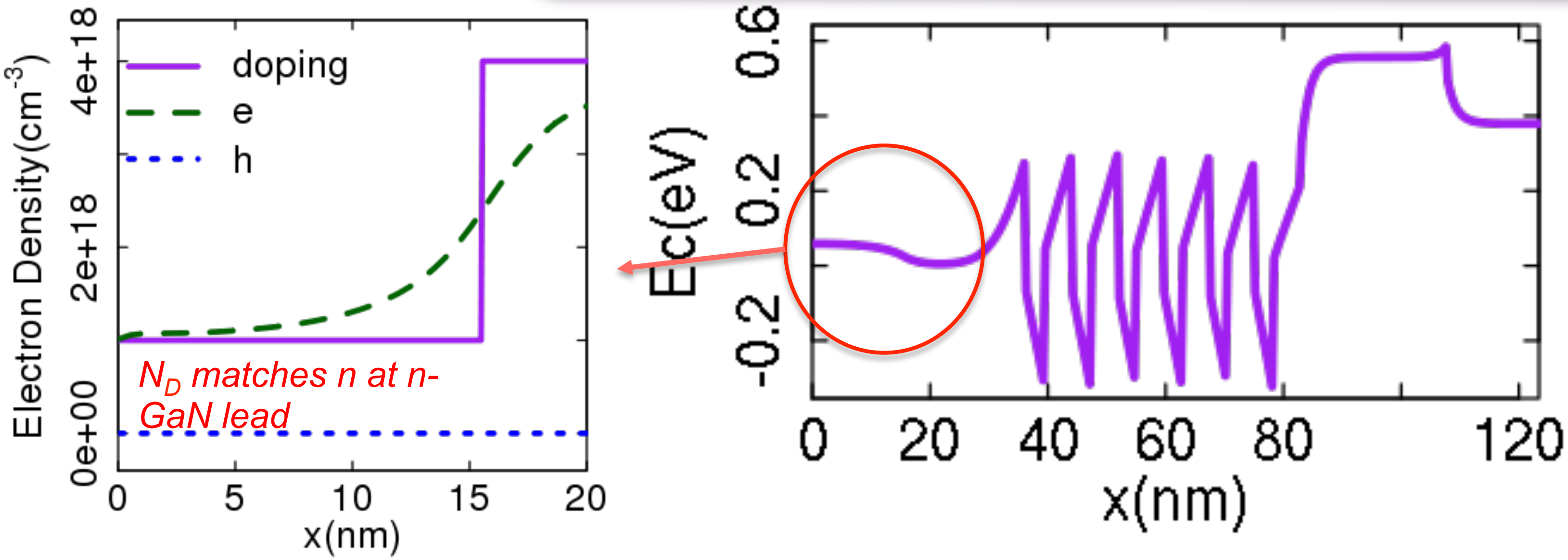

Normalized Emission Spectrum

Comparison of Ionized Doping Density with electron/hole Density

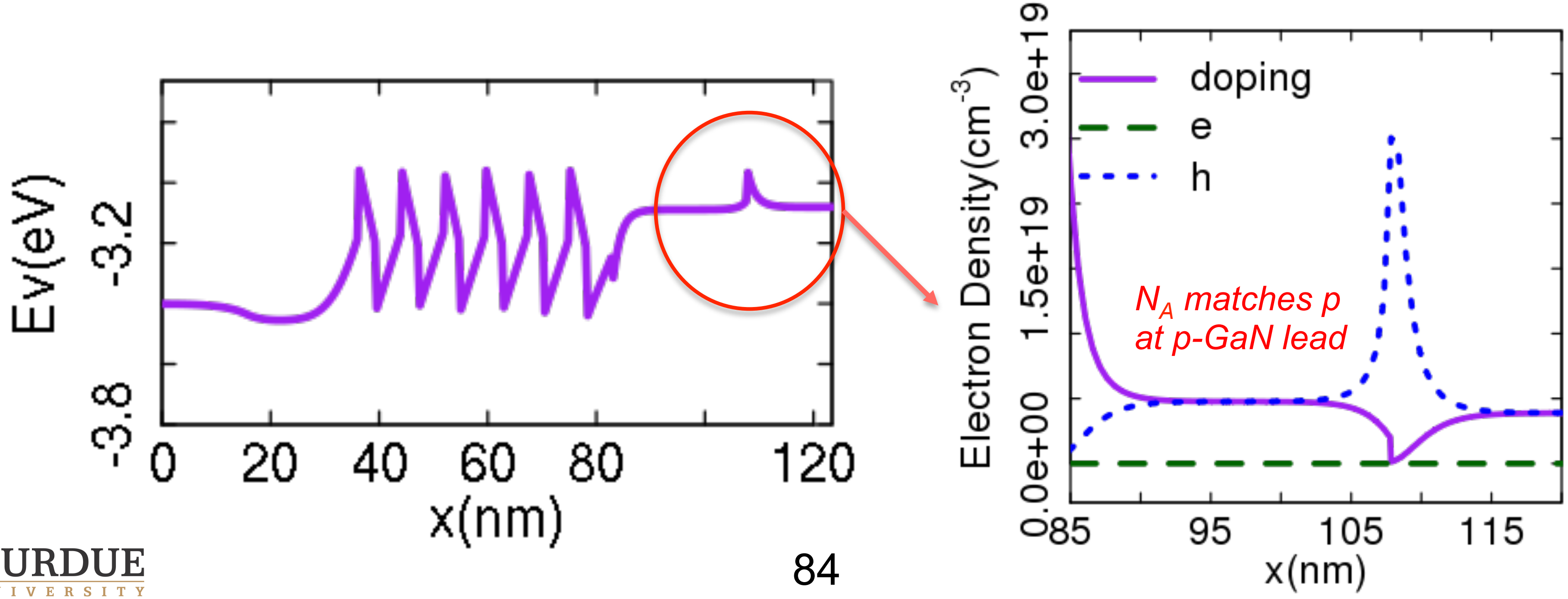


Charge density in the two leads matches (ionized) doping density

