NEMO: From Esoteric Quantum Theory to Industrial Transistor Designs and Global Impact

Gerhard Klimeck
Purdue University

How did we get from Quantum Transport in RTDs to billions of chips with billions of nanotransistors?

Challenges at the Frontier of Quantum Transport Modeling (NEMO & nanoHUB)

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- Starting Point - Specific measurable device challenges
- Modelling goals shared beyond specific devices
- Transferrable approaches shared beyond specific devices

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- Starting Point - Specific measurable device challenges

- Modelling goals shared beyond specific devices
  - Qualitatively and quantitatively guide physics experiments
  - Design and engineer real devices
  - Predictive not just "descriptive" or tightly calibrated
  - Realistically scaled and extended devices (beyond conceptual stick diagrams)
  - Transferrable approaches beyond a single device or material
- Transferrable approaches shared beyond specific devices

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- Transferrable approaches shared beyond specific devices
  - Multi-physics & multi-scale segmentation or partition
  - Smart choices of basis sets
  - Scalable compute times & accuracy (quick & dirty ⇔ detailed)
  - Usability and access to users (incl. computing hardware)

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(NEMO & nanoHUB)

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These Meta-Goals and Meta-Approaches define
The Frontiers of Modeling

Frontier of Modeling in Industry

- Transferrable approaches shared beyond specific devices
  - Multi-physics & multi-scale segmentation or partition
  - Smart choices of basis sets
  - Scalable compute times & accuracy (quick & dirty ⇔ detailed)
  - Usability and access to users (incl. computing hardware)

NEMO5

Core Code / Theory Development

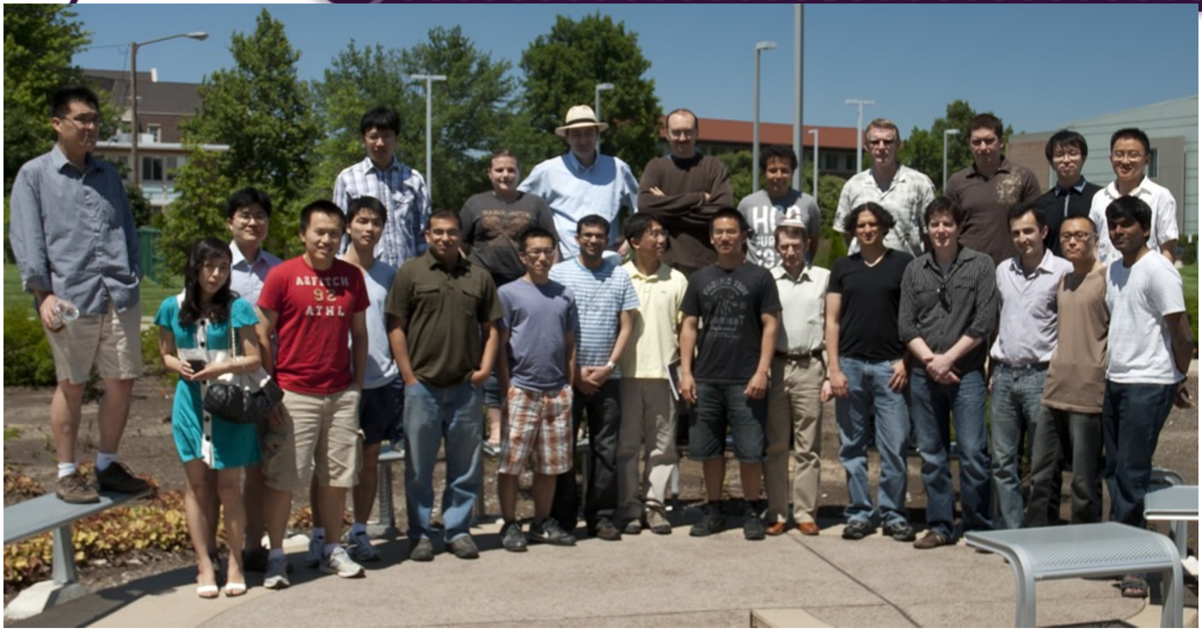
- NEMO-1D (Texas Instruments ‘94-’98, JPL ‘98-’03)
  - »Roger Lake, R. Chris Bowen
- NEMO3D (NASA JPL, Purdue, ’98-’07)
  - »R. Chris Bowen, Fabiano Oyafuso, Seungwon Lee
- NEMO3D-peta (Purdue, ’06-’11)
  - »Hoon Ryu, Sunhee Lee
- OMEN (ETH, Purdue, ‘06-’11)
  - »Mathieu Luisier
- NEMO5 (Purdue, ‘09-..)
  - » active professionals: M. Povolotsky, T. Kubis, J. Fonseca, B. Novakovic, R. Rahman, (formerly A. Ajoy, H-H Park, S. Steiger)

23+ active students: Tarek Ameen, James Charles, Junzhe Geng, Kaspar Haume, Yu He, Ganesh Hegde, Yuling Hsueh, Hesam Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Lemus, Daniel Mejia, Kai Miao, Samik Mukherjee, Seung Hyun Park, Ahmed Reza, Mehdi Salmani, Parijat Sengupta, Saima Sharmin, Yaohua Tan, Archana Tankasala, Daniel Valencia, Evan Wilson,

Tillmann Kubis

PURDUE UNIVERSITY

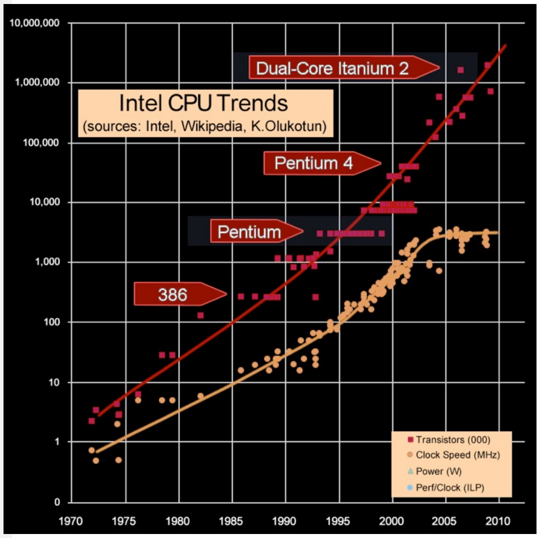
Thanks to



Research Group
@Purdue
@NASA JPL 1998-2003
@Texas Instruments 1994-1998

Tillmann Kubis

Moore's Law End:
falsely predicted dead many times

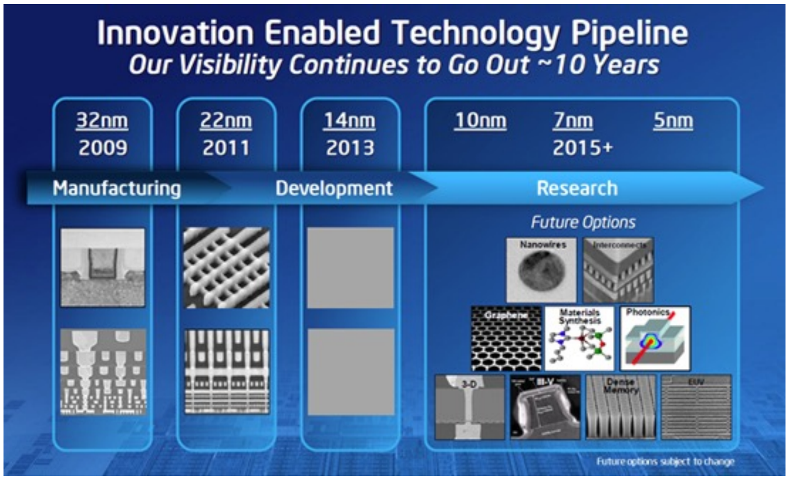


http://jai-on-asp.blogspot.com

2005: free lunch is over, updated 2009

Clock Speeds stopped scaling in 2005

2009 Intel Road Map - Atomistic Dimensions in Sight



Innovation Enabled Technology Pipeline

Our Visibility Continues to Go Out ~10 Years

32nm 2009
22nm 2011
14nm 2013
10nm
7nm 2015+
5nm

Manufacturing
Development
Research

Future Options

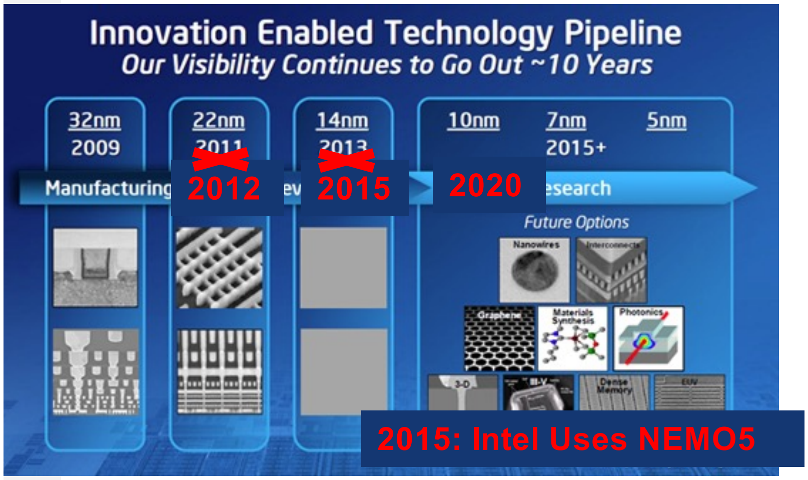
Future options subject to change

nm Node	22	14	10	7	5
Node atoms	176	122	80	56	40
Electrons	160-190	64-80	30-38	18-23	11-15

2009 All TCAD tools are Atom-Agnostic

Device Scaling Reaches Atomic Limits

2009 Intel Road Map - Atomistic Dimensions in Sight



Innovation Enabled Technology Pipeline

Our Visibility Continues to Go Out ~10 Years

32nm 2009 | 22nm ~~2011~~ 2012 | 14nm ~~2013~~ 2015 | 10nm 7nm 2015+ 5nm 2020

Manufacturing | Development | Research

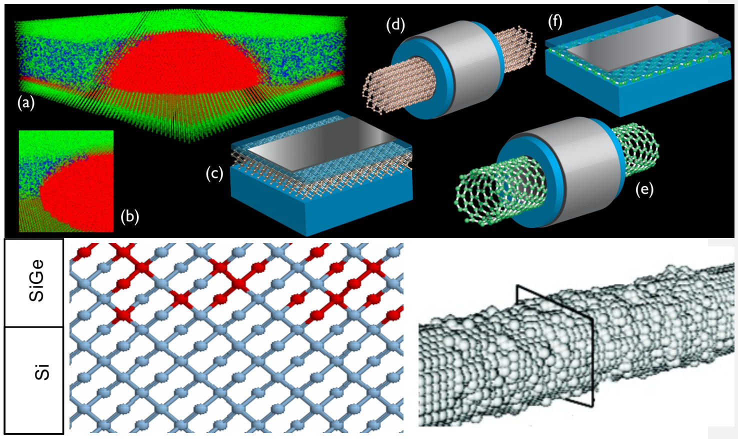
2015: Intel Uses NEMO5

nm Node	22	14	10	7	5
Node atoms	176	122	80	56	40
Electrons	160-190	64-80	30-38	18-23	11-15

2009 All TCAD tools are Atom-Agnostic

Since 1994: NEMO Development

Atomistic Quantum Transport for Extended Devices



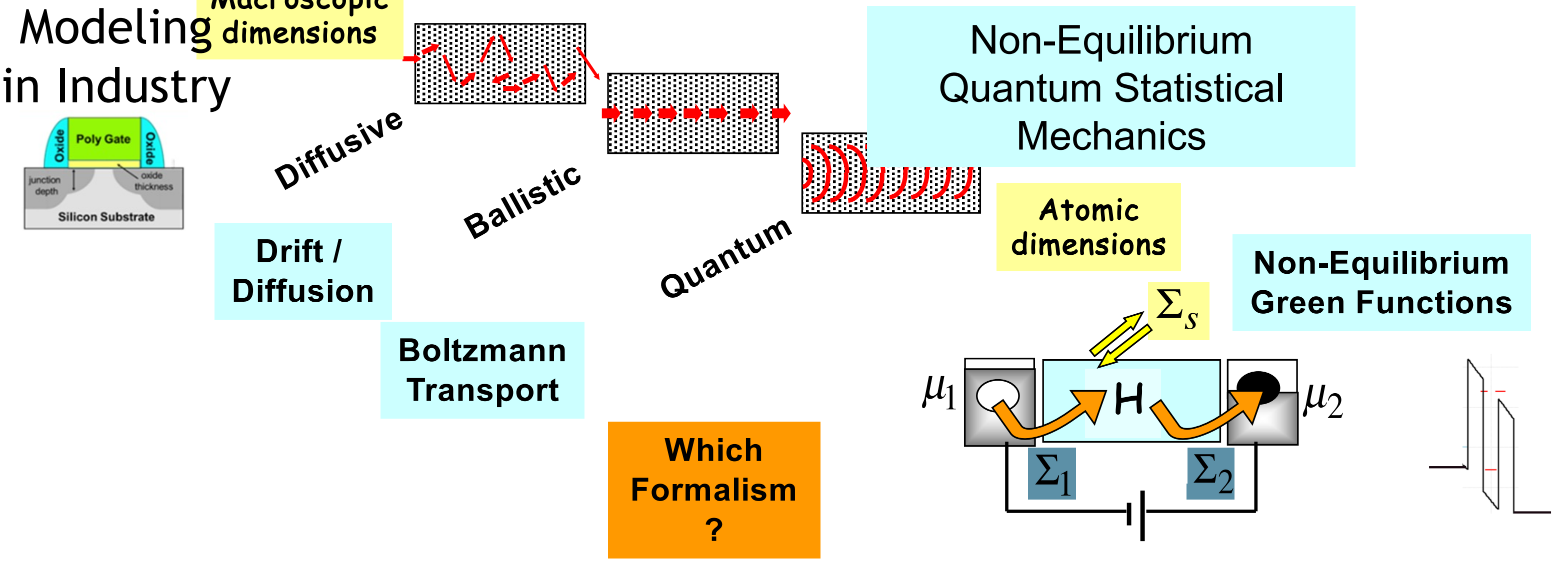
29 years development

- **Texas Instruments (1994-98)**
- **NASA JPL (1998-2004)**
- **Purdue (2004 – present)**

NEMO5

- Transferrable approaches shared beyond specific devices

Frontier of Modeling in Industry



Macroscopic dimensions

Drift / Diffusion

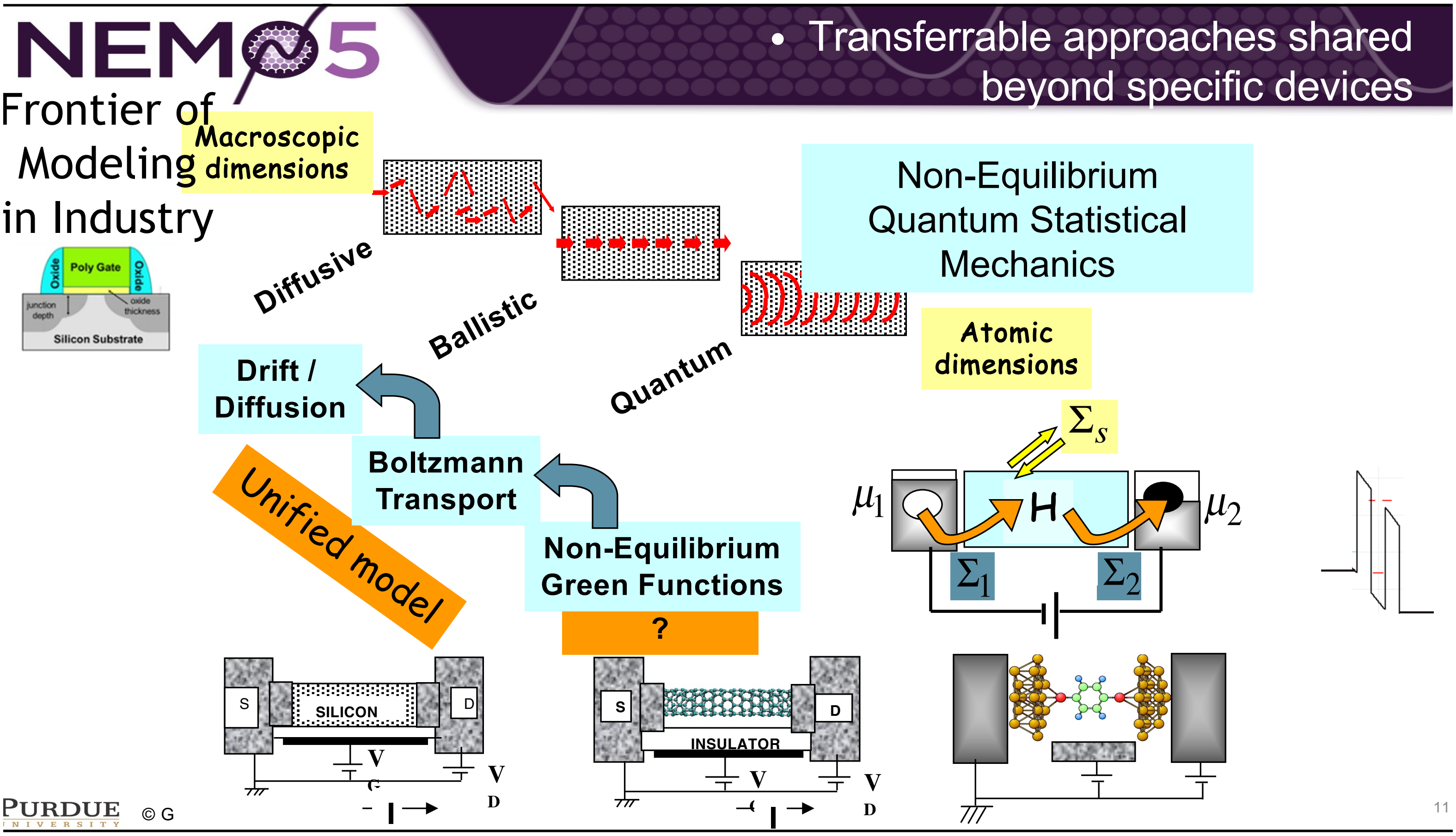
Boltzmann Transport

Which Formalism ?

Non-Equilibrium Quantum Statistical Mechanics

Atomic dimensions

Non-Equilibrium Green Functions



Frontier of Modeling in Industry

- Transferrable approaches shared beyond specific devices

Macroscopic dimensions

Atomic dimensions

Non-Equilibrium Quantum Statistical Mechanics

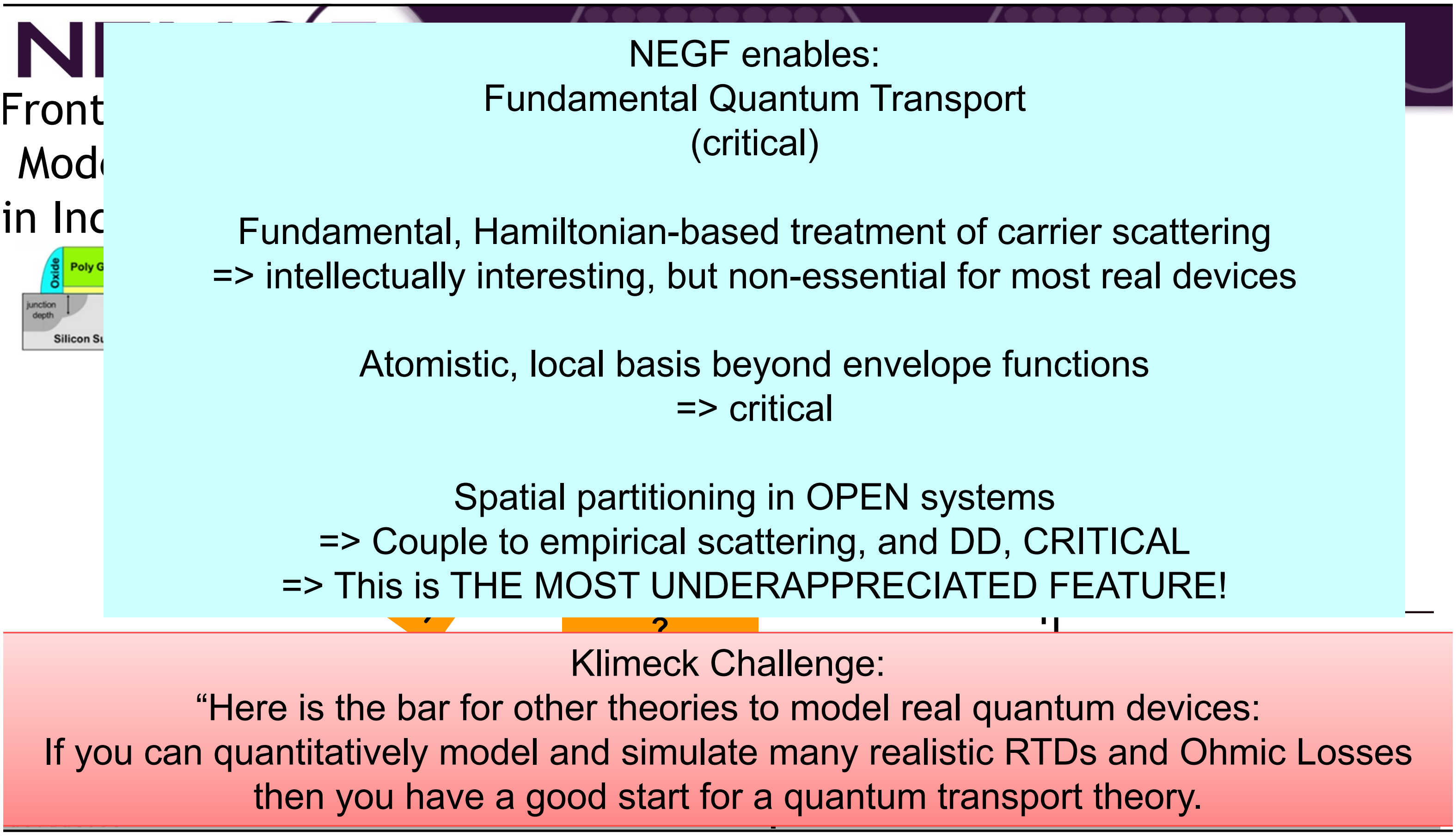
Drift / Diffusion

Boltzmann Transport

Non-Equilibrium Green Functions

?