Comparison of Ionized Doping Density with electron/hole Density

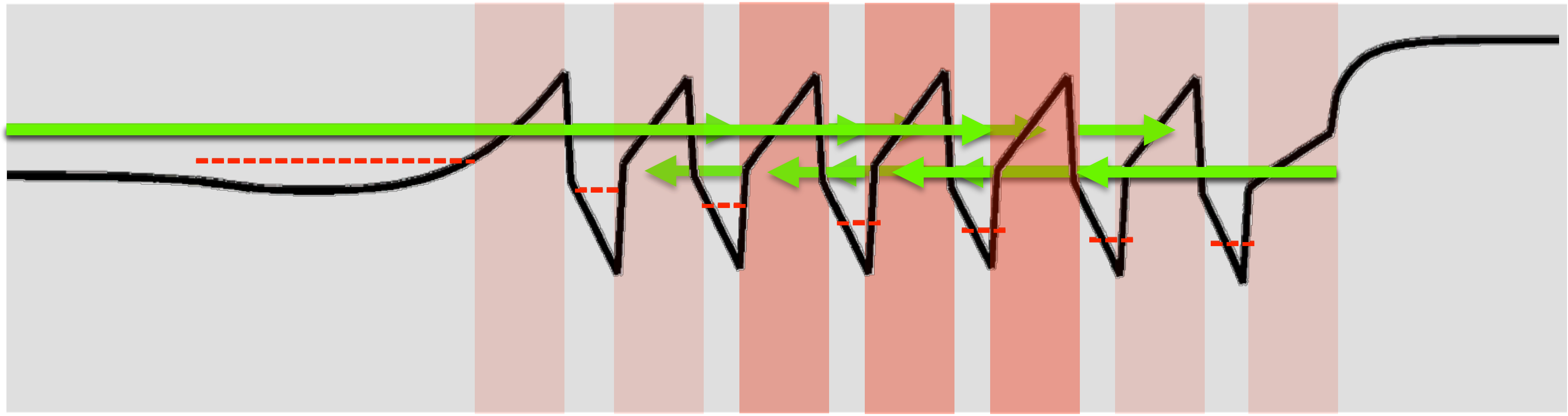


N_D matches n at n-GaN lead



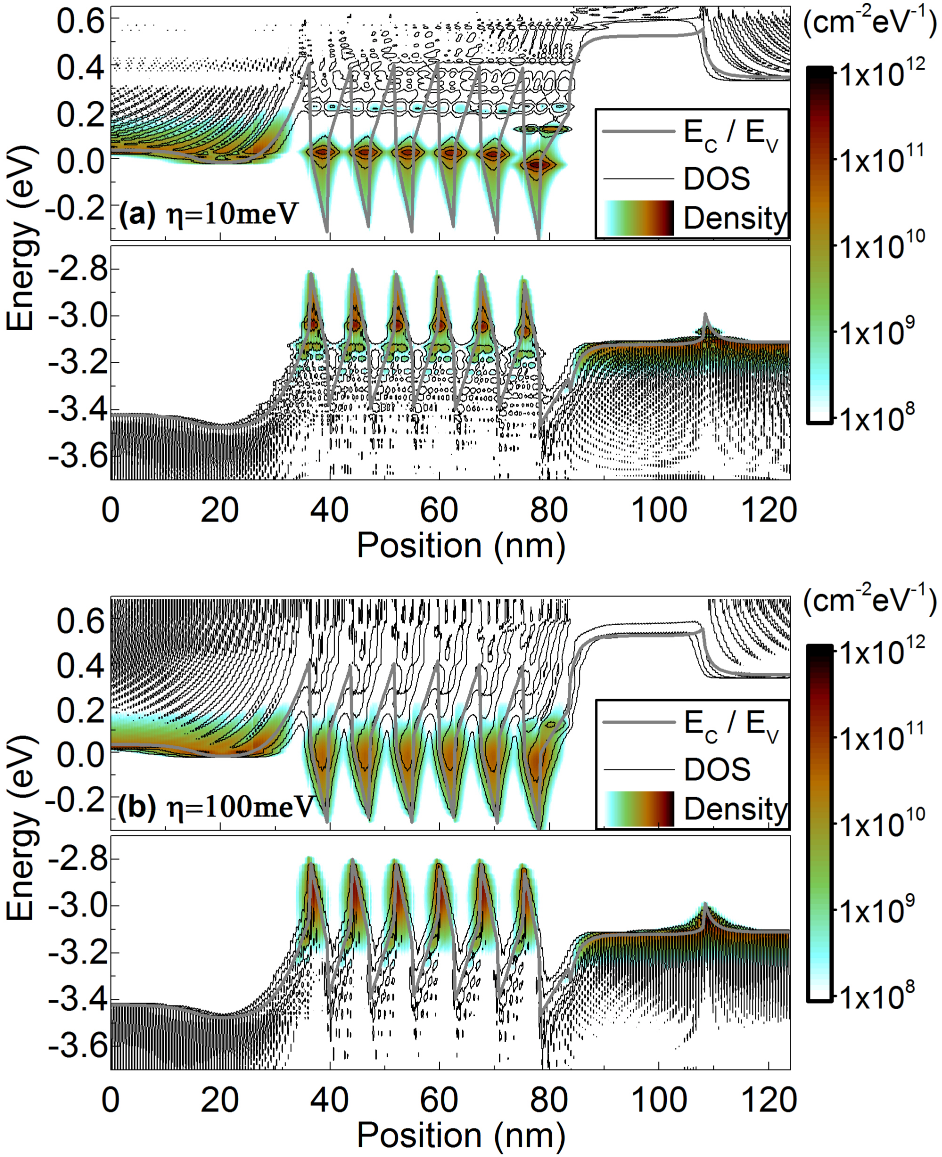
N_A matches p at p-GaN lead

Multi-Scale, Multi-Physics Modeling – Sophisticated Injection Mechanism



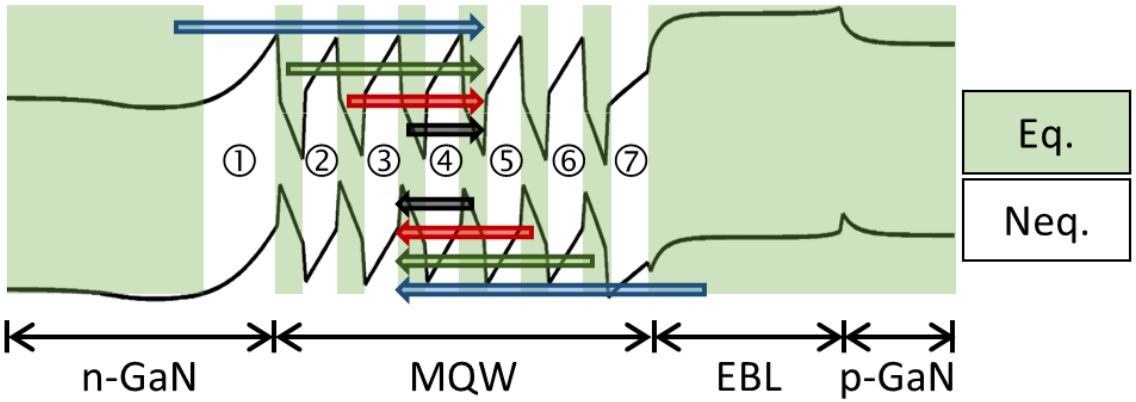
- Sophisticated injection:
  - Each well knows about the distributed presence of the others
- Critical quantum transport region reduced → Dramatic reduction in computation (~N^2)