Unified model



NEGF enables:
Fundamental Quantum Transport
(critical)

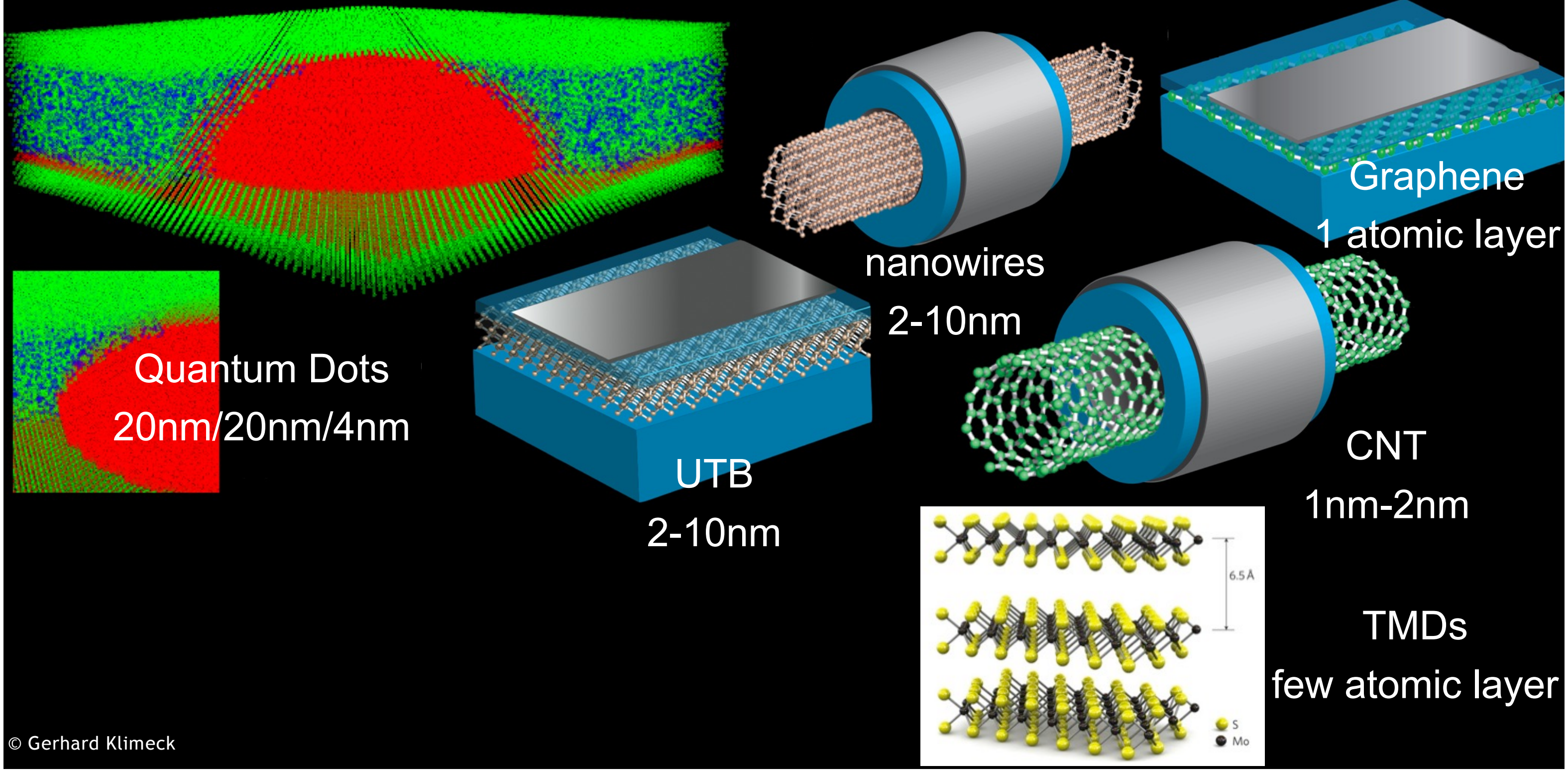
Fundamental, Hamiltonian-based treatment of carrier scattering
=> intellectually interesting, but non-essential for most real devices

Atomistic, local basis beyond envelope functions
=> critical

Spatial partitioning in OPEN systems
=> Couple to empirical scattering, and DD, CRITICAL
=> This is THE MOST UNDERAPPRECIATED FEATURE!

Klimeck Challenge:
“Here is the bar for other theories to model real quantum devices:
If you can quantitatively model and simulate many realistic RTDs and Ohmic Losses
then you have a good start for a quantum transport theory.

Modelling goals shared beyond specific devices



Quantum Dots
20nm/20nm/4nm

UTB
2-10nm

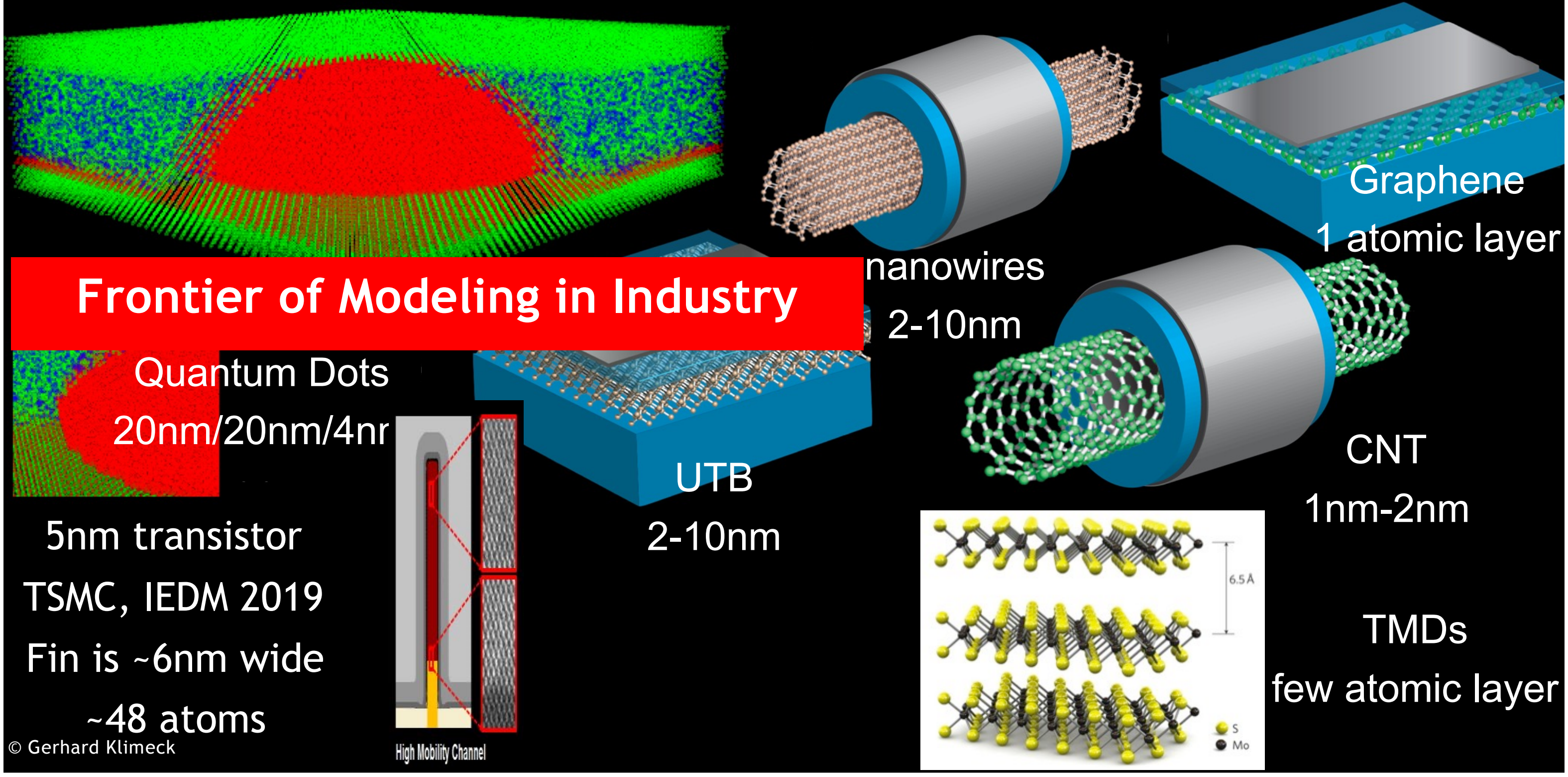
nanowires
2-10nm

Graphene
1 atomic layer

CNT
1nm-2nm

TMDs
few atomic layer

Modelling goals shared beyond specific devices



Frontier of Modeling in Industry

Quantum Dots
20nm/20nm/4nr

5nm transistor
TSMC, IEDM 2019
Fin is ~6nm wide
~48 atoms

UTB
2-10nm

nanowires
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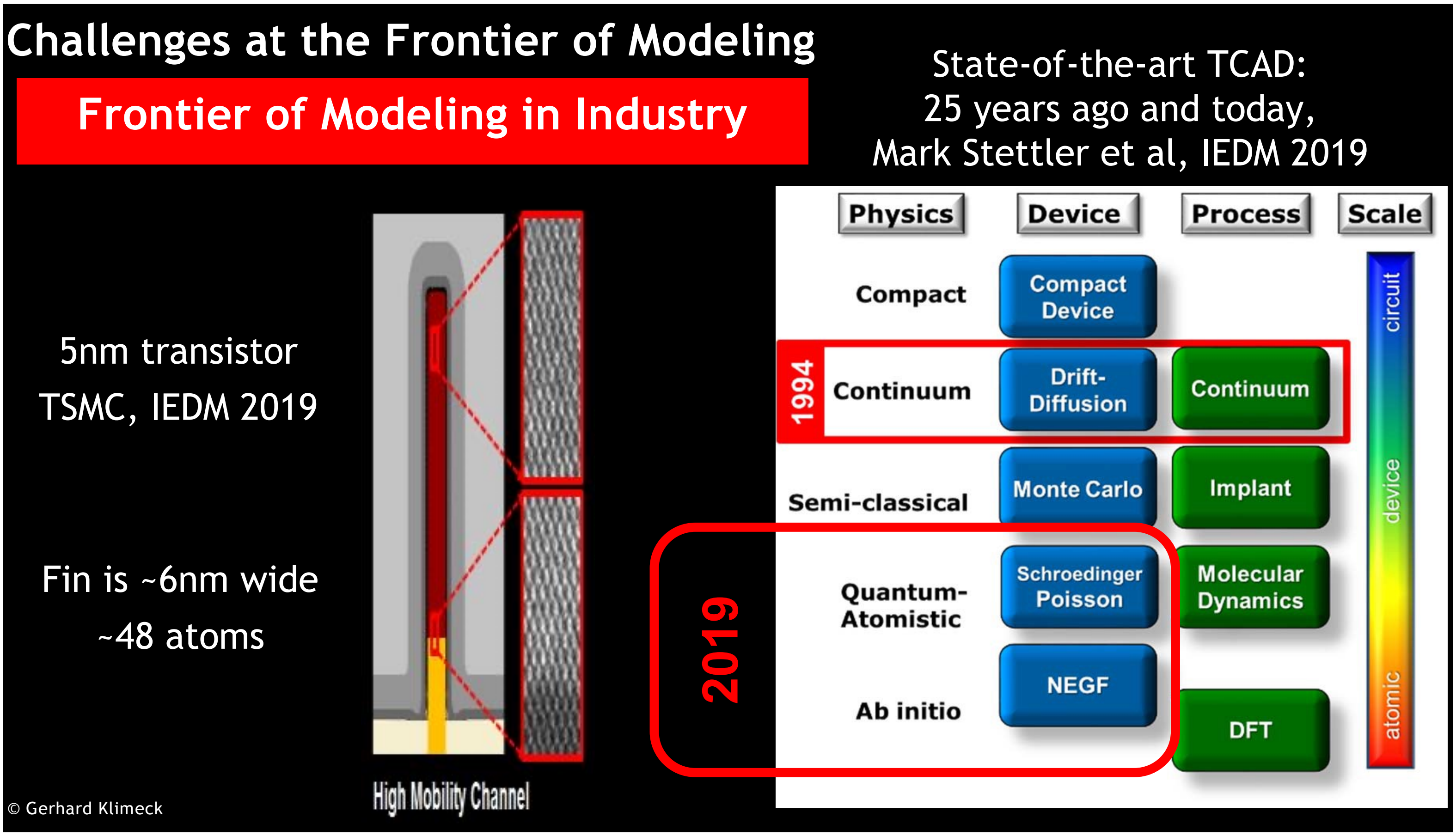


Challenges at the Frontier of Modeling

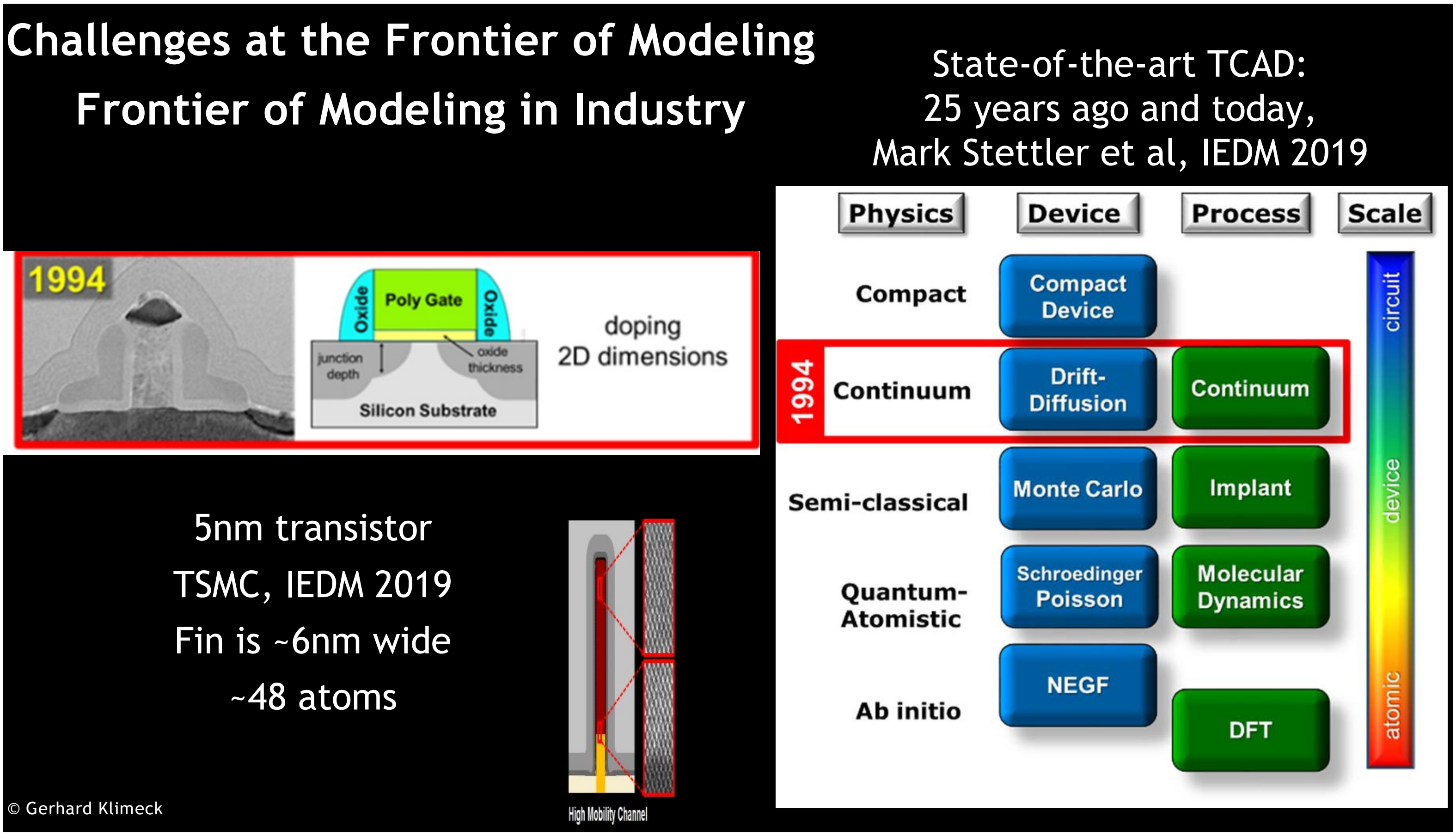
Frontier of Modeling in Industry

5nm transistor
TSMC, IEDM 2019

Fin is ~6nm wide
~48 atoms

State-of-the-art TCAD:
25 years ago and today,
Mark Stettler et al, IEDM 2019

Physics	Device	Process	Scale
Compact	Compact Device		circuit
1994 Continuum	Drift-Diffusion	Continuum	
Semi-classical	Monte Carlo	Implant	device
2019 Quantum-Atomistic	Schroedinger Poisson	Molecular Dynamics	
Ab initio	NEGF	DFT	atomic



Challenges at the Frontier of Modeling

Frontier of Modeling in Industry

doping
2D dimensions

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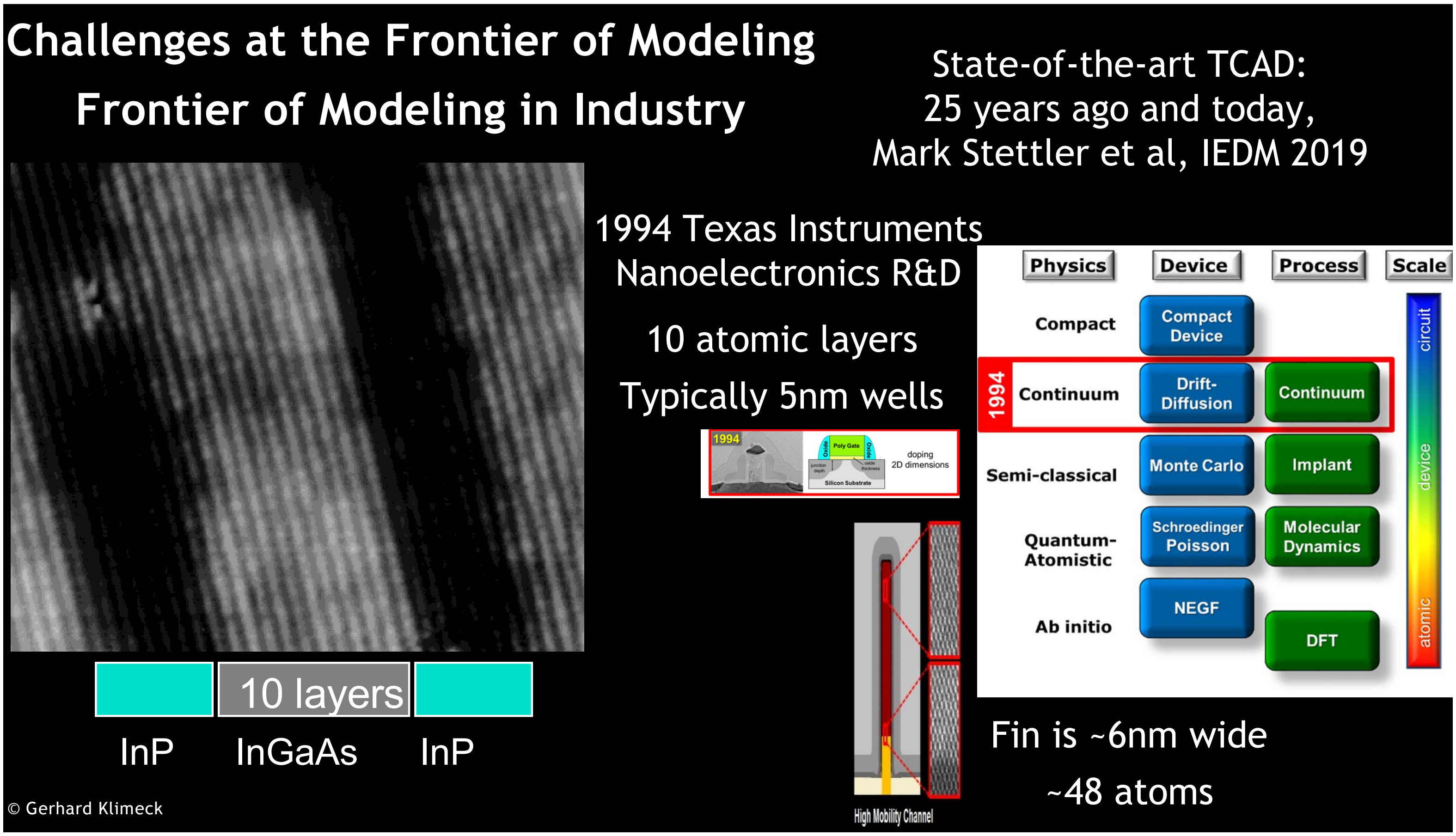

Challenges at the Frontier of Modeling

Frontier of Modeling in Industry

State-of-the-art TCAD:
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1994 Texas Instruments
Nanoelectronics R&D

10 atomic layers

Typically 5nm wells

Physics		Device	Process
Compact		Compact Device	
Continuum	1994	Drift-Diffusion	Continuum
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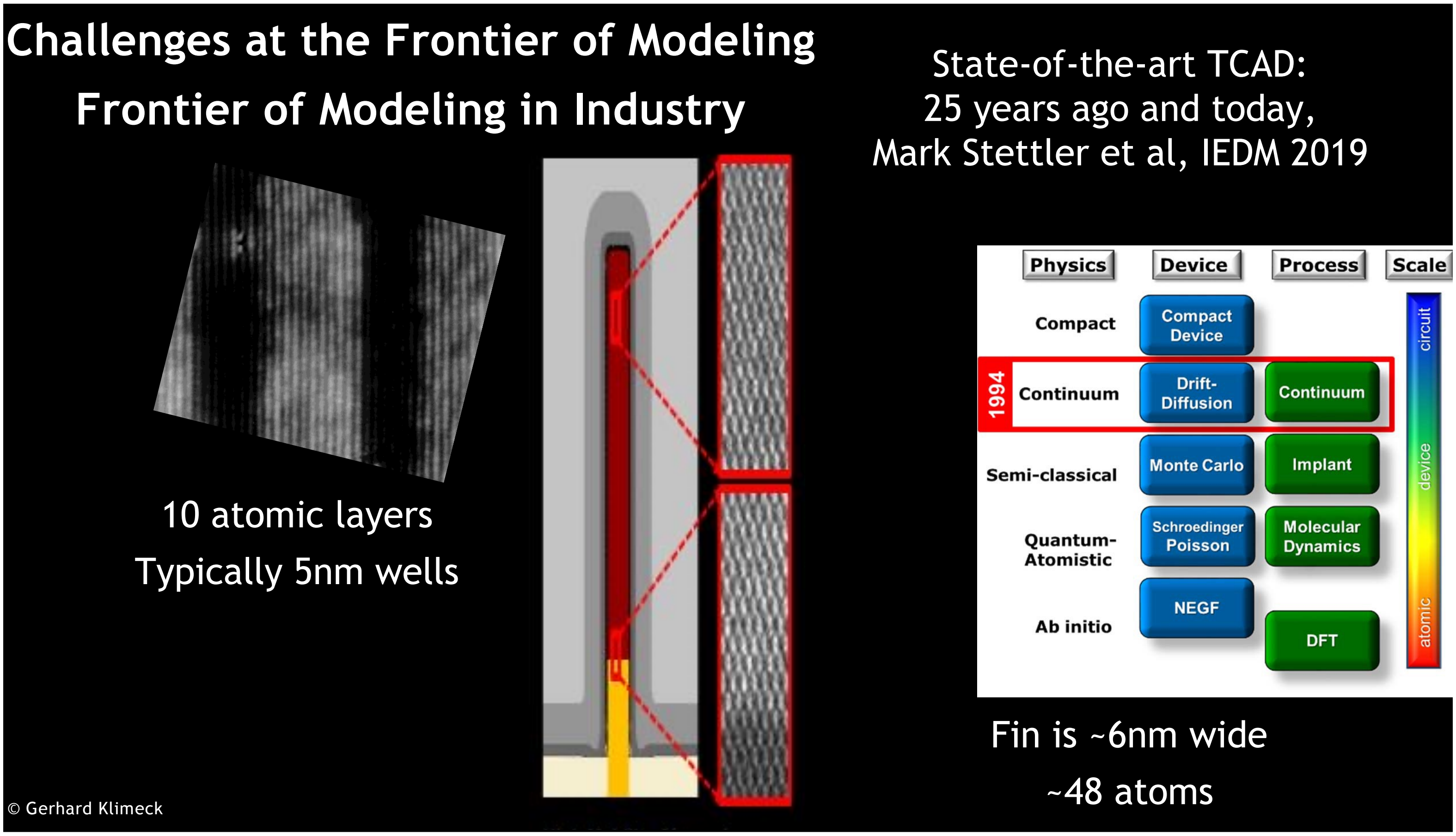
Scale