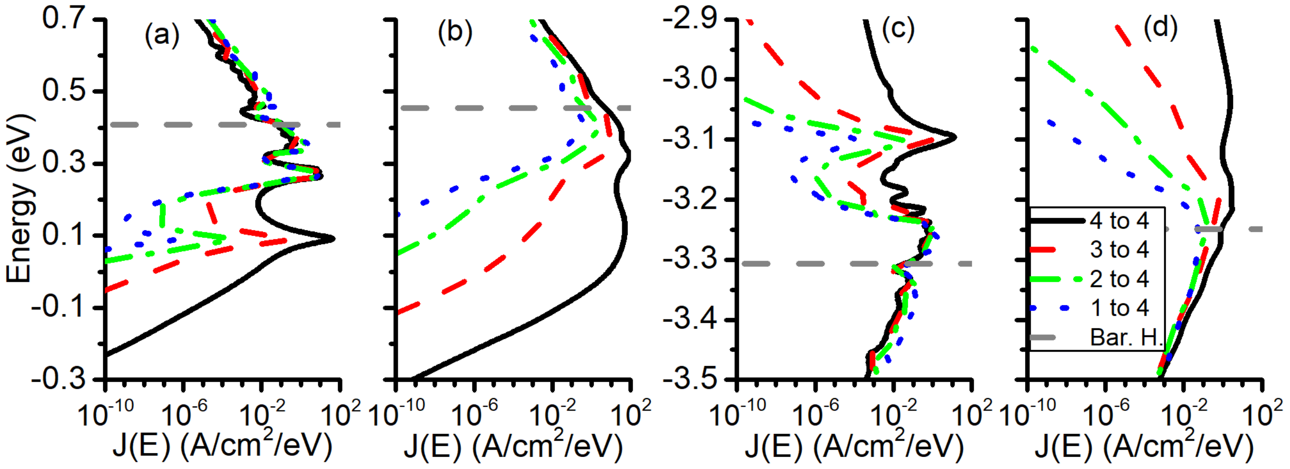
DOS comparison 10 vs. 100meV



1. Energy-resolved electron, hole density of states (contour lines) filled with electrons and holes (color contours). The bulk-based conduction and valence band edges serve as a guide to the eye and only enter the calaculation in the definition of the empirical scattering strength η. States in the QW are broadenend due to η and coupled to each other. (a) η=10meV is a typical broadening in GaAs and InP based devices. The quantum well states are broadened but still distinct. (b) η=100meV is a broadening that corresponds to experimental optical linewidth measurements. The various hole states are all cross coupled and also the electron states broaden energetically to about half the height of the quantum wells. These broadened states serve as injectors and receptors for tunneling across the barriers. η =100meV leads to the quantitative agreement with experimental data shown below and is used in all other simulations presented here.