Fin is ~6nm wide

~48 atoms



Challenges at the Frontier of Modeling

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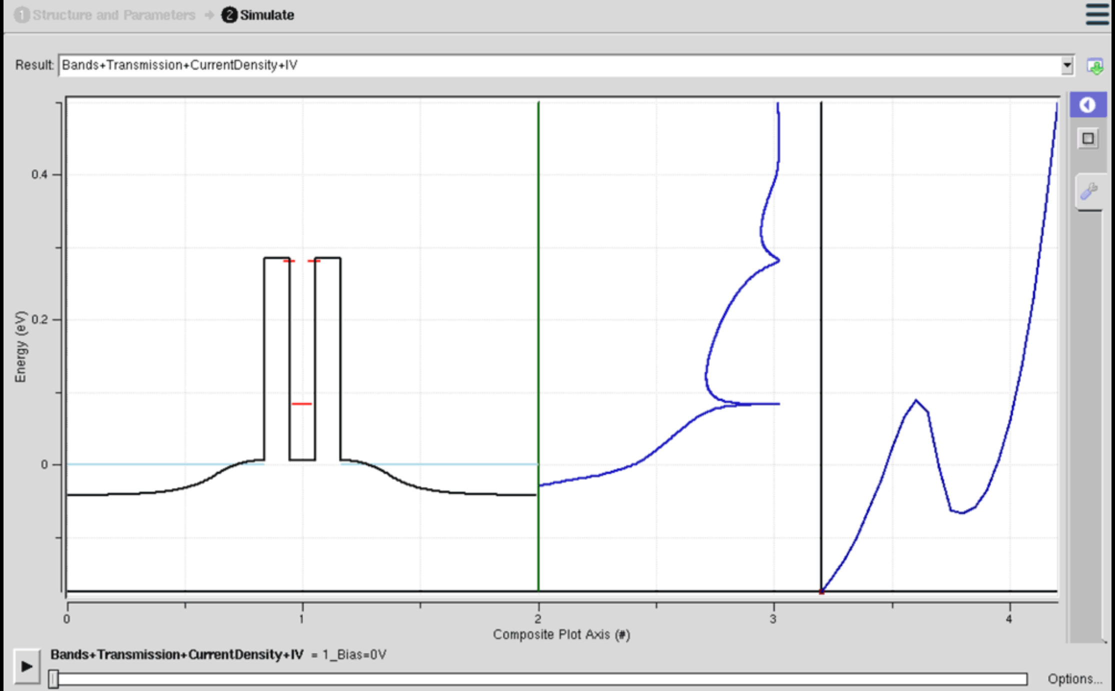
Frontier of Modeling in Industry
1994

A Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD
nanohub.org/tools/rtdnegf



Result: Bands+Transmission+CurrentDensity+IV

Bands+Transmission+CurrentDensity+IV = 1_Bias=0V

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Texas Instruments UTD

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Frontier of Modeling in Industry

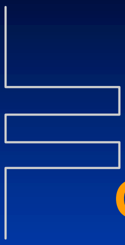
A Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD

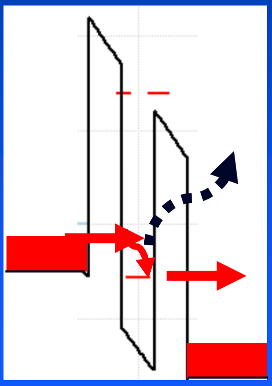
WHOLE field was convinced: valley current due to SCATTERING inside the RTD

WRONG!

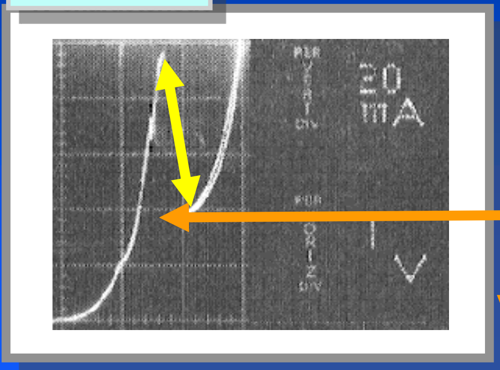
Wrong Basis Set & Contacts

20 nm	GaAs	$N_D = 2\ 10^{18}\ cm^{-3}$
200 nm	GaAs	$N_D = 2\ 10^{15}\ cm^{-3}$
18 nm	GaAs	
5 nm	$Al_{0.4}Ga_{0.6}As$	
5 nm	GaAs	
5 nm	$Al_{0.4}Ga_{0.6}As$	
18 nm	GaAs	
200 nm	GaAs	$N_D = 2\ 10^{15}\ cm^{-3}$
20 nm	GaAs	$N_D = 2\ 10^{18}\ cm^{-3}$





Experimental IV characteristic



Goals

Increase
Peak/Valley R
>1,000
Typically 3

Reduce
Valley Current
(Leakage)

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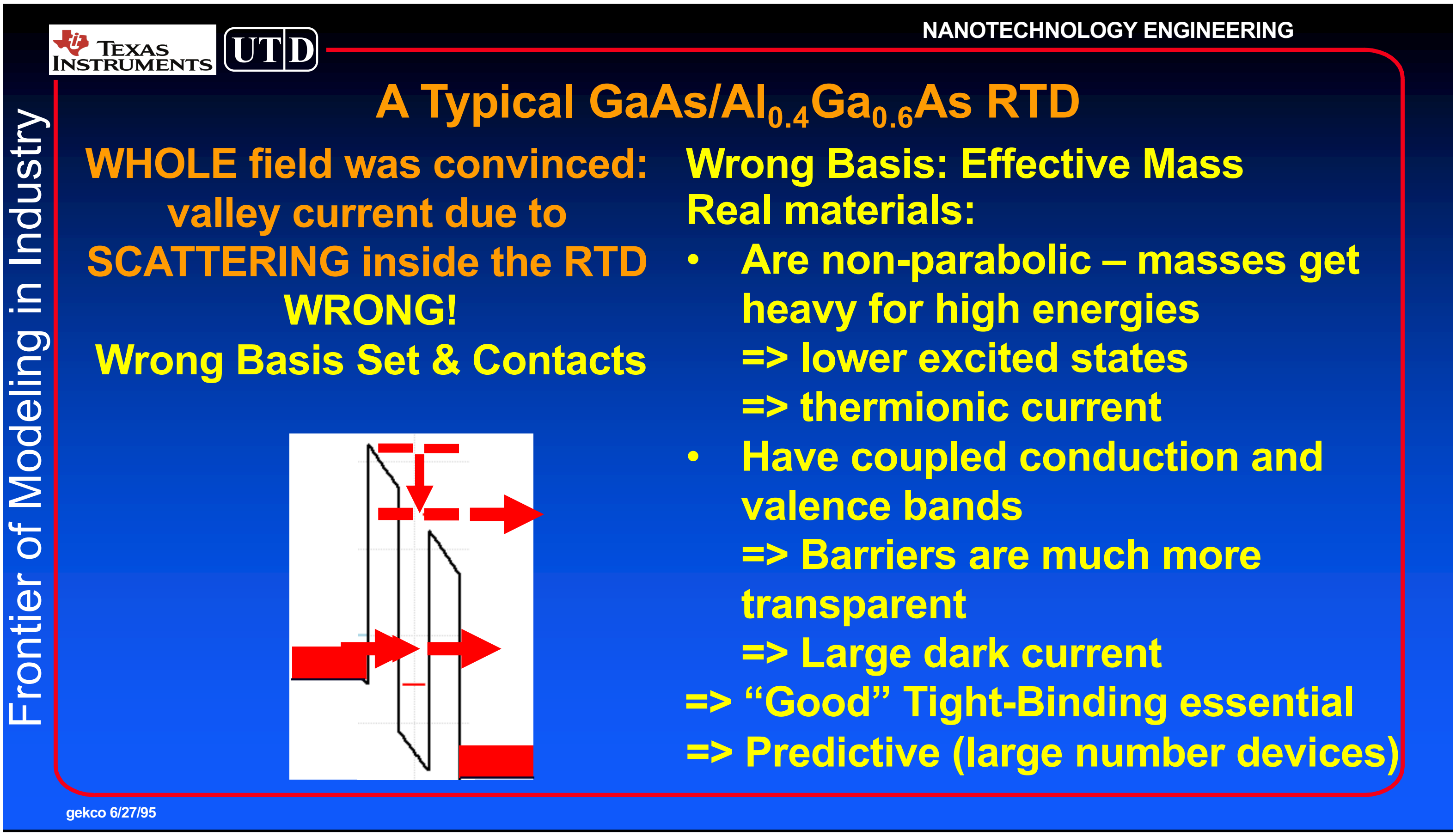

NANOTECHNOLOGY ENGINEERING

Frontier of Modeling in Industry

A Typical GaAs/Al$_{0.4}$Ga$_{0.6}$As RTD

WHOLE field was convinced:
valley current due to
SCATTERING inside the RTD
WRONG!
Wrong Basis Set & Contacts

Wrong Basis: Effective Mass
Real materials:

- Are non-parabolic – masses get heavy for high energies
  => lower excited states
  => thermionic current
- Have coupled conduction and valence bands
  => Barriers are much more transparent
  => Large dark current

=> “Good” Tight-Binding essential
=> Predictive (large number devices)

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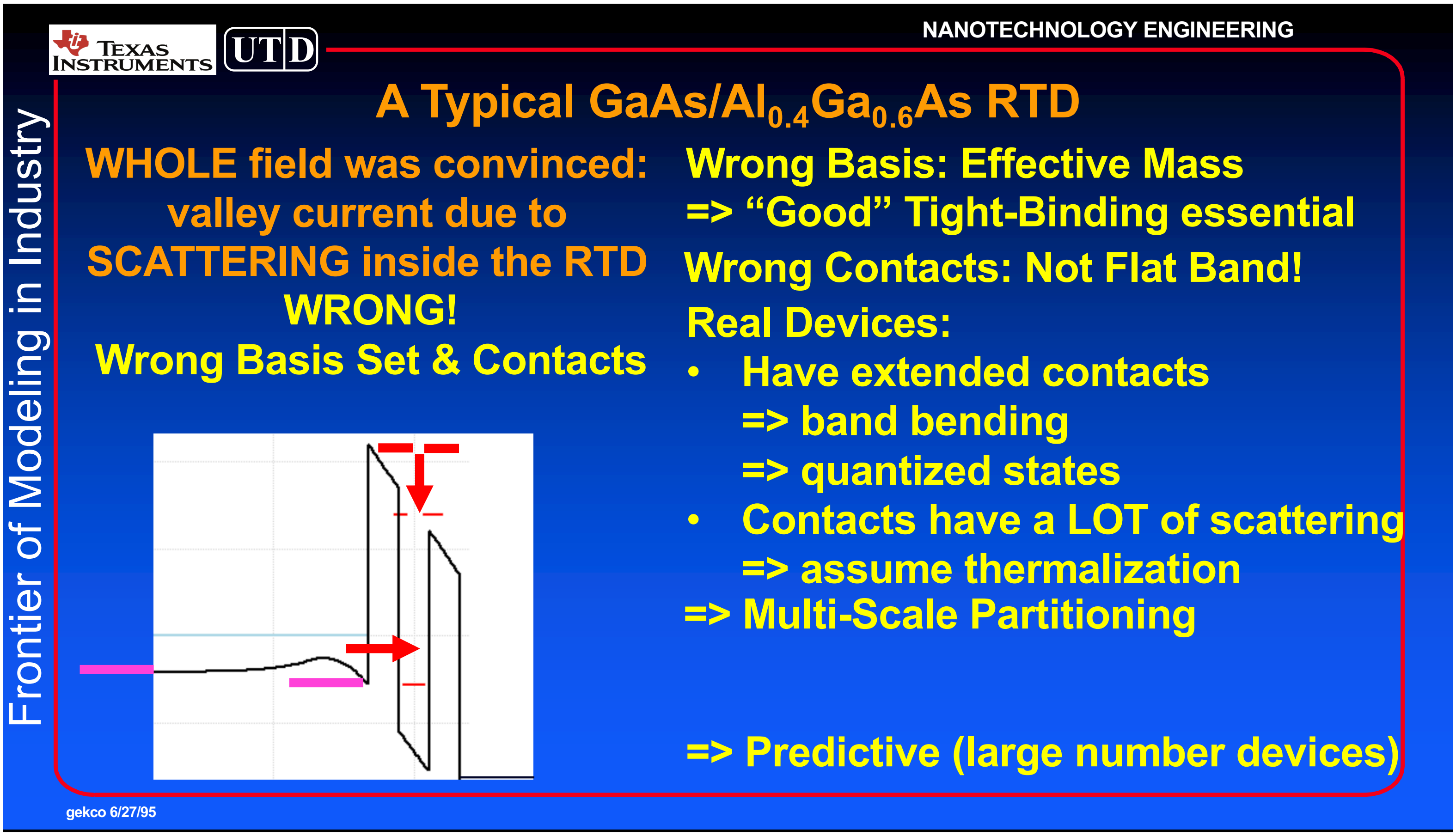

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Wrong Basis Set & Contacts

Wrong Basis: Effective Mass
=> “Good” Tight-Binding essential
Wrong Contacts: Not Flat Band!
Real Devices:

- Have extended contacts
  => band bending
  => quantized states
- Contacts have a LOT of scattering
  => assume thermalization

=> Multi-Scale Partitioning

=> Predictive (large number devices)

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A Typical GaAs/Al$_{0.4}$Ga$_{0.6}$As RTD

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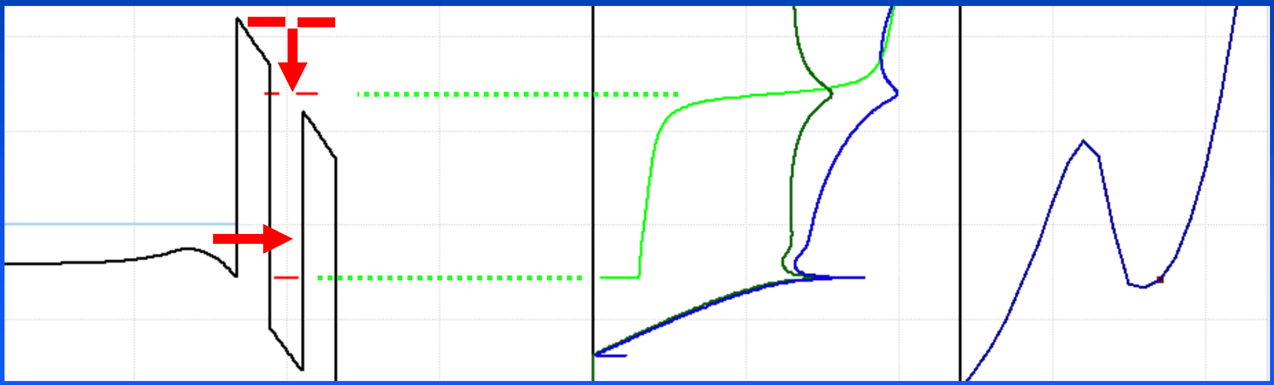

A Typical GaAs/Al$_{0.4}$Ga$_{0.6}$As RTD

15 nm Device?

20 nm GaAs $N_D = 2\ 10^{18}$ cm^{-3}
200 nm GaAs $N_D = 2\ 10^{15}$ cm^{-3}
18 nm GaAs
5 nm Al$_{0.4}$Ga$_{0.6}$As
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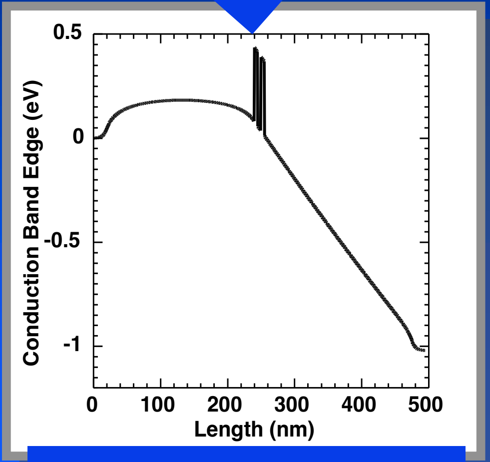
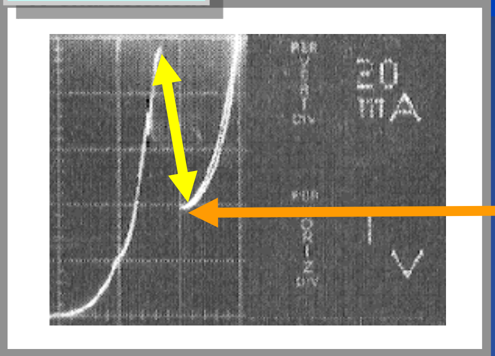


500 nm Device?

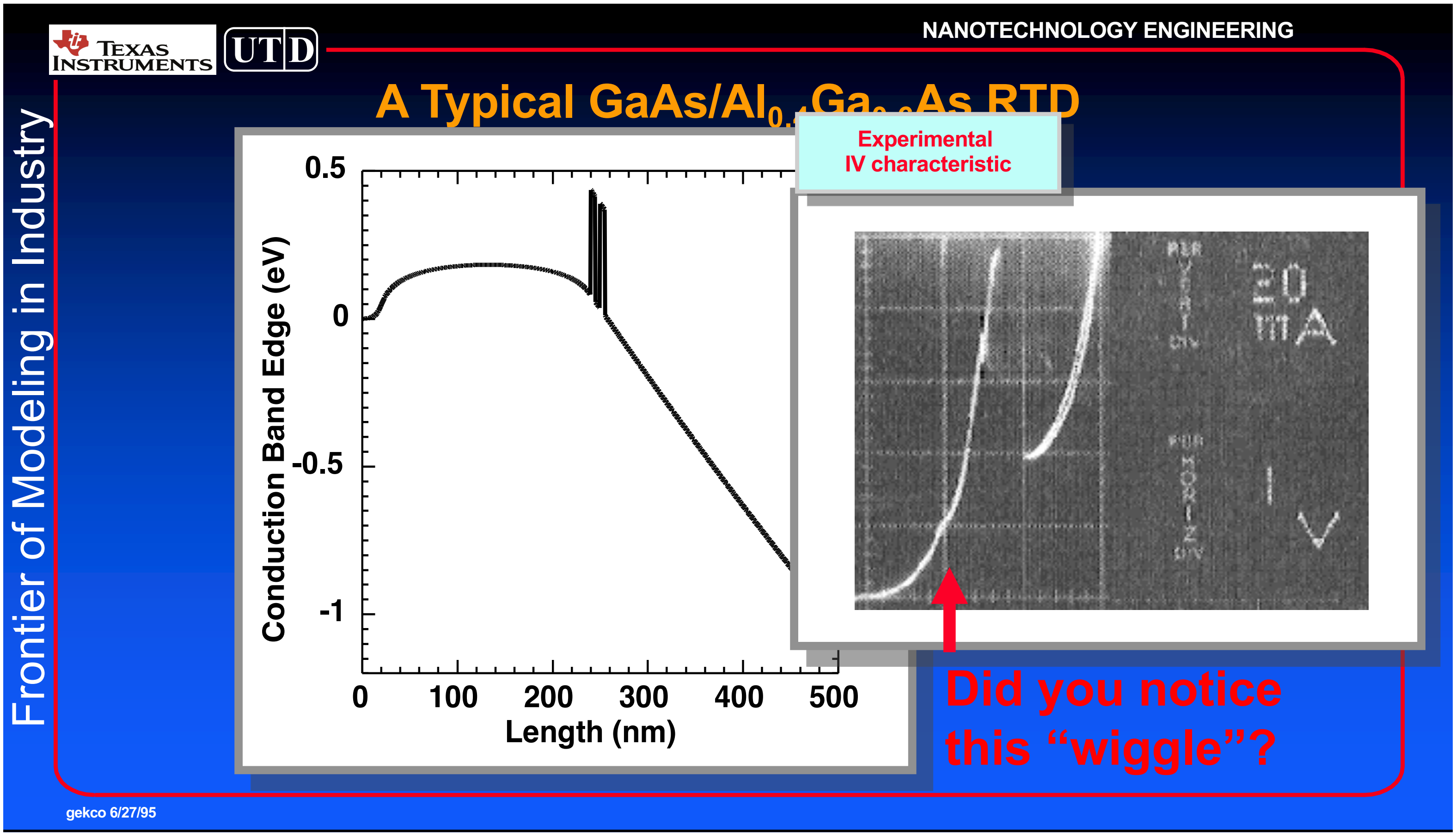
Experimental
IV characteristic



Goals

Increase
Peak/Valley R
>1,000
Typically 3

Reduce
Valley Current
(Leakage)



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A Typical GaAs/Al$_{0.4}$Ga$_{0.6}$As RTD

Experimental
IV characteristic

Did you notice
this “wiggle”?