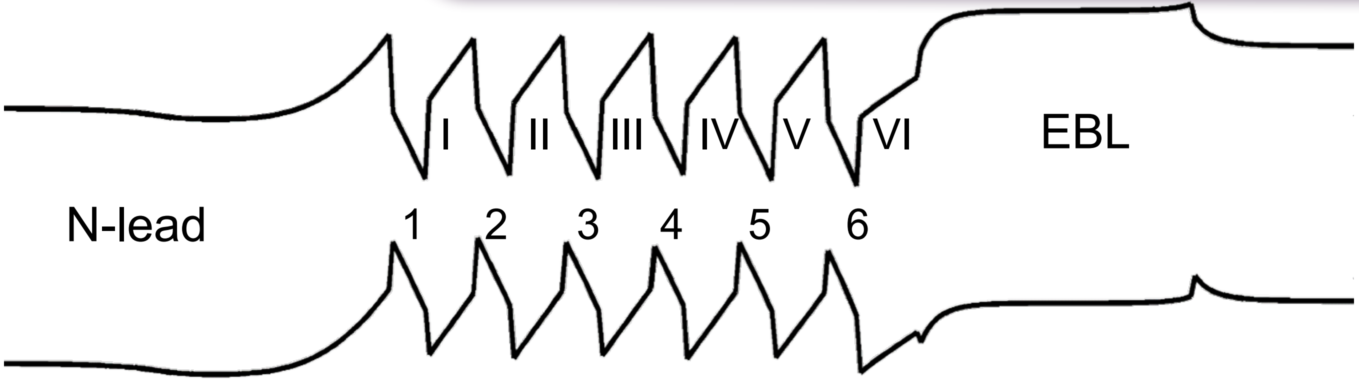
E-current density long range

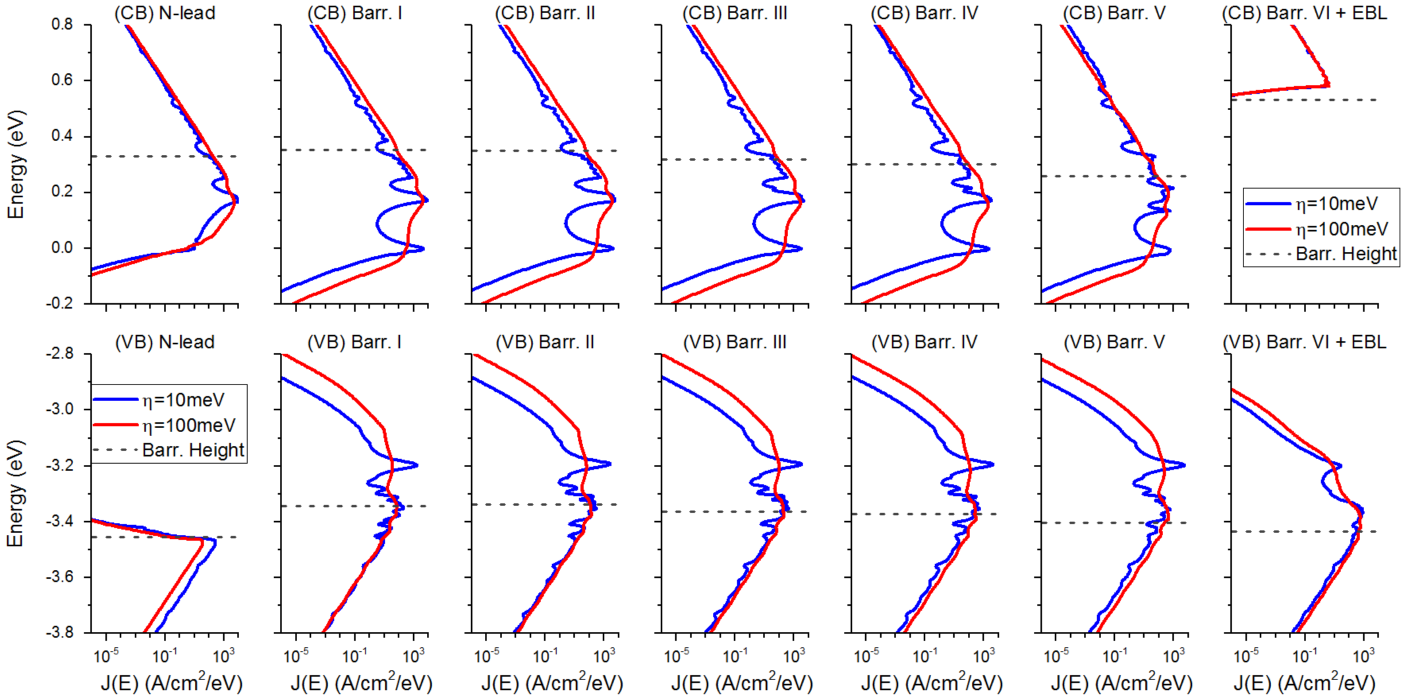


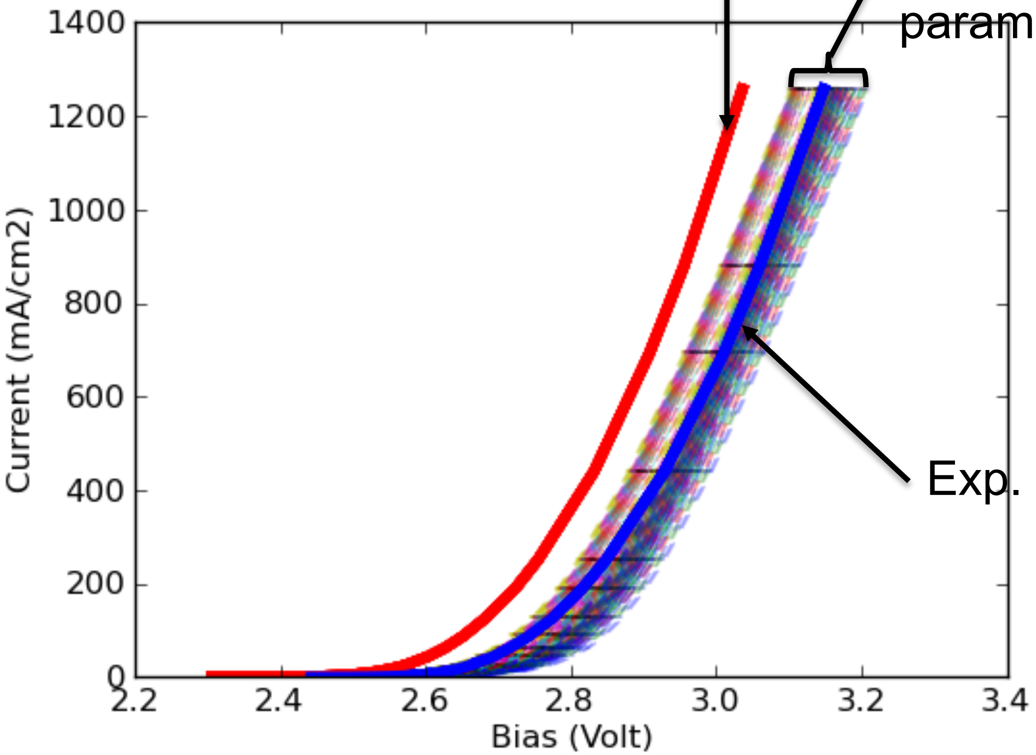


Energy-resolved current density across the middle barrier (No. 4 in Fig. 6.1) for η=0.01 (a,c) and η=0.1eV (b,d). Barrier heights are marked with grey dashed lines.