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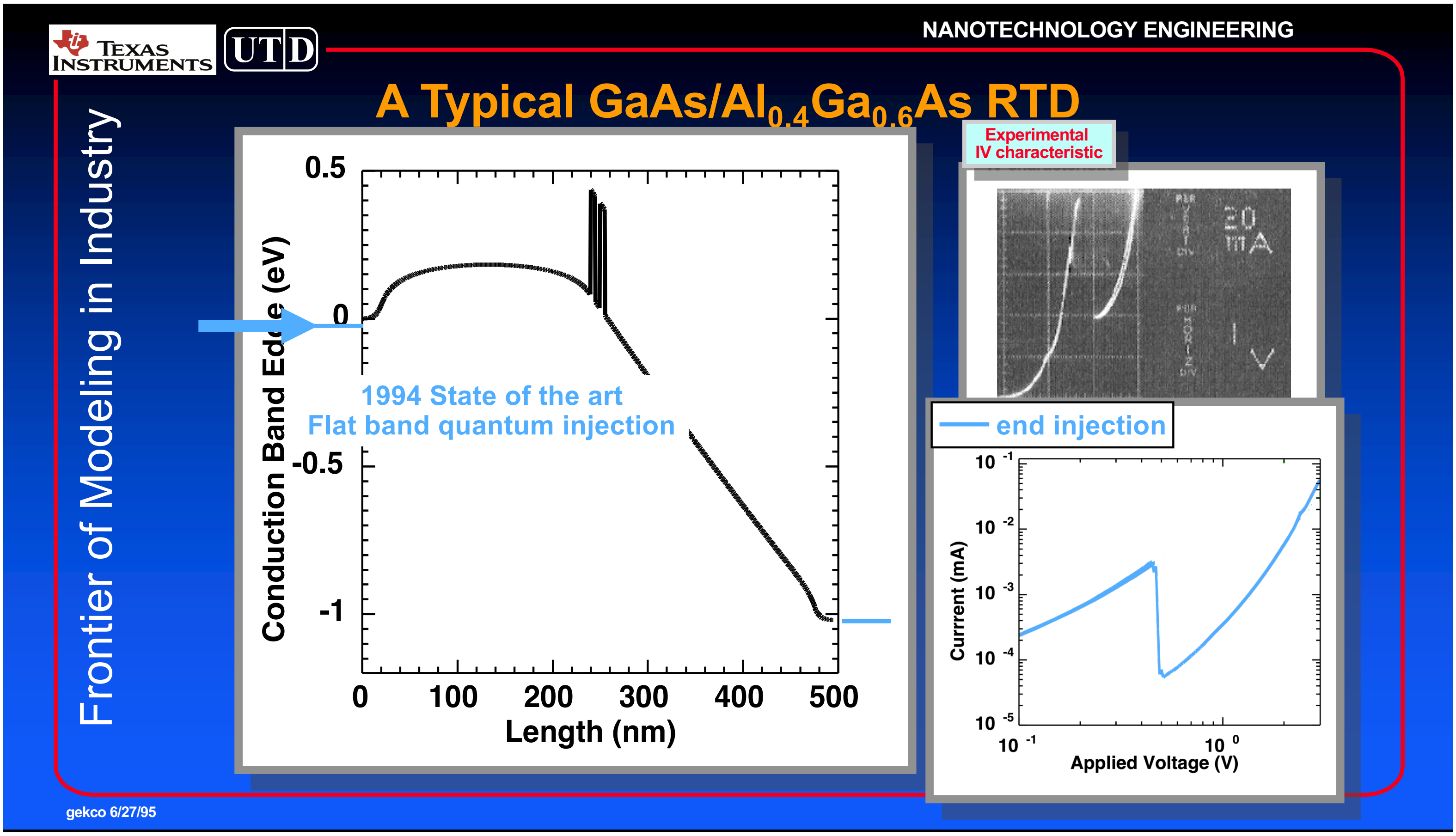

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A Typical GaAs/Al$_{0.4}$Ga$_{0.6}$As RTD

Experimental
IV characteristic

1994 State of the art
Flat band quantum injection

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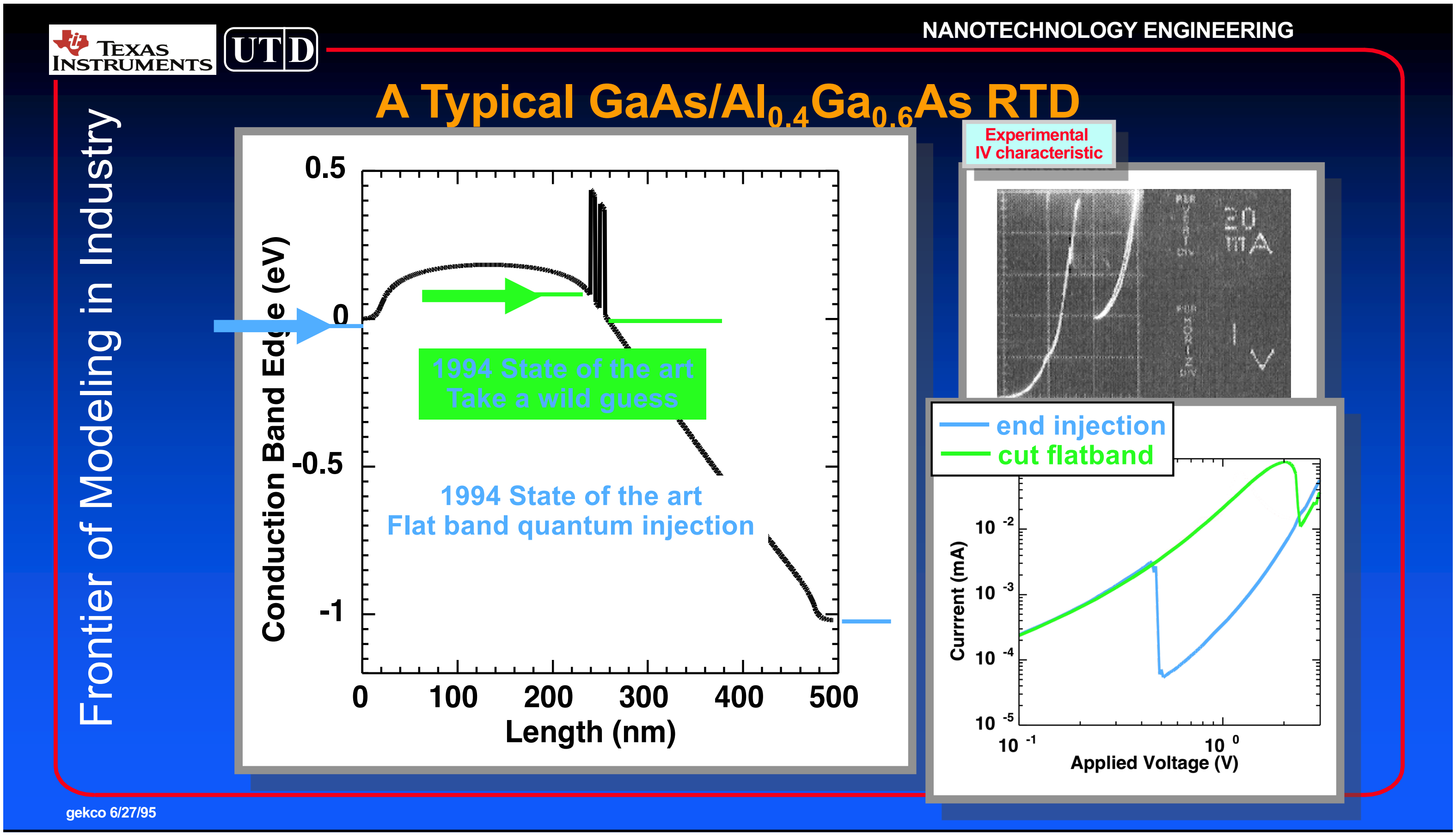

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A Typical GaAs/$Al_{0.4}Ga_{0.6}As$ RTD

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1994 State of the art
Take a wild guess

1994 State of the art
Flat band quantum injection

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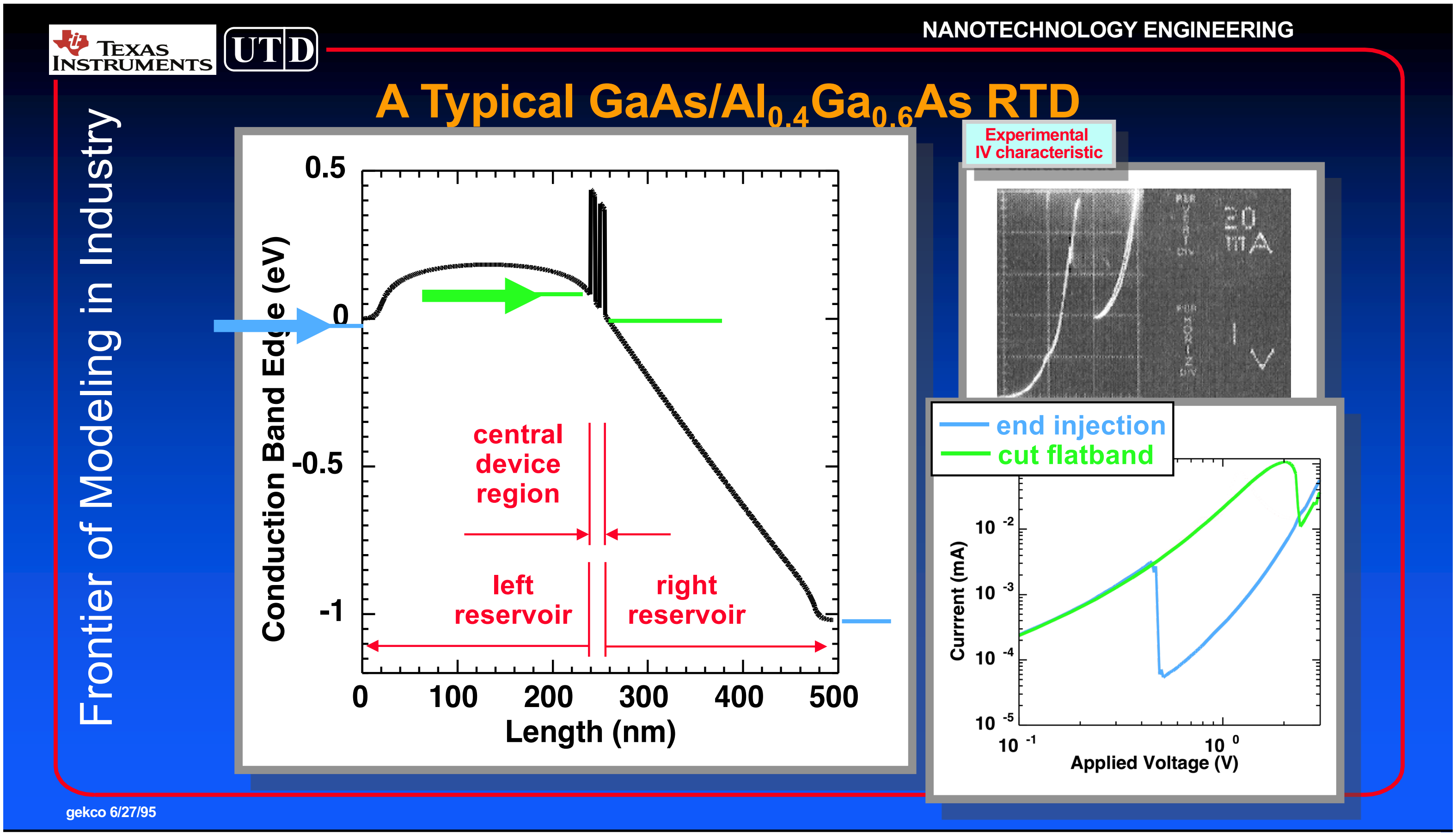

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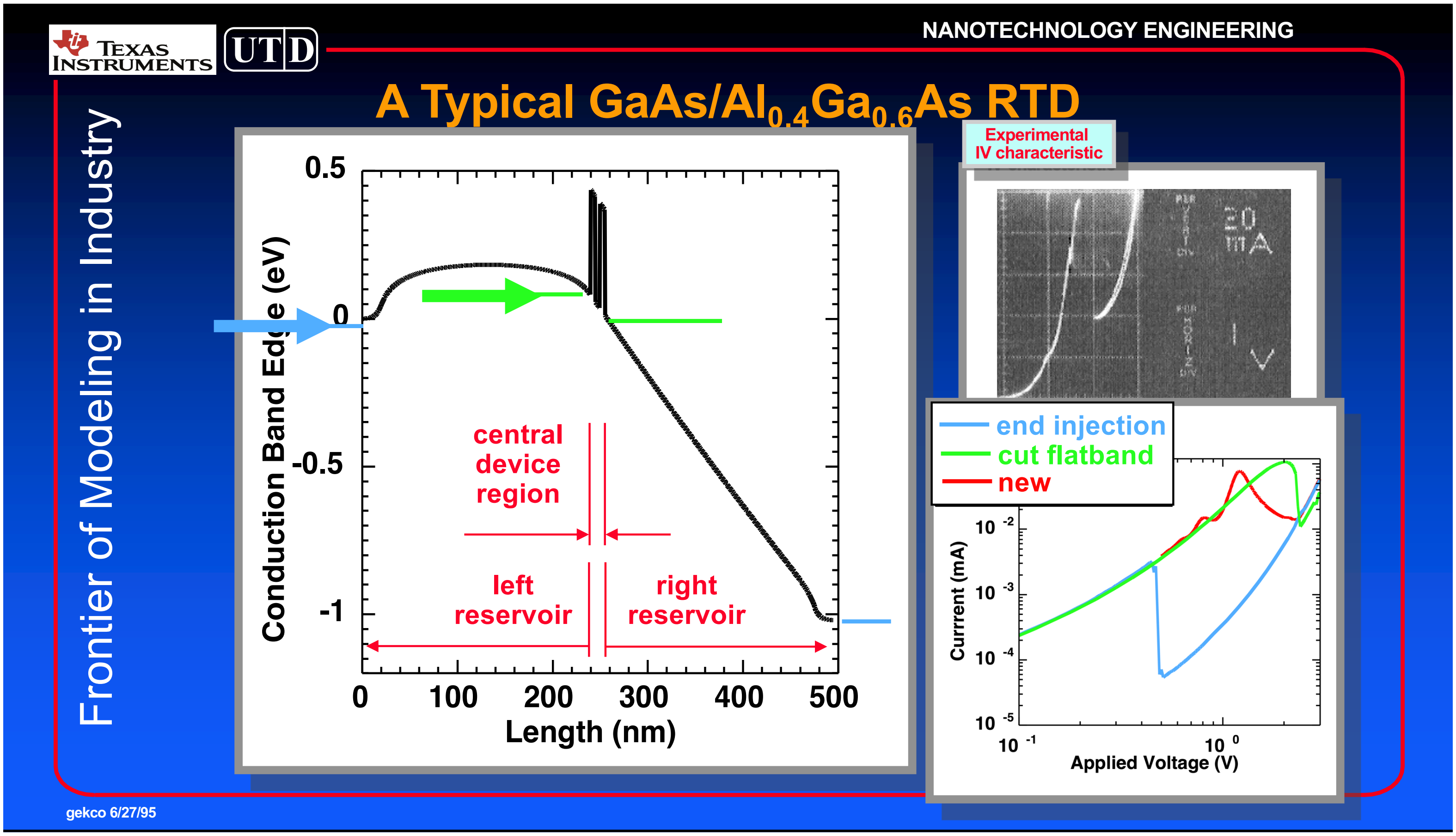

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Frontier of Modeling in Industry

Experimental IV characteristic

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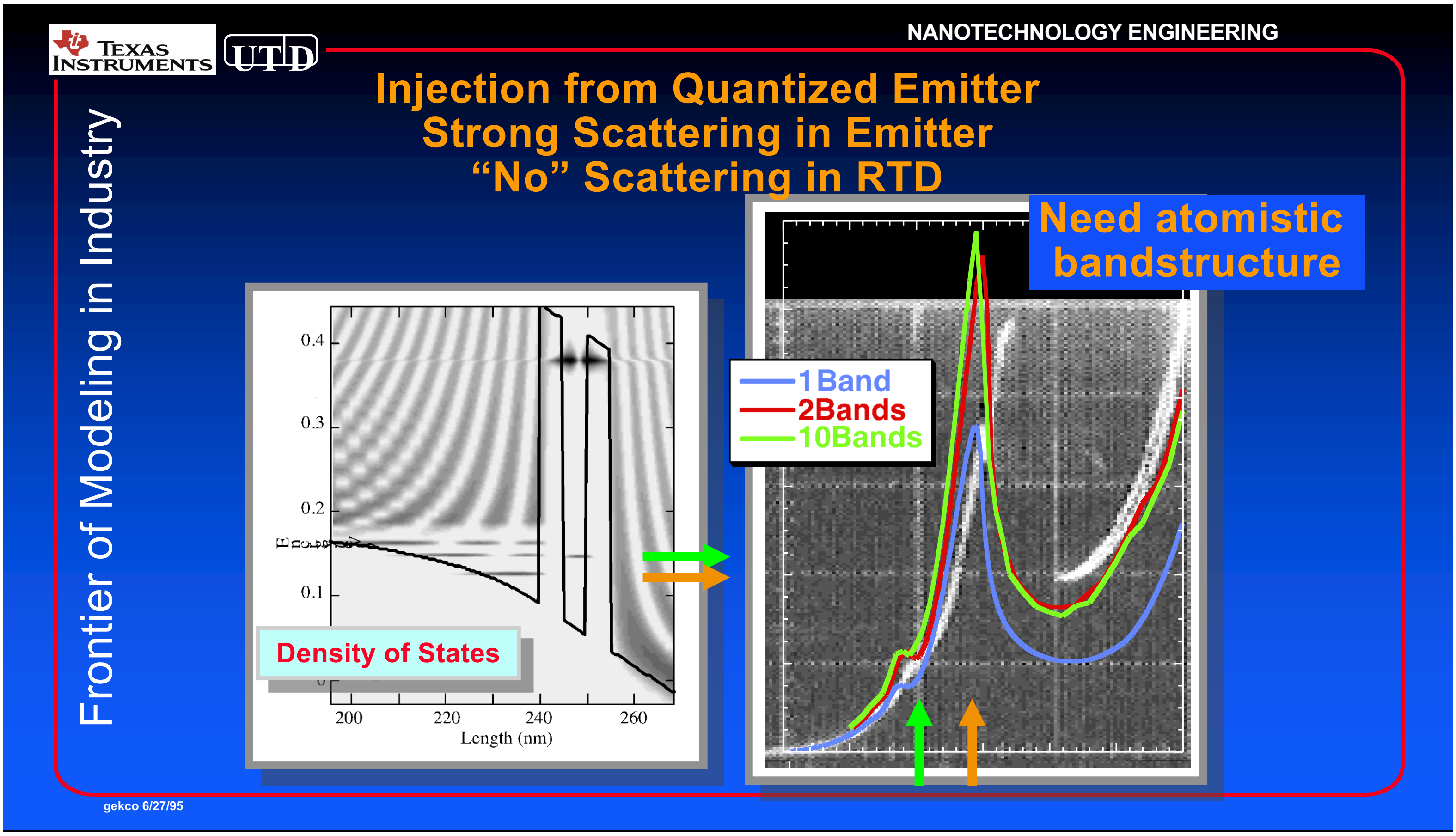

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Injection from Quantized Emitter
Strong Scattering in Emitter
“No” Scattering in RTD

Frontier of Modeling in Industry

Need atomistic bandstructure

Density of States

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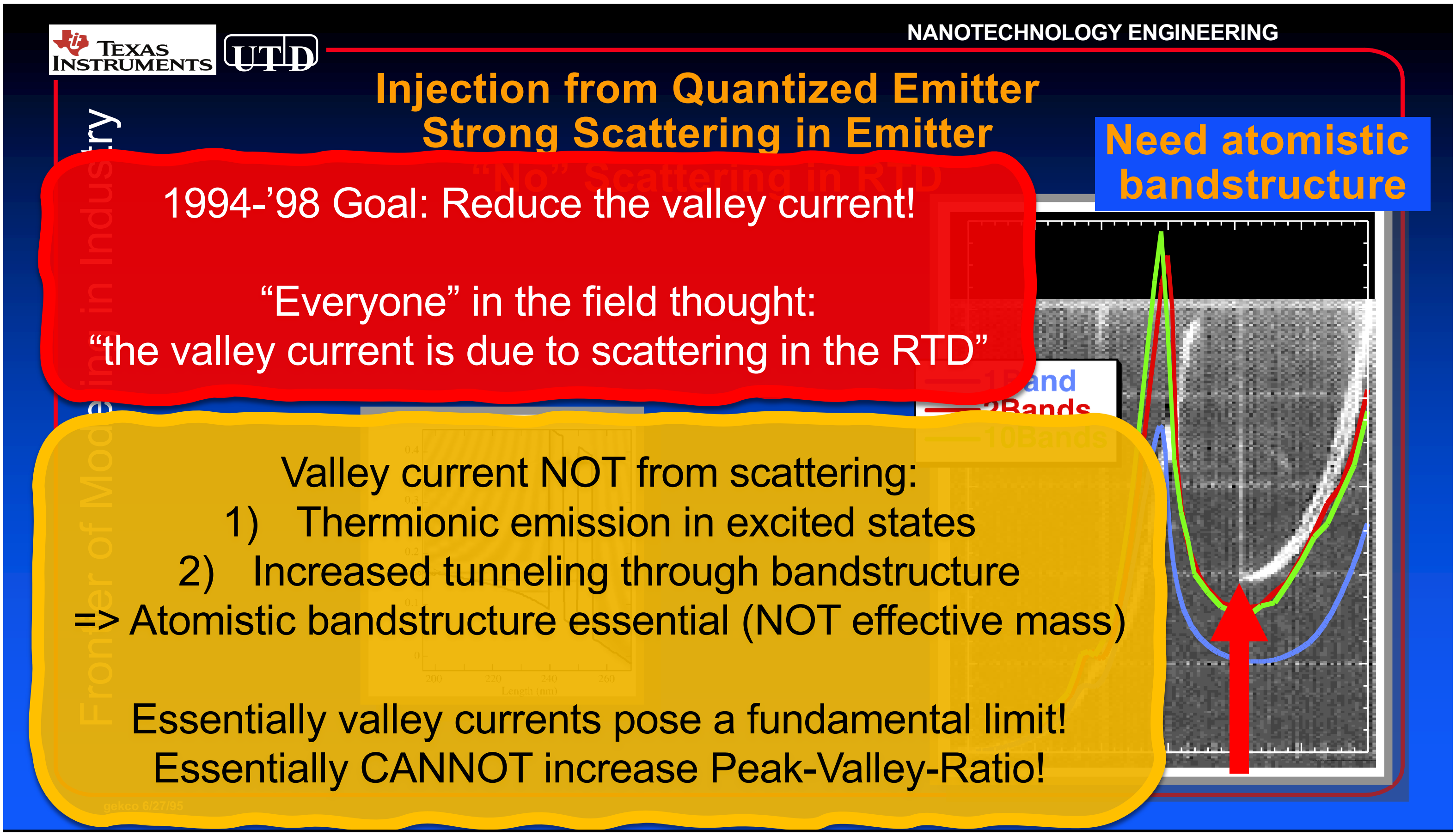

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Injection from Quantized Emitter
Strong Scattering in Emitter
"No" Scattering in RTD

Need atomistic bandstructure

1994-'98 Goal: Reduce the valley current!

"Everyone" in the field thought:
"the valley current is due to scattering in the RTD"

Valley current NOT from scattering:
1) Thermionic emission in excited states
2) Increased tunneling through bandstructure
=> Atomistic bandstructure essential (NOT effective mass)

Essentially valley currents pose a fundamental limit!
Essentially CANNOT increase Peak-Valley-Ratio!

Frontier of Modeling in Industry

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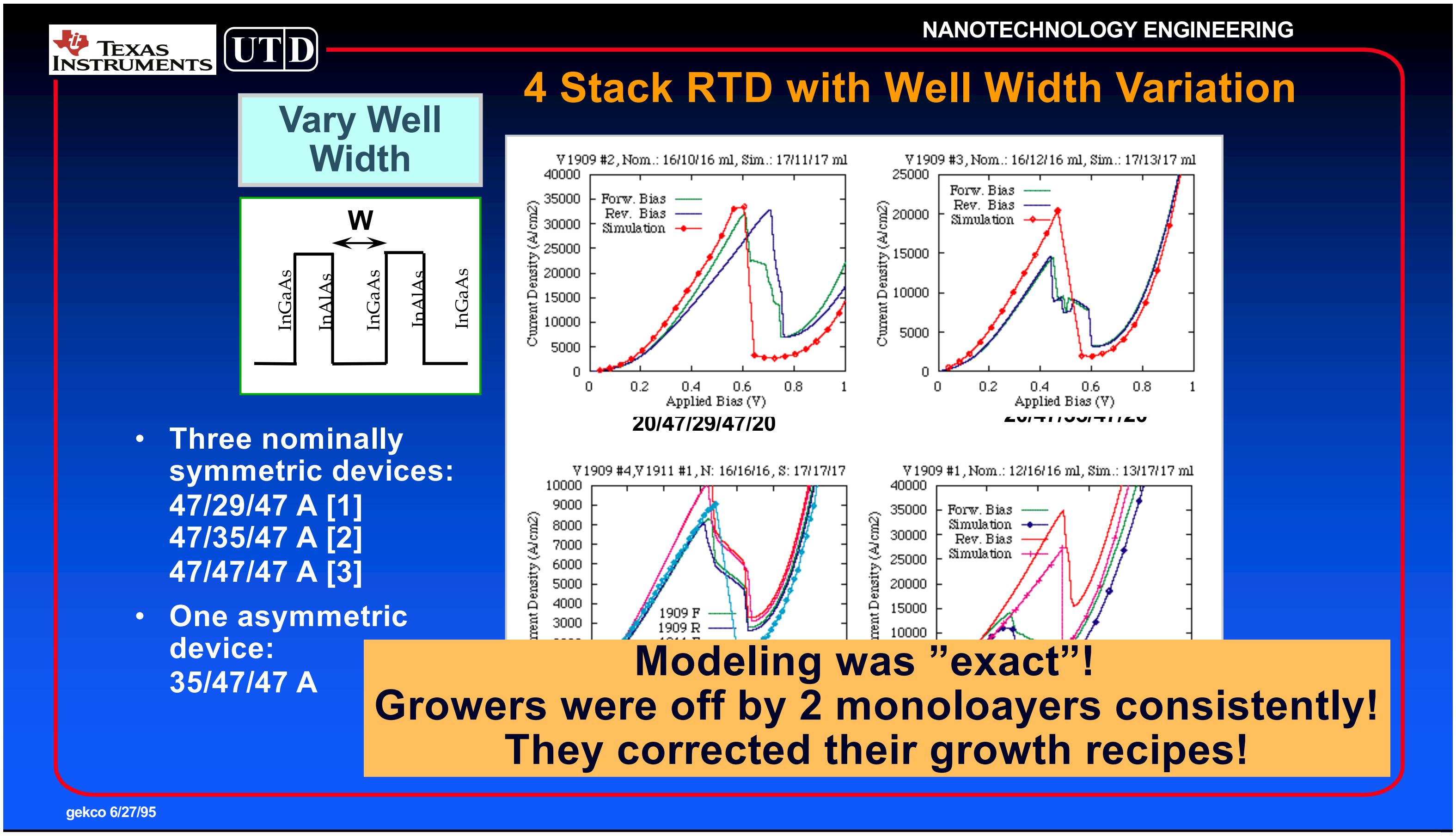

NANOTECHNOLOGY ENGINEERING

4 Stack RTD with Well Width Variation

Vary Well Width

20/47/29/47/20

- **Three nominally symmetric devices:**
  47/29/47 A [1]
  47/35/47 A [2]
  47/47/47 A [3]
- **One asymmetric device:**
  35/47/47 A

Modeling was "exact"!
Growers were off by 2 monoloayers consistently!
They corrected their growth recipes!

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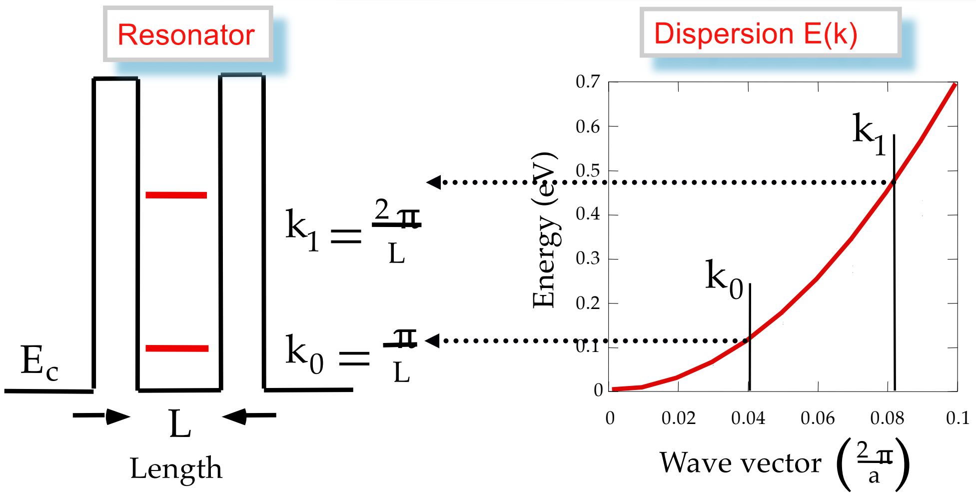
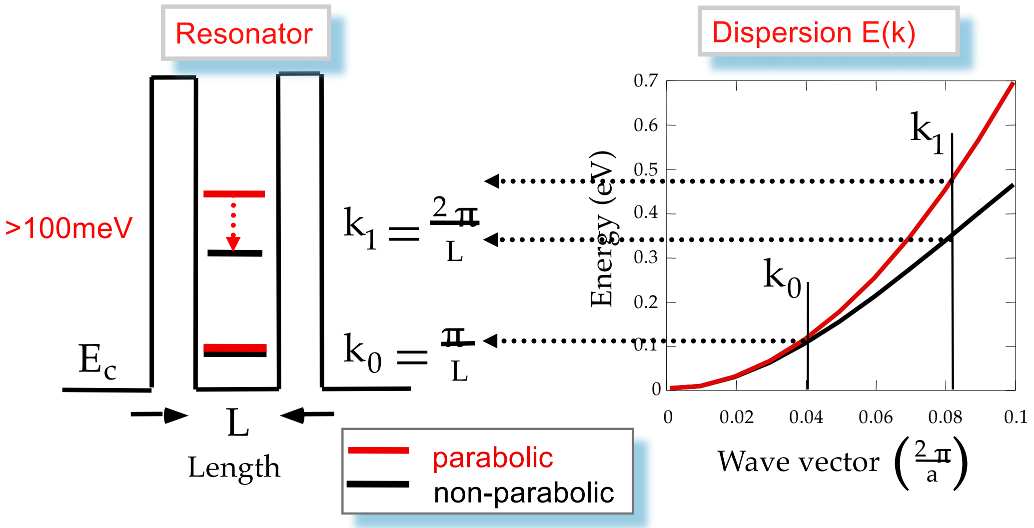
Resonator State Quantization

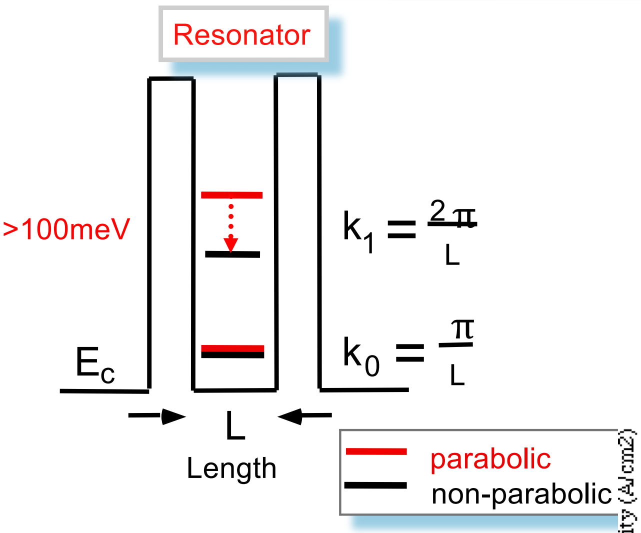


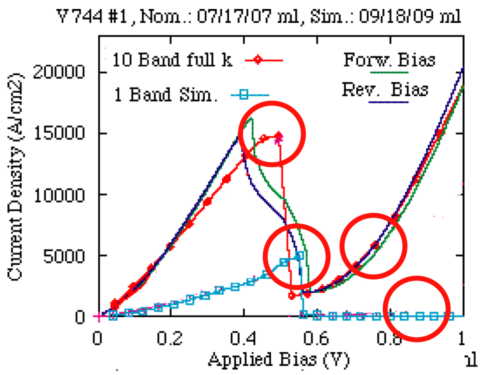
Resonator State Quantization
Effects of Band Non-Parabolicity

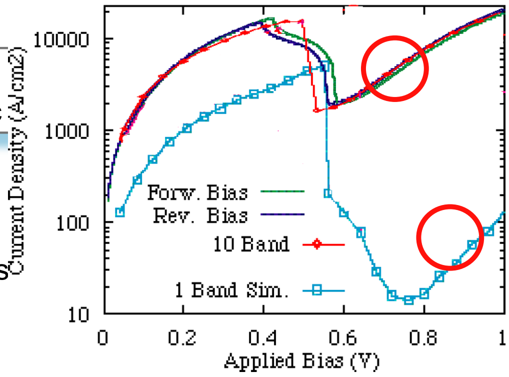


- Second state lowered by >100mev ~ 4kT

Effects of Band Non-Parabolicity on I-V Characteristics

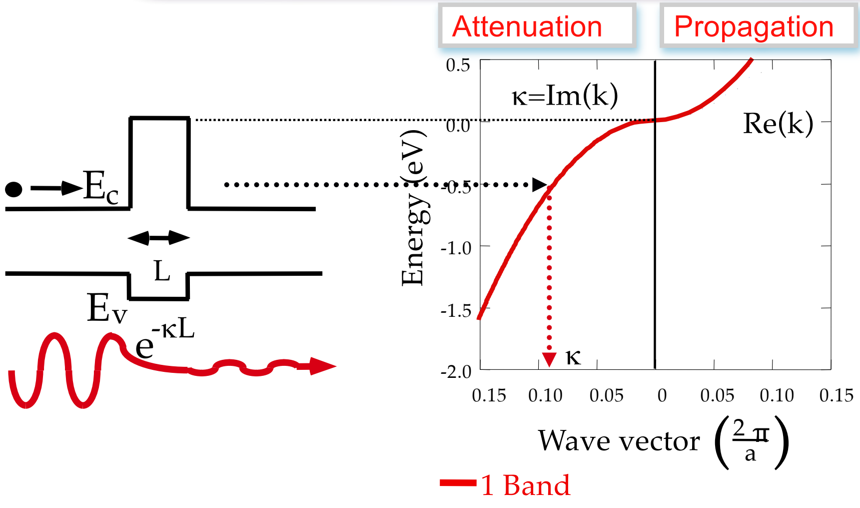




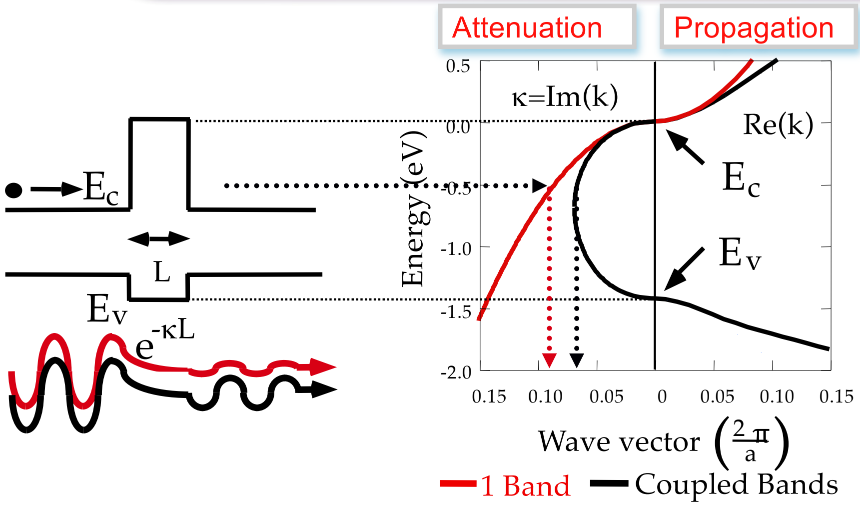


- Second state lowered by >100mev ~ 4kT
- Second diode turn-on at lower voltages
- Valley current mostly due to thermal excitations
- k_0 about equal - Why is peak current different?

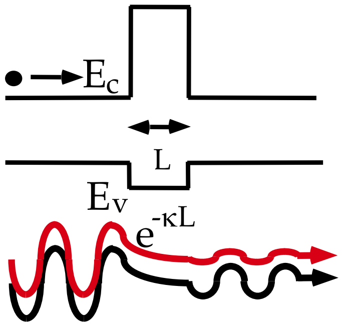
Wave Attenuation in Barriers Single Parabolic Band

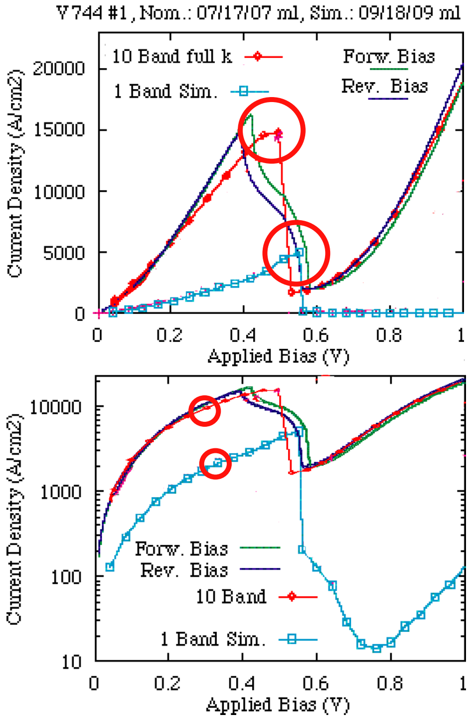


Wave Attenuation in Barriers
Coupled Bands



Band Warping in Barriers
Impact on I-V Characteristics





Non-Parabolicity:

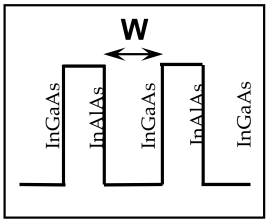
- Second state lowered by >100mev ~ 4kT
- Second diode turn-on at lower voltages
- Valley current mostly due to thermal excitations

Complex Band Coupling:

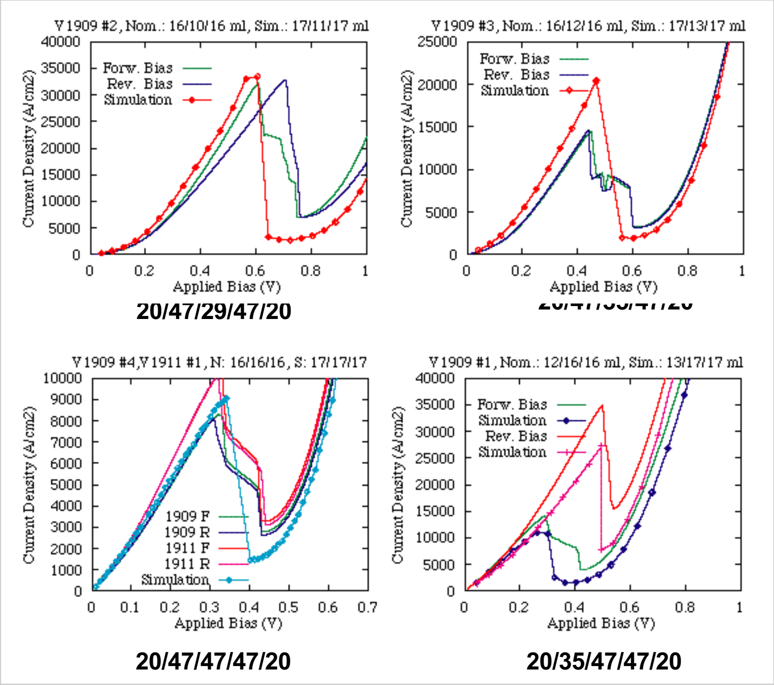
- RTD more transparent - correct peak current

4 Stack RTD with Well Width Variation

Vary Well Width



- Three nominally symmetric devices:
  47/29/47 A [1]
  47/35/47 A [2]
  47/47/47 A [3]
- One asymmetric device:
  35/47/47 A



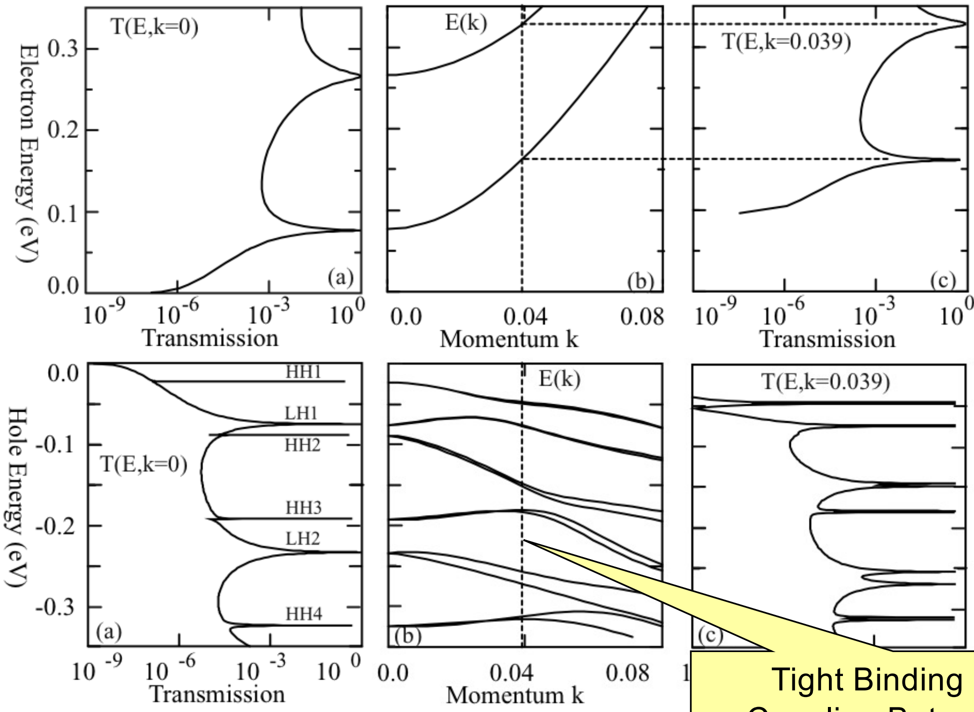
20/47/29/47/20

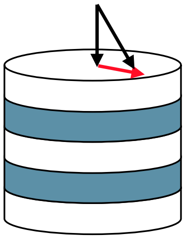
20/47/35/47/20

20/47/47/47/20

20/35/47/47/20

Quantum Transport in non-parabolic, strained, and coupled bands



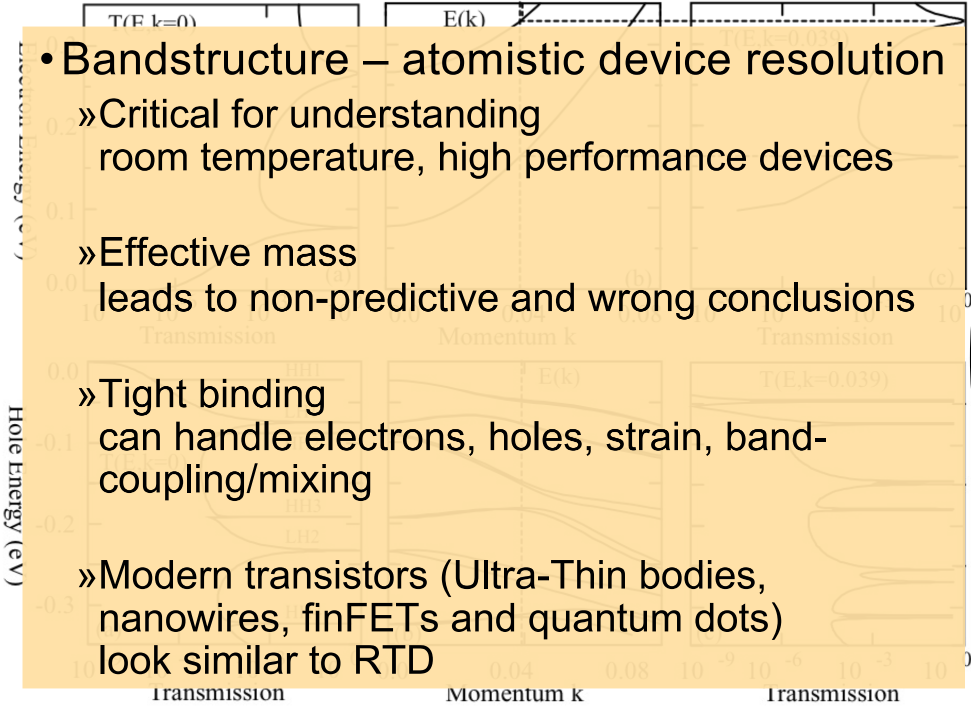


Electron:
- Dispersion looks parabolic, but is NOT
- Transmission looks replicated, but is NOT

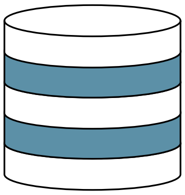
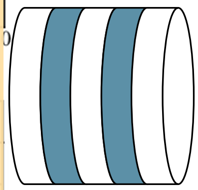
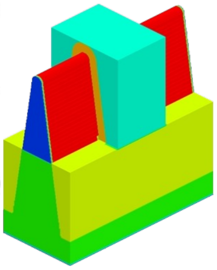
Holes:
- LH, HH, SO coupled
- Dispersion "complicated"
- Transmission

Tight Binding Handles
Coupling Between Bands
Strain, Non-Parabolicity

Quantum Transport in non-parabolic, strained, and coupled bands

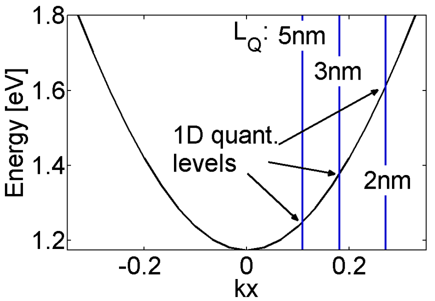


- Bandstructure – atomistic device resolution
  - »Critical for understanding room temperature, high performance devices
  - »Effective mass leads to non-predictive and wrong conclusions
  - »Tight binding can handle electrons, holes, strain, band-coupling/mixing
  - »Modern transistors (Ultra-Thin bodies, nanowires, finFETs and quantum dots) look similar to RTD

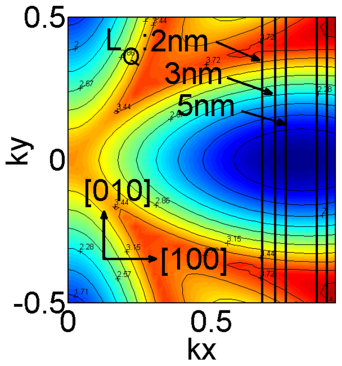
The effect of quantization

$$\left.\begin{array}{ll} E_n = \dfrac{\hbar^2\pi^2}{2m_i L^2} & \text{(2D-quantization)} \\ E = \dfrac{\hbar^2 k^2}{2m_i} & \text{(parabolic mass)} \end{array}\right\} \rightarrow k = \frac{\pi}{L}$$