E-current density







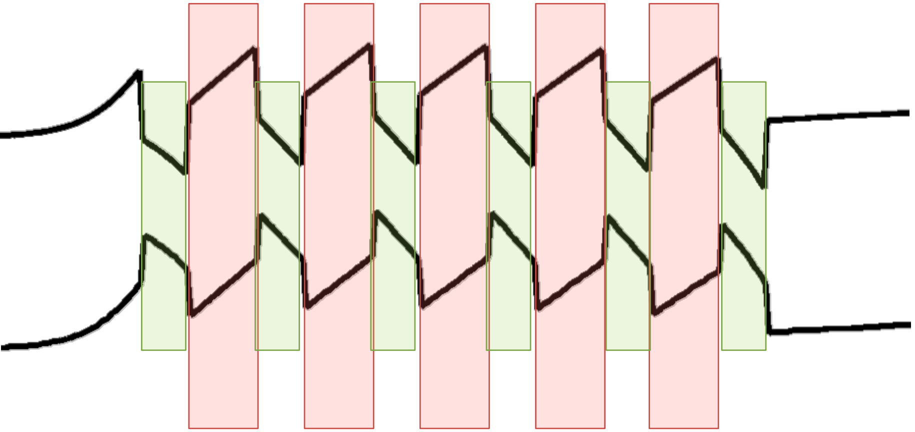
Exp. 85C

Simulation results over all possible A,B,C parameters

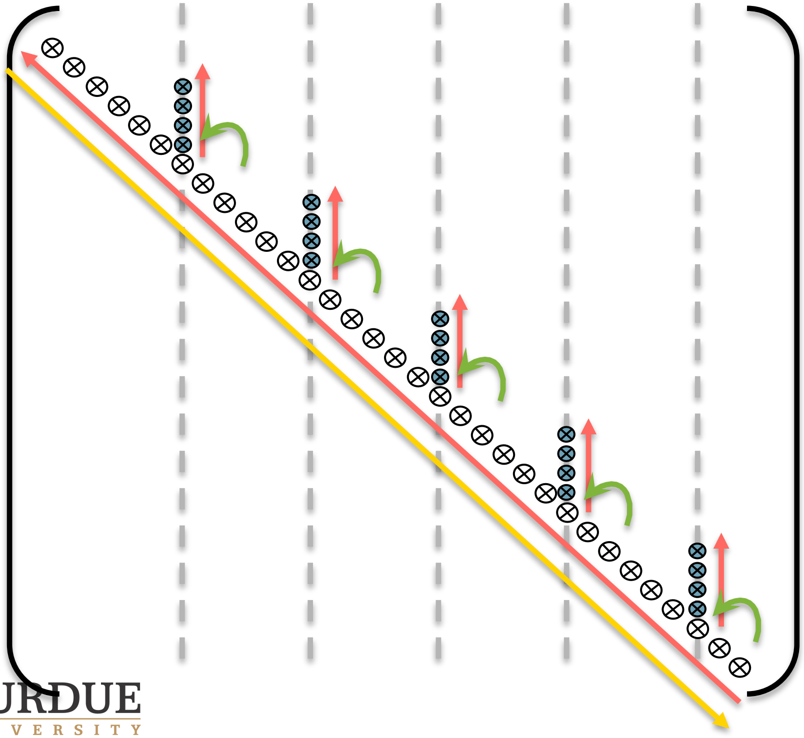
Exp. 25C

Backup slides for “scattering in barrier” future plan

Incorporating Scattering in the Barriers
- Overview of the current approach



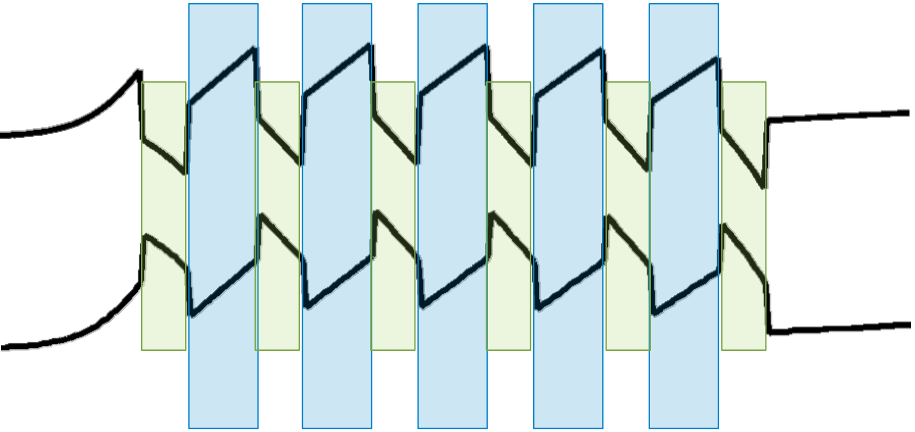
- Barrier: coherent transport
- Well: equilibrium