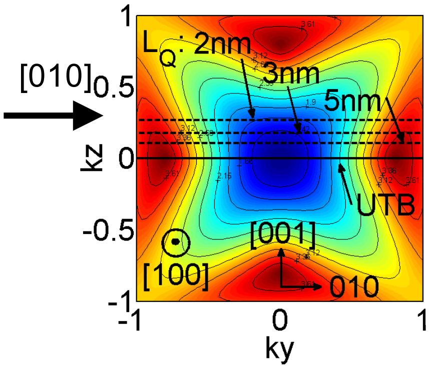


Abhijeet Paul

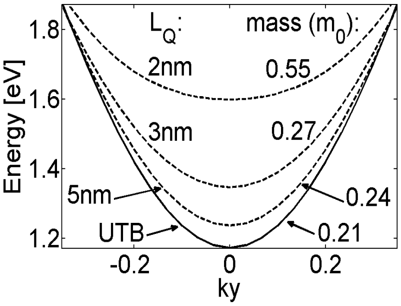
Quantization and Anisotropy

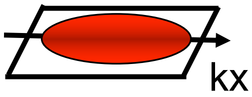


(b)

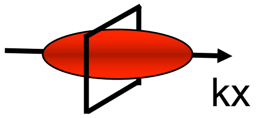


(c)

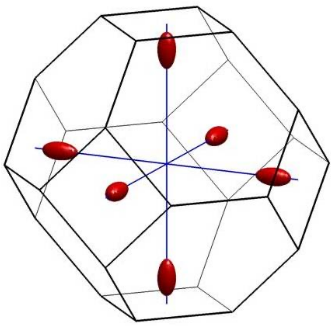




“Cut” through the ellipsoid (x-y plane)

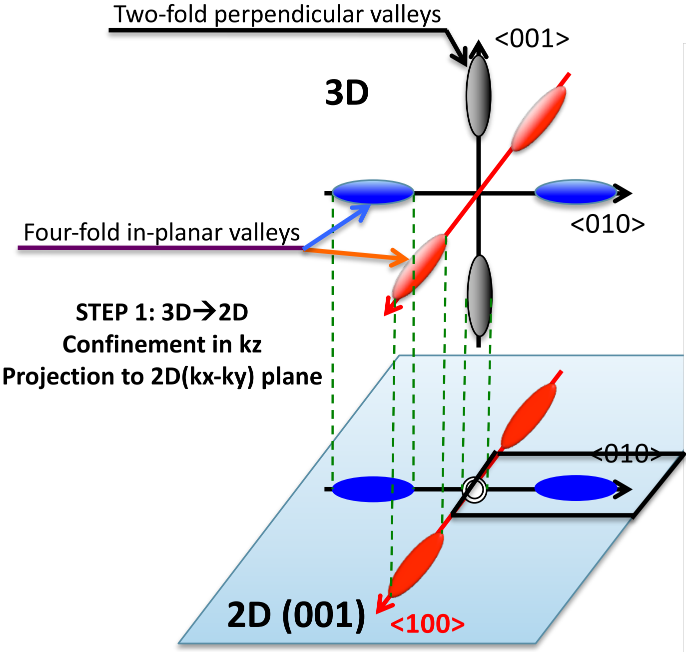


Cut through the 3nm kx line



Band Projection in [100] Si:P Quantum Wells

- 3D→2D→1D projection of Si [100] nanowire



Two-fold perpendicular valleys

<001>

3D

<010>

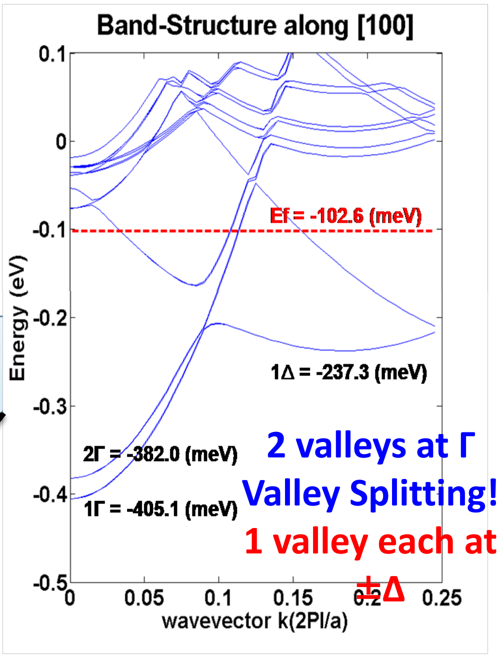
Four-fold in-planar valleys

STEP 1: 3D→2D
Confinement in kz
Projection to 2D(kx-ky) plane

<010>

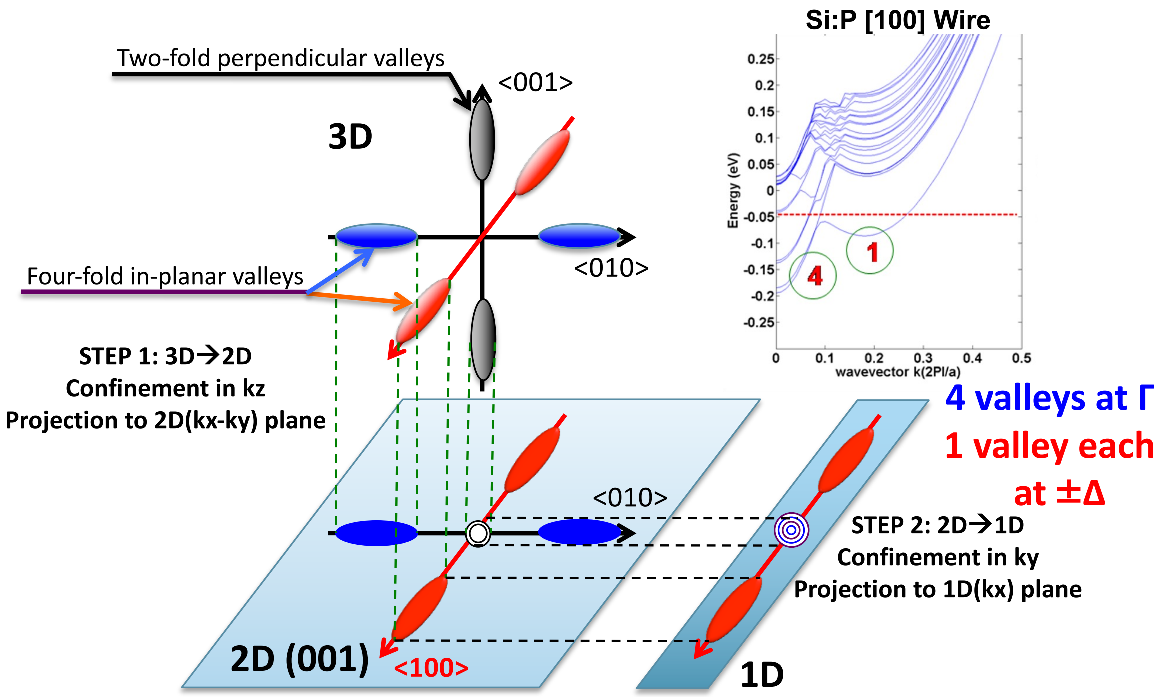
2D (001)

<100>



Band projection in [100] Si:P wires

- 3D→2D→1D projection of Si [100] nanowire



4 valleys at Γ

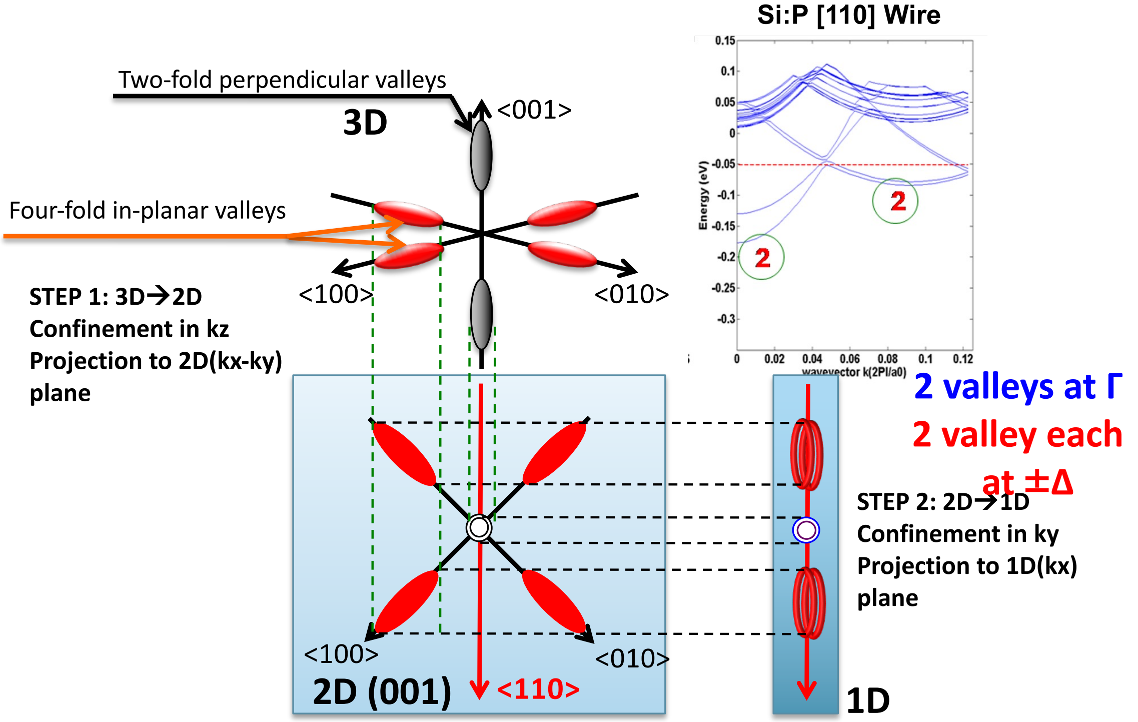
1 valley each at ±Δ

STEP 1: 3D→2D
Confinement in kz
Projection to 2D(kx-ky) plane

STEP 2: 2D→1D
Confinement in ky
Projection to 1D(kx) plane

Band projection in [110] Si:P wires

- 3D→2D→1D projection of Si [110] nanowire



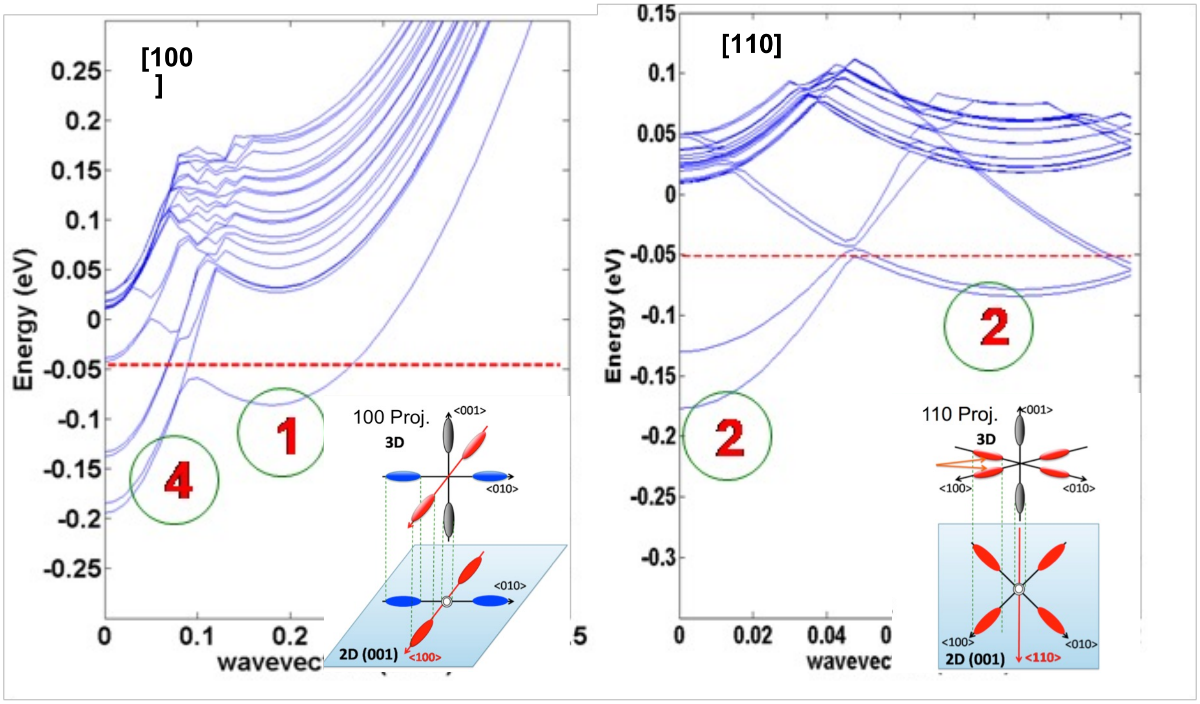
2 valleys at Γ

2 valley each at ±Δ

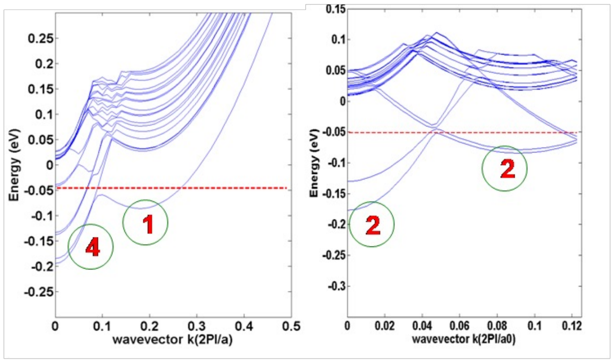
STEP 1: 3D→2D
Confinement in kz
Projection to 2D(kx-ky) plane

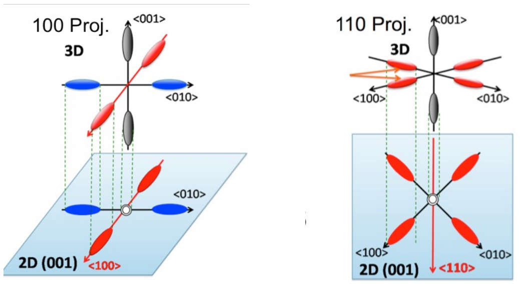
STEP 2: 2D→1D
Confinement in ky
Projection to 1D(kx) plane

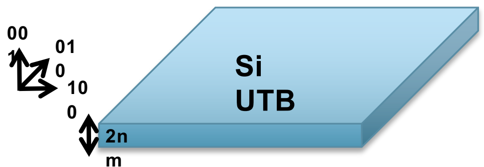
Band Projection in [100]/[110] Si:P Quantum Wire

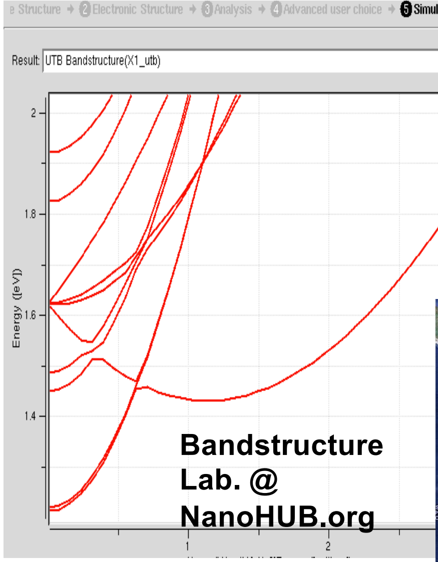


Band-Projection: A comparison to Si UTB









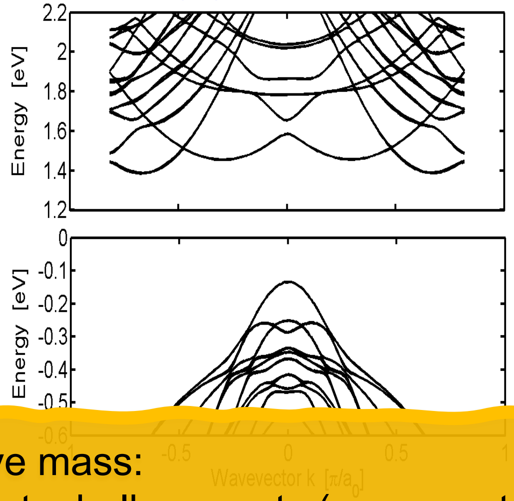
Bandstructure Lab. @ NanoHUB.org

>10,800 users

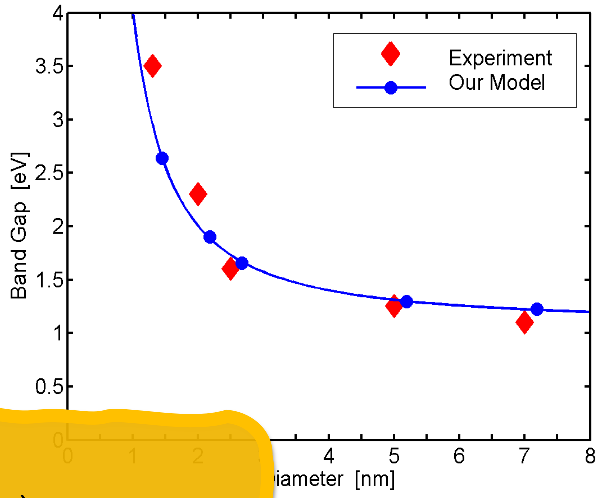
NEMO5

Circular 112 Wire Comparison with Experiment

Si, CW [112], D=3.0nm



Si, CW [112]



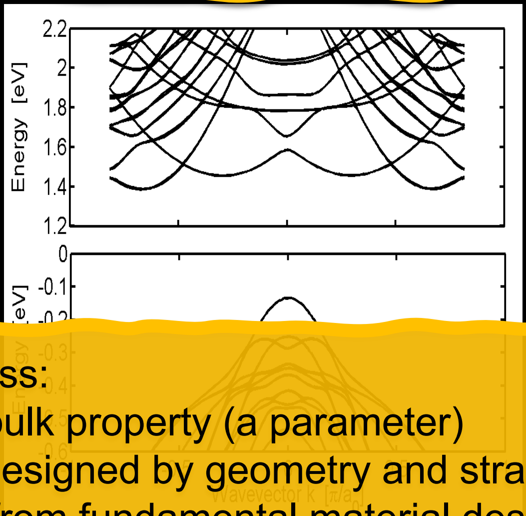
Effective mass:
- Is not a bulk property (a parameter)
- Can be designed by geometry and strain
- Derived from fundamental material description

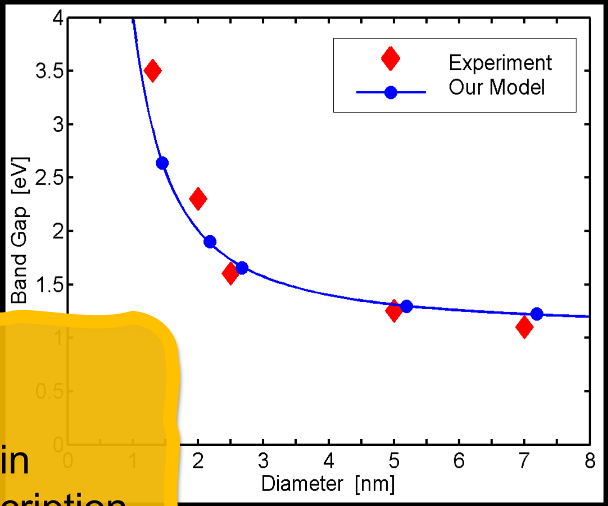
Our tight-binding calculation provides good agreement with experiment data (*Ma et al., Science 299, 1874, 2003*.)

PURDUE UNIVERSITY © Gerhard Klimeck

Frontier of Modeling

- Transferrable approaches shared beyond specific devices
  - Multi-physics & multi-scale segmentation or partition
  - Smart choices of basis sets
  -
  -





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© Gerhard Klimeck

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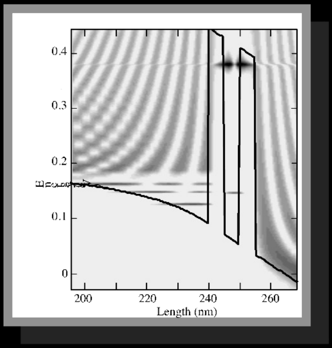
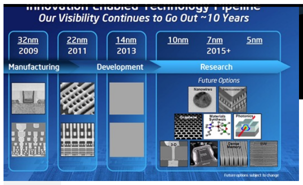


Shared in the whole spatial domain:

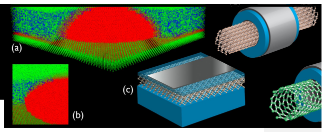
- Non-Equilibrium –Open System => Non-Hermitian
- Quantum mechanical dynamics w/ spatial variations
- "No" approximation in the quantum mechanics

Spatial partitioning into:

- Strong vs. weak scattering (kinetics)



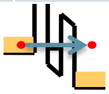
NEMO1D - First Industrial NEGF Tool
Atomistic Basis

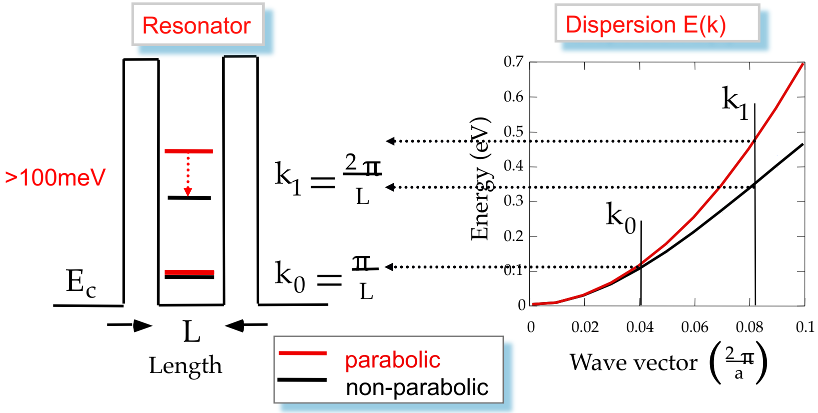


Transferrable approaches shared beyond specific devices

TI&JPL
1994-2003

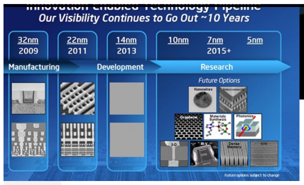
	NEMO-1D
Transport	Yes
Dimensions	1D
Atoms	~1,000
Substrate, Crystals	[100] Cubic, ZB
Strain	-
Multi-physics Multi-Scale	Scattering Domains
Parallel Comp.	3 levels 23,000 cores



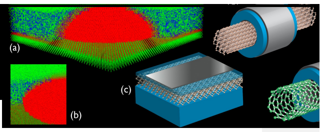


- Second state lowered by >100mev ~ 4kT

1996: 1D atomistic, full bandstructure chain, 5nm central features in 150nm device



NEMO1D - First Industrial NEGF Tool Atomistic Basis



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Atoms	~1,000
Substrate, Crystals	[100] Cubic, ZB
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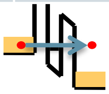
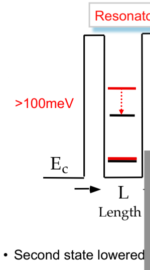
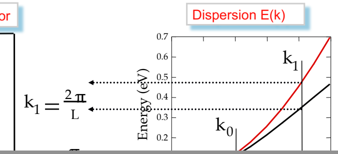
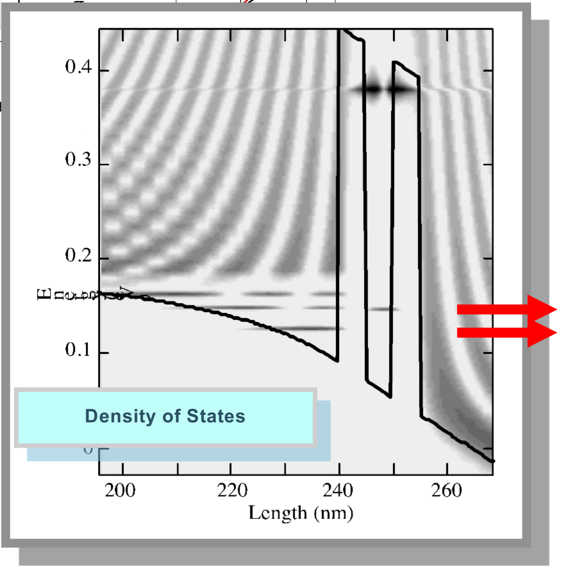
Parallel Comp.	3 levels 23,000 cores





- Second state lowered





Density of States

1996: 1D atomistic, full bandstructure chain, 5nm central features in 150nm device

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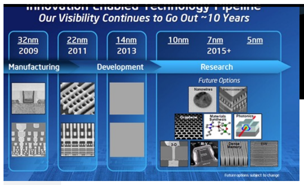
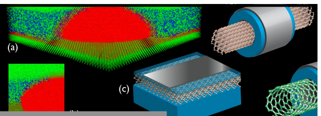


NEMO1D - First Industrial NEGF Tool Atomistic Basis



Transferrable approaches shared beyond specific devices

TI&JPL
1994-2003

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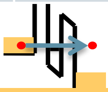
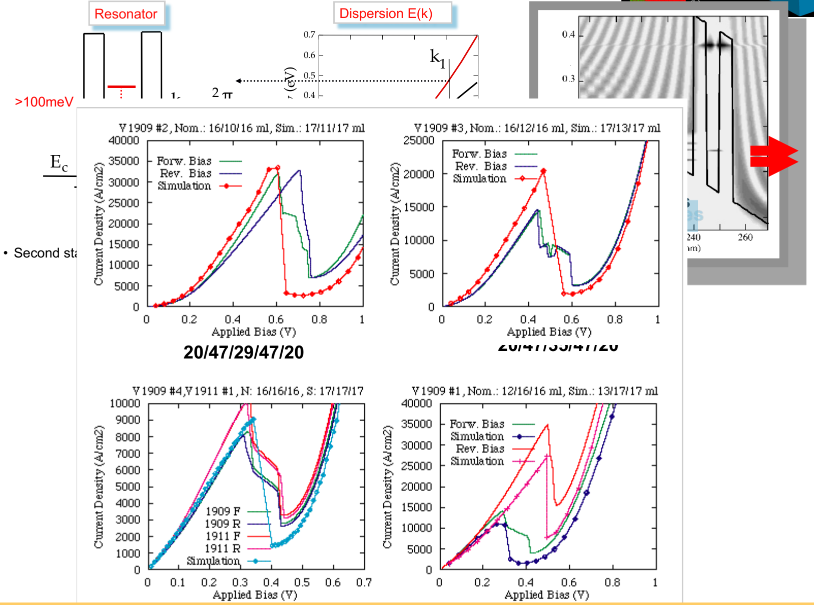
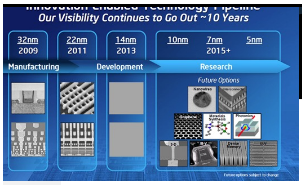
Strain	-
Multi-physics Multi-Scale	Scattering Domains
Parallel Comp.	3 levels 23,000 cores



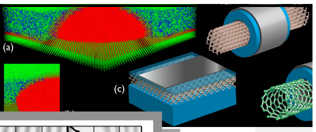


NEMO theory team CORRECTED the growth recipes of experimentalists
Experiments were off by TWO ATOMIC MONOLAYERS

1996: 1D atomistic, full bandstructure chain, 5nm central features in 150nm device



NEMO1D - First Industrial NEGF Tool Impact on Si Technology



Transferrable approaches shared beyond specific devices

TI&JPL
1994-2003

	NEMO-1D
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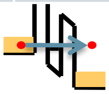
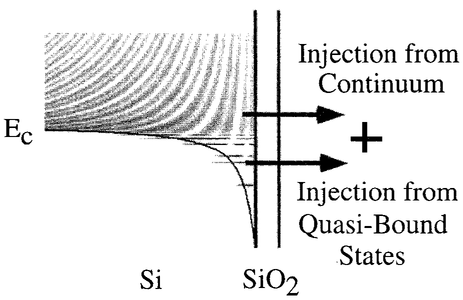
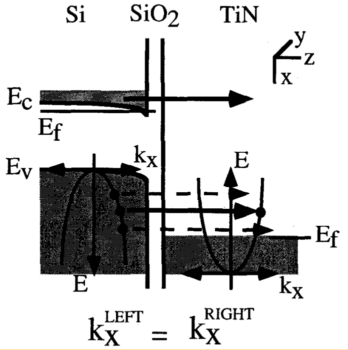
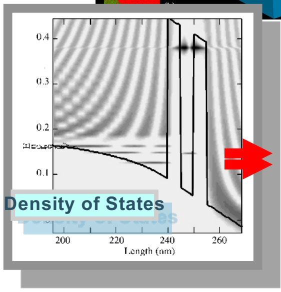
Dimensions	1D
Atoms	~1,000
Substrate, Crystals	[100] Cubic, ZB
Strain	-
Multi-physics Multi-Scale	Scattering Domains
Parallel Comp.	3 levels 23,000 cores

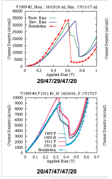


Tunneling Simulation

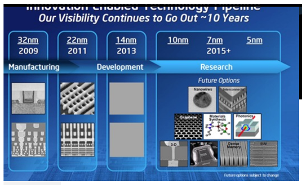




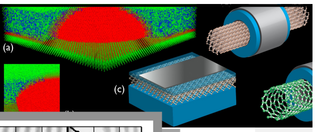




1997 IEDM: **Texas Instruments uses NEMO1D to calibrate Oxide thickness in Si/SiO2/TiN**



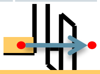
NEMO1D - First Industrial NEGF Tool Change Industrial Practice



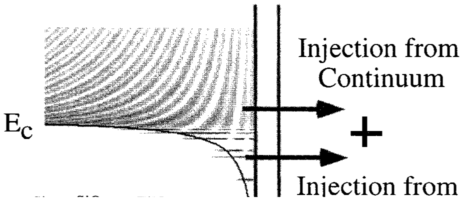
Transferrable approaches shared beyond specific devices

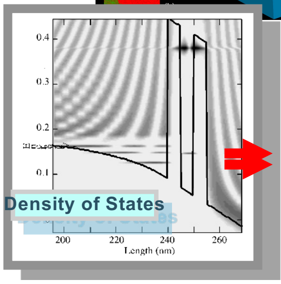
TI&JPL
1994-2003

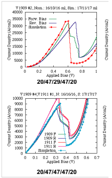
	NEMO-1D
Transport	Yes
Dimensions	1D
Atoms	~1,000
Substrate, Crystals	[100] Cubic, Z
Strain	-
Multi-physics Multi-Scale	Scatterir Domains
Parallel Comp.	3 levels 23,000 c

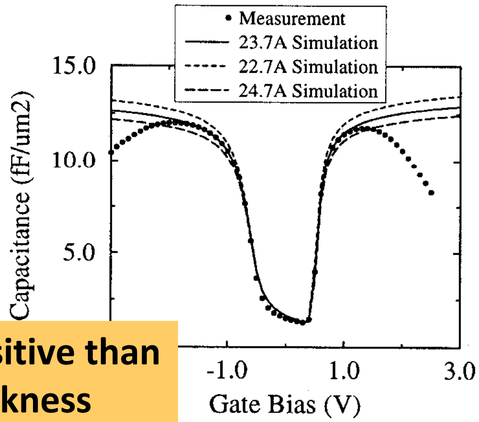


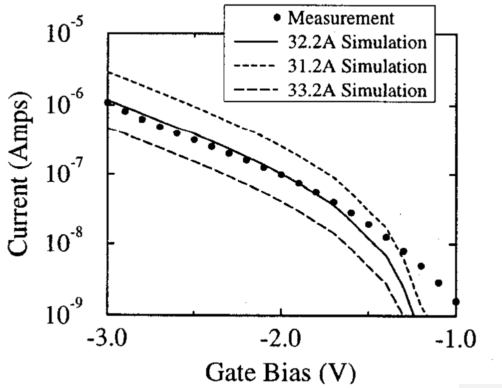
Tunneling Simulation





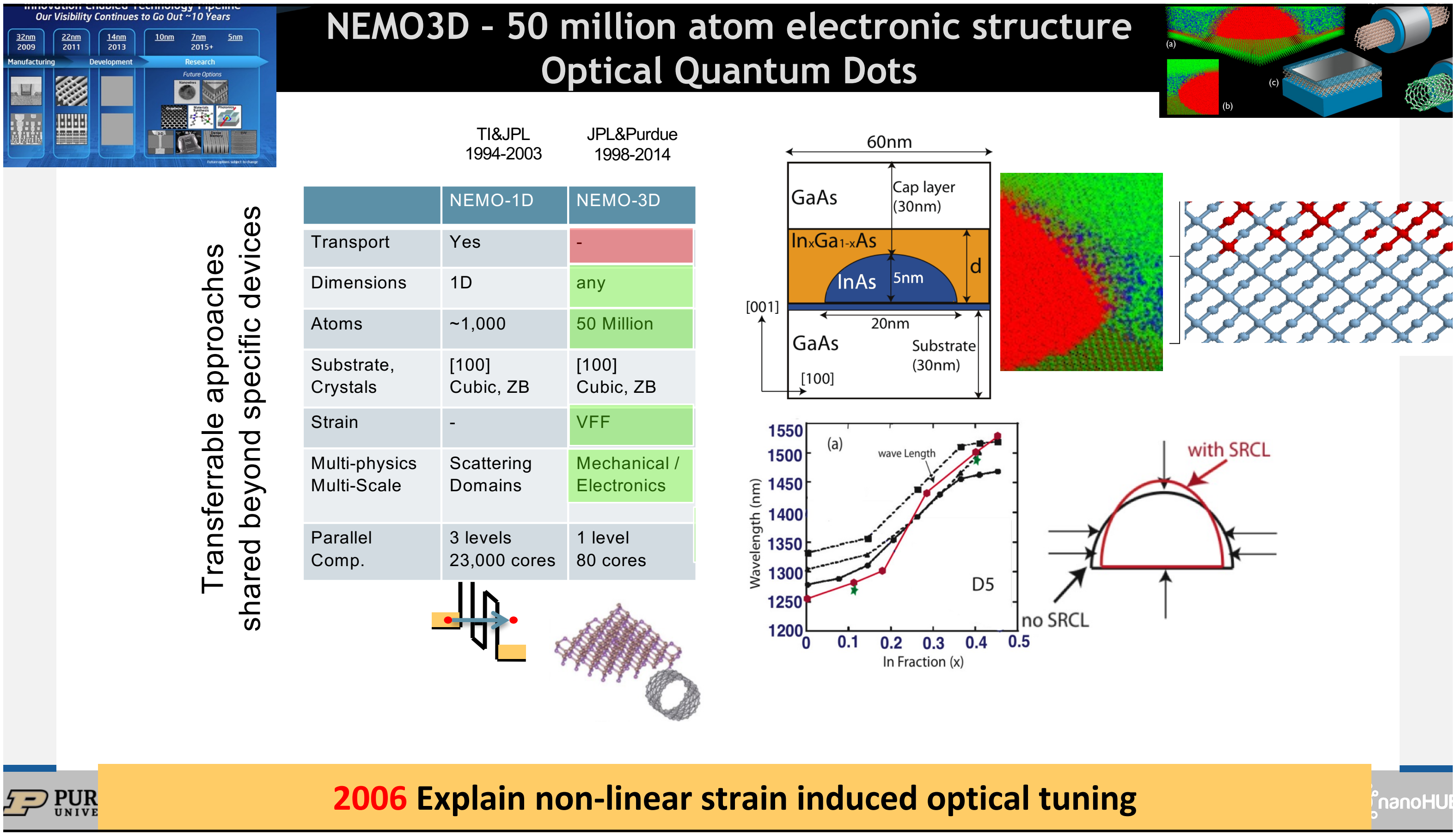






1997 IEDM: **I-V much more sensitive than C-V to determine oxide thickness**

1997 IEDM: **Texas Instruments uses NEMO1D to calibrate Oxide thickness in Si/SiO2/TiN**

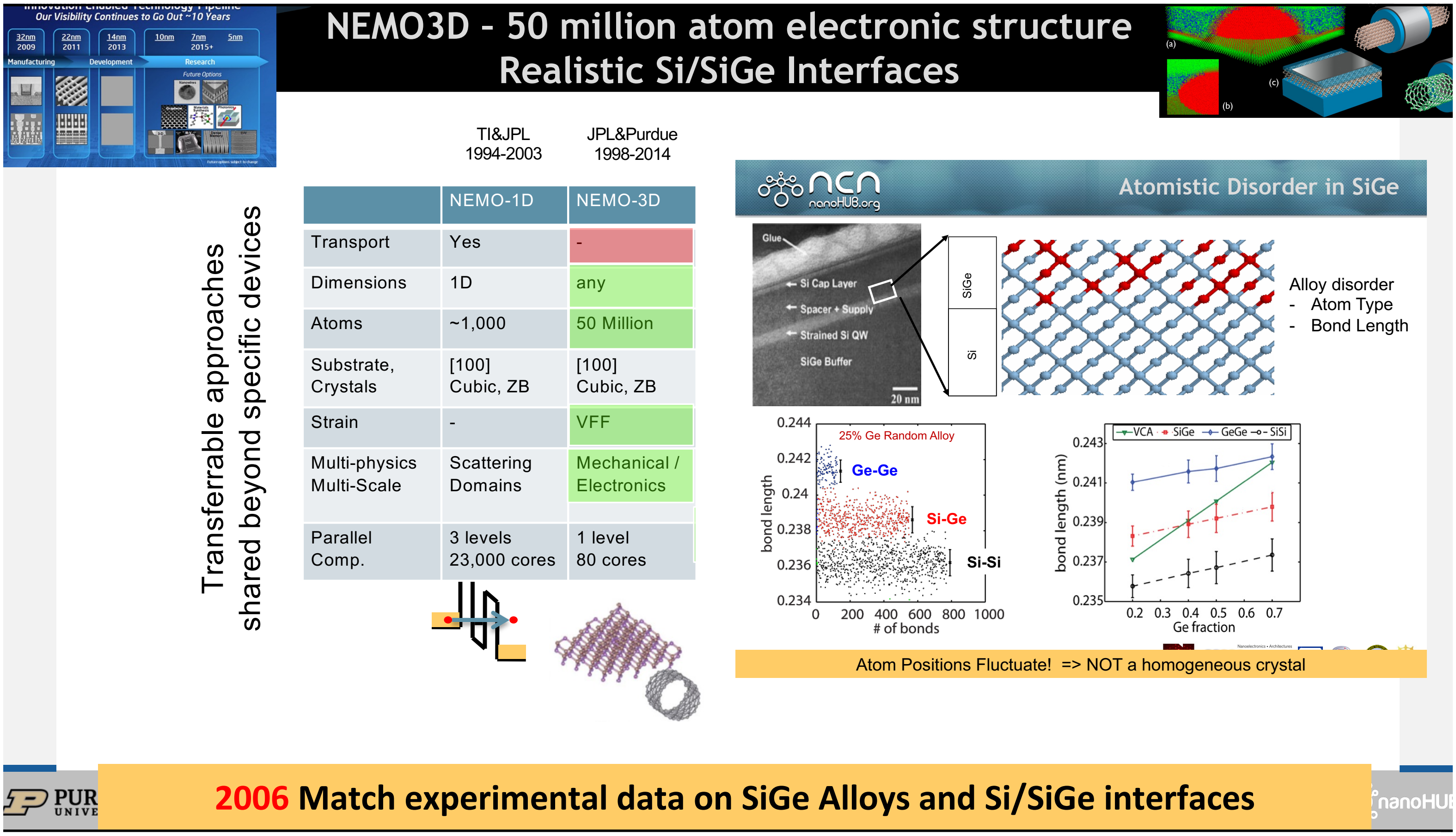


NEMO3D - 50 million atom electronic structure Optical Quantum Dots

Transferable approaches shared beyond specific devices

	NEMO-1D	NEMO-3D
	TI&JPL 1994-2003	JPL&Purdue 1998-2014
Transport	Yes	-
Dimensions	1D	any
Atoms	~1,000	50 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB
Strain	-	VFF
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores

2006 Explain non-linear strain induced optical tuning



NEMO3D - 50 million atom electronic structure Realistic Si/SiGe Interfaces

Transferable approaches shared beyond specific devices

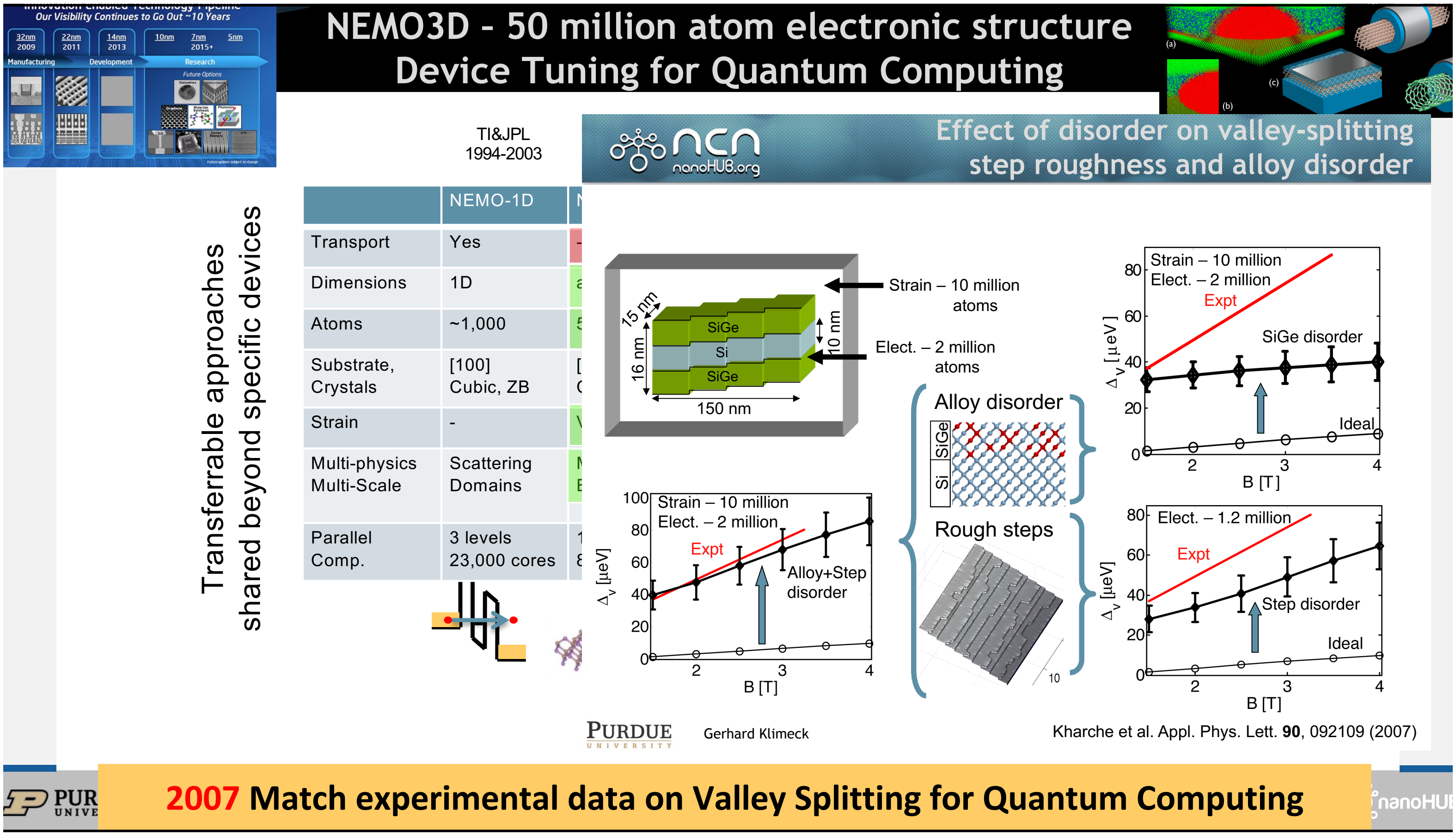
	NEMO-1D	NEMO-3D
	TI&JPL 1994-2003	JPL&Purdue 1998-2014
Transport	Yes	-
Dimensions	1D	any
Atoms	~1,000	50 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB
Strain	-	VFF
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores

Atomistic Disorder in SiGe

Alloy disorder
- Atom Type
- Bond Length

Atom Positions Fluctuate! => NOT a homogeneous crystal

2006 Match experimental data on SiGe Alloys and Si/SiGe interfaces



NEMO3D - 50 million atom electronic structure Device Tuning for Quantum Computing

Transferrable approaches shared beyond specific devices

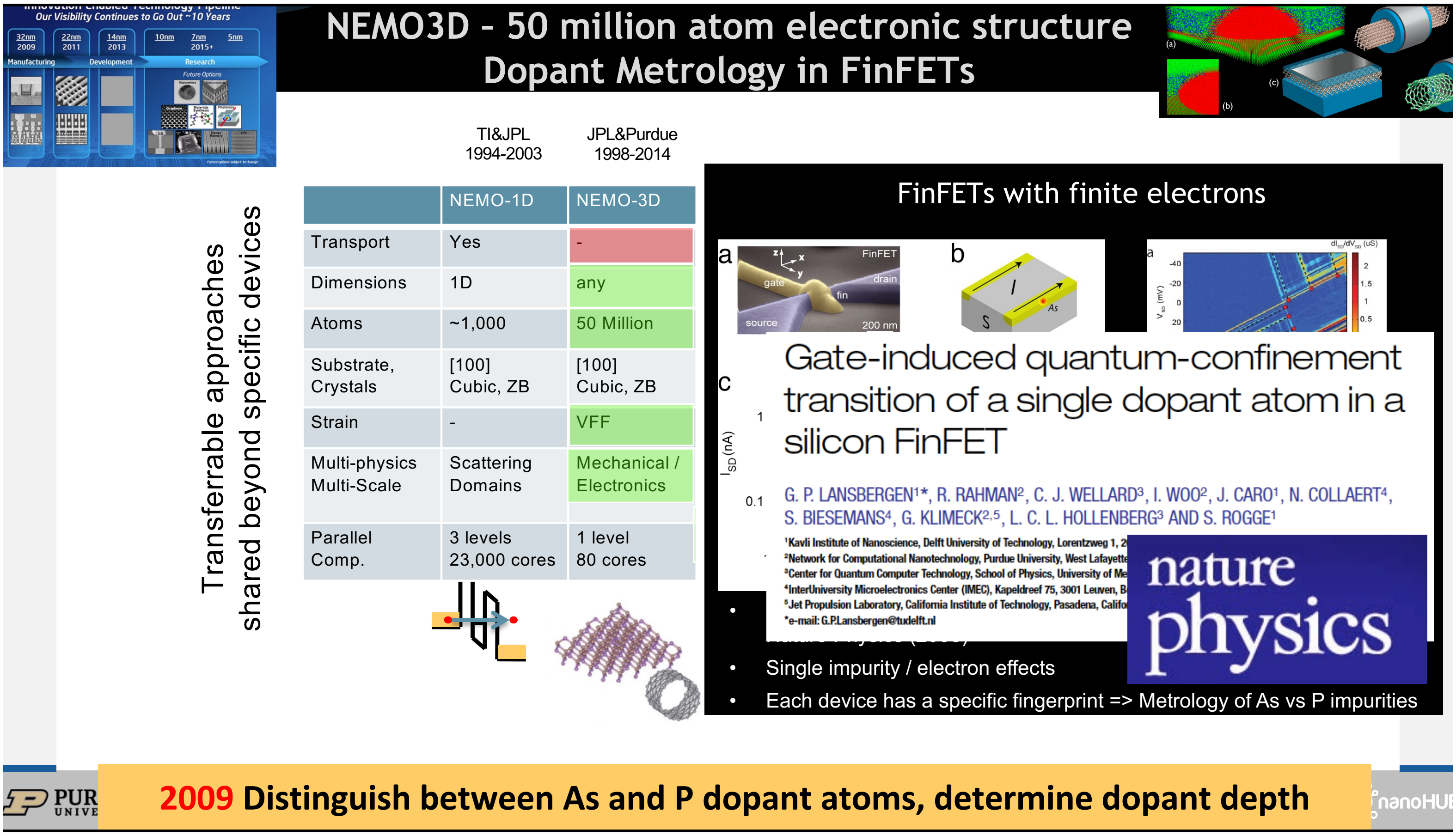
	TI&JPL 1994-2003	
	NEMO-1D	N
Transport	Yes	-
Dimensions	1D	a
Atoms	~1,000	5
Substrate, Crystals	[100] Cubic, ZB	[C
Strain	-	V
Multi-physics Multi-Scale	Scattering Domains	M E
Parallel Comp.	3 levels 23,000 cores	1 8