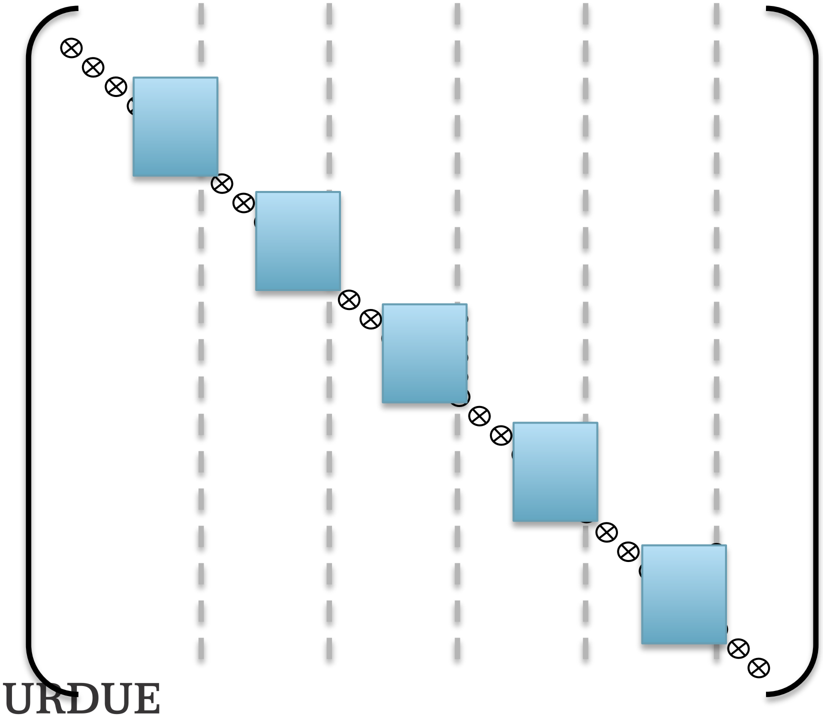
One forward RGF solver: provides g^R (the left-connected Green's function, diagonal only)

One backward MEQ solver: provides full G^R (diagonal + off-diagonal), also provides Σ^R for calculating transmission.

Incorporating Scattering in the Barriers -Update of code/algorithm I



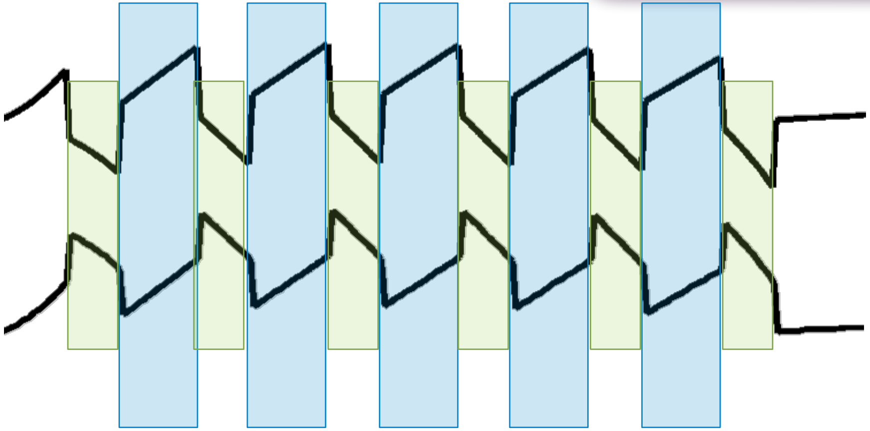
- Barrier: full scattering
- Well: equilibrium

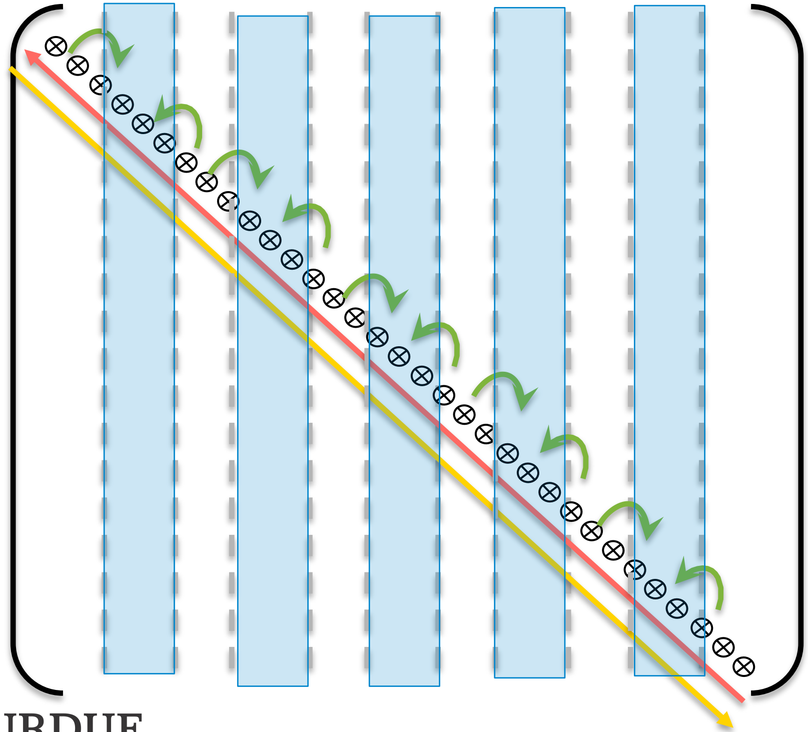


Will require additional self-consistent Born (scBorn) modules:

- One scBorn for each barrier region.
- scBorn module will solve additional matrices:
  - Additional off-diagonal G^R elements
  - Σ^R and $\Sigma^<$ for each subdomain (slab)
  - Σ for each scattering
  - $G^<$
  - Σ^R, $\Sigma^<$, G^R, $G^<$ needs to be solved multiple times until converged

Incorporating Scattering in the Barriers
-Update of code/algorithm II





Implementing full scattering:

1. First solve the original forward RGF and backward MEQ:
   - Equilibrium regions' calculations remain the same
   - Backward MEQ solver will provide region boundary Σ^R's to the scBorn.
2. Create scBorn for each non-eq region
   - Σ^R provided by Backward MEQ solver
   - Calculates Σ^R, $\Sigma^<$, G^R, $G^<$ self-consistently
3. Once every scBorn is converged, calculate and update quantities such as density and current in each region.
4. Solve Newton-Raphson for overall current convergence. Each iteration will repeat steps 1-3

Estimate of additional numerical load

- Additional Greensfunction elements for scBorn (2.5x for local and up to 150x for nonlocal)
- Calculating scattering Σ's (10x for local and 1000x for nonlocal pop)
- Additional iterations for scBorn convergence between Σ^R, $\Sigma^<$, G^R and $G^<$ (10x)
- Current conservation including scattering does not allow to recycle transmission for current conservation (10 x)
- **Overall additional numerical load (x3~7 orders of magnitude)**

LED with scBorn in neq-regions is a research project
Industrially relevant solution not available yet

Implementation roadmap

Implementation Steps:	If Junzhe were to implement this:
First solve the original forward RGF and backward MEQ	Ready
Create scBorn for each non-eq region	Create, initialize, solve compatibility-related issues (1 month)
Once every scBorn is converged, calculate and update quantities such as density and current in each region.	Control convergence, add interfaces, verify code flow (5 months)
Solve Newton-Raphson for overall current convergence. Each iteration will repeat steps 1-3	Embed 3 into Newton-Raphson and use J instead of T(transmission) – setup enough iterations, develop efficient algorithm and iteration scheme (5 months)

Junzhe is expected to graduate on 7/12 – new student requires training and more help – factor 1.5x – 3x slow down