Effect of disorder on valley-splitting step roughness and alloy disorder

PURDUE UNIVERSITY Gerhard Klimeck

Kharche et al. Appl. Phys. Lett. **90**, 092109 (2007)

2007 Match experimental data on Valley Splitting for Quantum Computing



NEMO3D - 50 million atom electronic structure Dopant Metrology in FinFETs

Transferrable approaches shared beyond specific devices

	TI&JPL 1994-2003	JPL&Purdue 1998-2014
	NEMO-1D	NEMO-3D
Transport	Yes	-
Dimensions	1D	any
Atoms	~1,000	50 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB
Strain	-	VFF
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores

FinFETs with finite electrons

Gate-induced quantum-confinement transition of a single dopant atom in a silicon FinFET

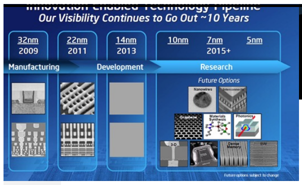
G. P. LANSBERGEN[1]*, R. RAHMAN[2], C. J. WELLARD[3], I. WOO[2], J. CARO[1], N. COLLAERT[4], S. BIESEMANS[4], G. KLIMECK[2,5], L. C. L. HOLLENBERG[3] AND S. ROGGE[1]

[1]Kavli Institute of Nanoscience, Delft University of Technology, Lorentzweg 1, 2
[2]Network for Computational Nanotechnology, Purdue University, West Lafayette
[3]Center for Quantum Computer Technology, School of Physics, University of Me
[4]InterUniversity Microelectronics Center (IMEC), Kapeldreef 75, 3001 Leuven, B
[5]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, Califo
*e-mail: G.P.Lansbergen@tudelft.nl

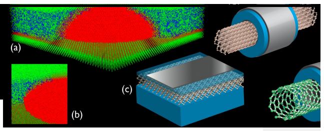
nature physics

- Single impurity / electron effects
- Each device has a specific fingerprint => Metrology of As vs P impurities

2009 Distinguish between As and P dopant atoms, determine dopant depth

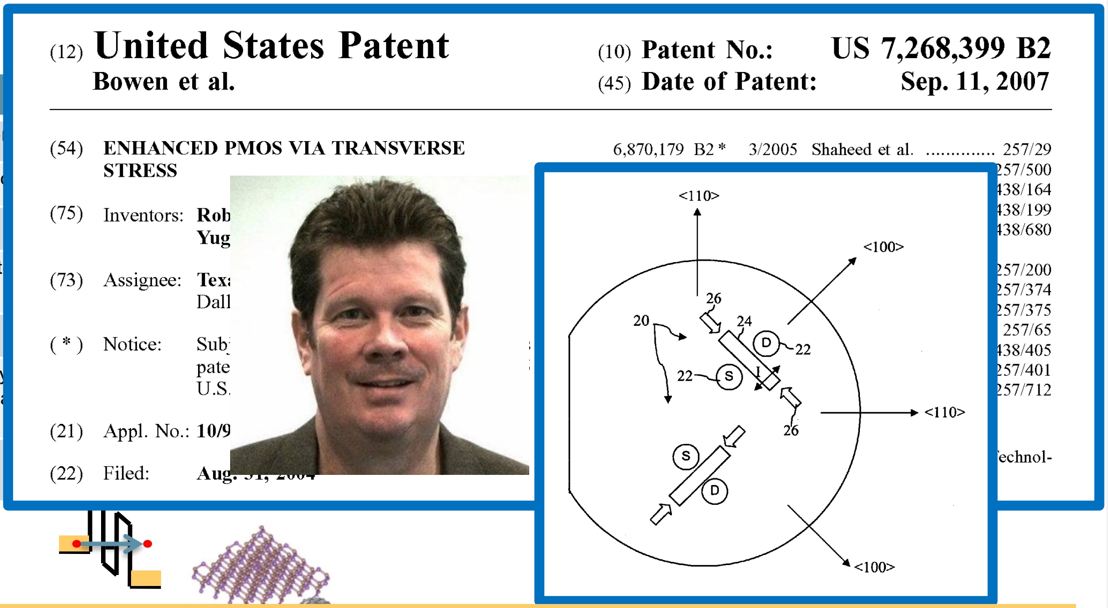


NEMO3D - Impact on 90nm, 65nm and beyond Rotated Substrate



Transferrable approaches
shared beyond specific devices

Transpo
Dimensi
Atoms
Substrat
Crystals
Strain
Multi-phy
Multi-Sca
Parallel
Comp.



(12) **United States Patent**
Bowen et al.

(10) **Patent No.:** **US 7,268,399 B2**
(45) **Date of Patent:** **Sep. 11, 2007**

(54) **ENHANCED PMOS VIA TRANSVERSE STRESS**

(75) Inventors: **Rob**
Yug

(73) Assignee: **Tex**
Dall

(*) Notice: Sub
pate
U.S.

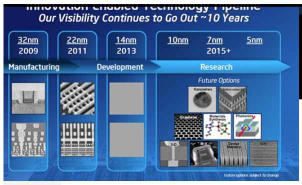
(21) Appl. No.: **10/9**

(22) Filed: **Aug. 31, 2004**

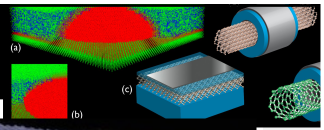
6,870,179 B2 * 3/2005 Shaheed et al. 257/29
257/500
438/164
438/199
438/680
257/200
257/374
257/375
257/65
438/405
257/401
257/712
echnol-

2004 Impacted Billions of Chips!

2004 Rotated substrate invented at TI based on NEMO3D

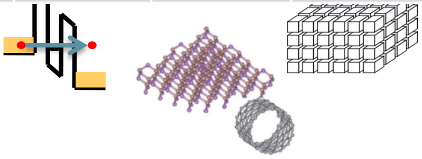


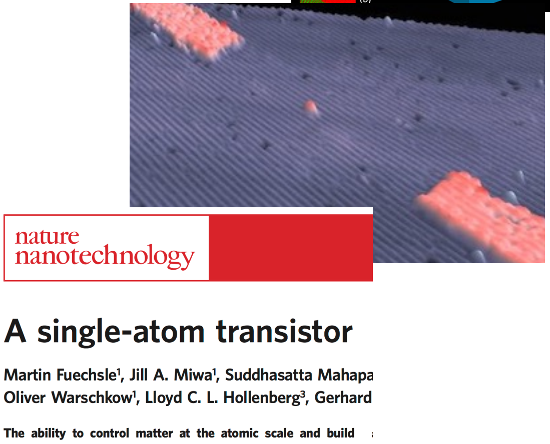
NEMO3Dpeta - wider parallel scaling Impact on Quantum Computing



Transferrable approaches
shared beyond specific devices

	TI&JPL 1994-2003	JPL&Purdue 1998-2014	Purdue 2007-2012
	NEMO-1D	NEMO-3D	NEMO3Dpeta
Transport	Yes	-	-
Dimensions	1D	any	any
Atoms	~1,000	50 Million	100 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic, ZB, WU
Strain	-	VFF	VFF
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics	Continuum & Single Electrons
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores



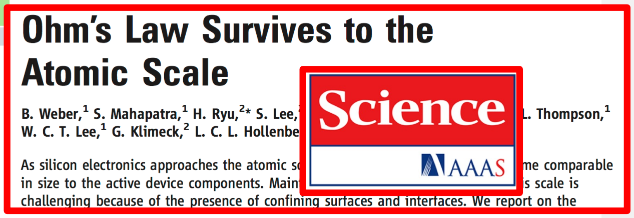


nature nanotechnology

A single-atom transistor

Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapa
Oliver Warschkow[1], Lloyd C. L. Hollenberg[3], Gerhard

The ability to control matter at the atomic scale and build



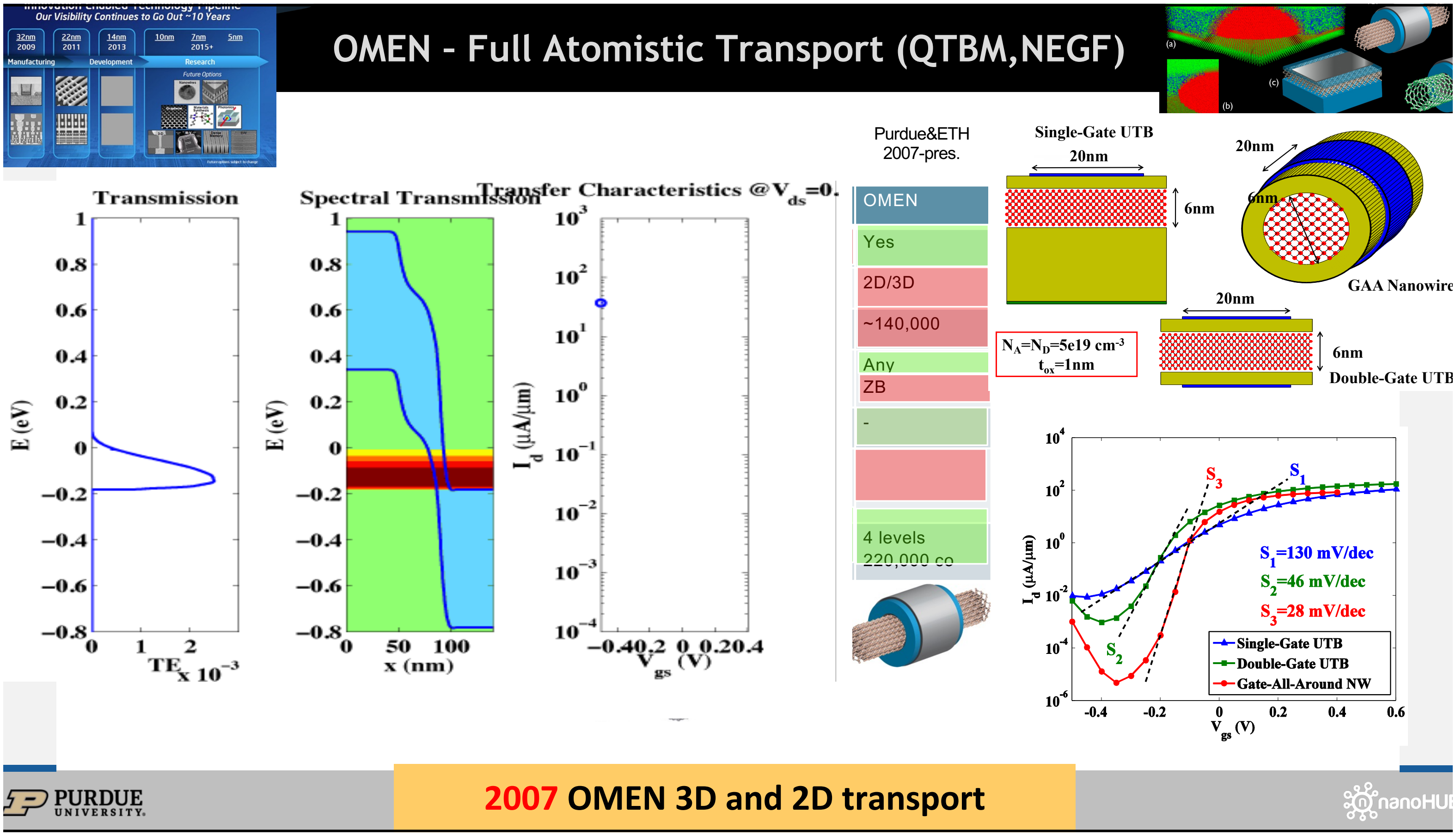
Ohm's Law Survives to the Atomic Scale

B. Weber,[1] S. Mahapatra,[1] H. Ryu,[2*] S. Lee, L. Thompson,[1]
W. C. T. Lee,[1] G. Klimeck,[2] L. C. L. Hollenbe

As silicon electronics approaches the atomic sc me comparable in size to the active device components. Main s scale is challenging because of the presence of confining surfaces and interfaces. We report on the

Science AAAS

2012 Full 3D electrostatics, disordered P patterns, transport in single P dopants



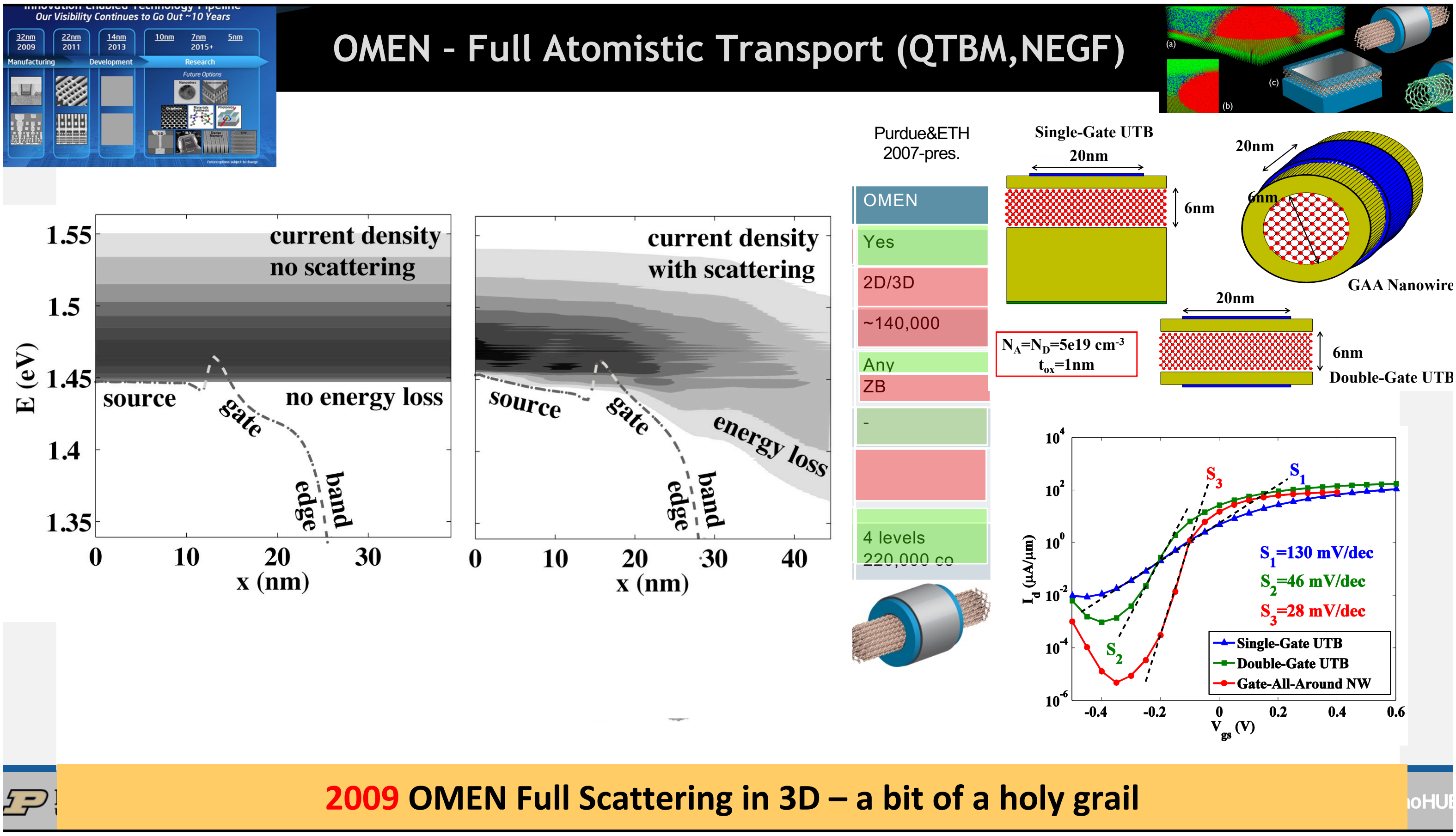
OMEN - Full Atomistic Transport (QTBM,NEGF)

Purdue&ETH
2007-pres.

- OMEN
- Yes
- 2D/3D
- ~140,000
- Any
- ZB
- -
- 4 levels
- 220,000 co

N_A=N_D=5e19 cm^{-3}
t_{ox}=1nm

2007 OMEN 3D and 2D transport



OMEN - Full Atomistic Transport (QTBM,NEGF)

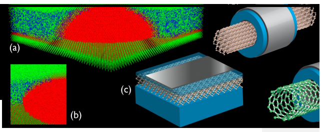
Purdue&ETH
2007-pres.

- OMEN
- Yes
- 2D/3D
- ~140,000
- Any
- ZB
- -
- 4 levels
- 220,000 co

N_A=N_D=5e19 cm^{-3}
t_{ox}=1nm

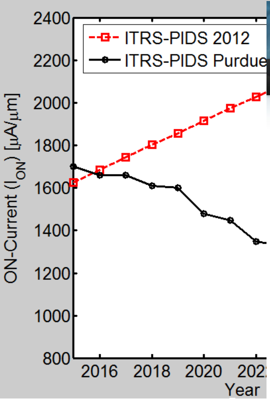
2009 OMEN Full Scattering in 3D – a bit of a holy grail

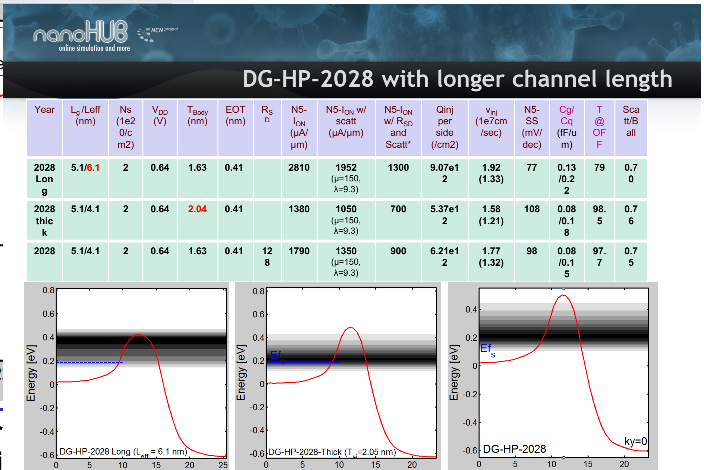
NEMO5 adopted for ITRS Roadmap - first physics-based model



Rewriting ITRS PIDS Tables

Nov 23, 2013





DG-HP-2028 with longer channel length

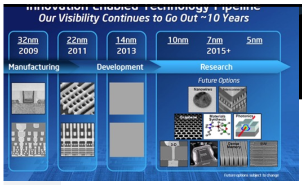
Year	L_g/Leff (nm)	Ns (1e20/cm2)	V_{DD} (V)	T_{Body} (nm)	EOT (nm)	R_{SD}	N5-I_{ON} (μA/μm)	N5-I_{ON} w/ scatt (μA/μm)	N5-I_{ON} w/ R_{SD} and Scatt*	Qinj per side (/cm2)	v_{inj} (1e7cm/sec)	N5-SS (mV/dec)	Cg/Cq (fF/um)	T @ OFF	Scatt/Ball
2028 Long	**5.1/6.1**	**2**	**0.64**	**1.63**	**0.41**		**2810**	**1952** (μ=150, λ=9.3)	**1300**	**9.07e12**	**1.92 (1.33)**	**77**	**0.13/0.22**	**79**	**0.70**
2028 thick	**5.1/4.1**	**2**	**0.64**	**2.04**	**0.41**		**1380**	**1050** (μ=150, λ=9.3)	**700**	**5.37e12**	**1.58 (1.21)**	**108**	**0.08/0.18**	**98.5**	**0.76**
2028	**5.1/4.1**	**2**	**0.64**	**1.63**	**0.41**	**128**	**1790**	**1350** (μ=150, λ=9.3)	**900**	**6.21e12**	**1.77 (1.32)**	**98**	**0.08/0.15**	**97.7**	**0.75**

Opposite to former prediction for continui increase in technolog see a trend of curre drop and increase in sub-threshold swing.

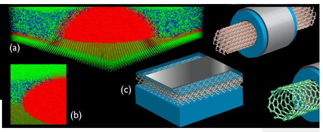
It's clear tunneling is a first order performance killer at the end of the roadmap.

NEMO5
Yes
any
100 Million
Any Any
MVFF, MD
Spin, **Thermal** Classical, Wannier
4 levels 200,000 cores

2013 First Physics-Based Device Simulation Projection in ITRS

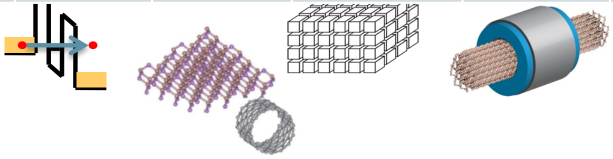


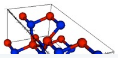
NEMO5 is expandable and scriptable Combines prior versions



Transferrable approaches shared beyond specific devices

	TI&JPL 1994-2003	JPL&Purdue 1998-2014	Purdue 2007-2012	Purdue&ETH 2007-pres.	
	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN	NEMO5
Transport	Yes	-	-	Yes	Yes
Dimensions	1D	any	any	2D/3D	any
Atoms	~1,000	50 Million	100 Million	~140,000	100 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic, ZB, WU	Any ZB	Any Any
Strain	-	VFF	VFF	-	MVFF, MD
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics	Continuum & Single Electrons		Spin, **Thermal** Classical, Wannier
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co	4 levels 200,000 cores



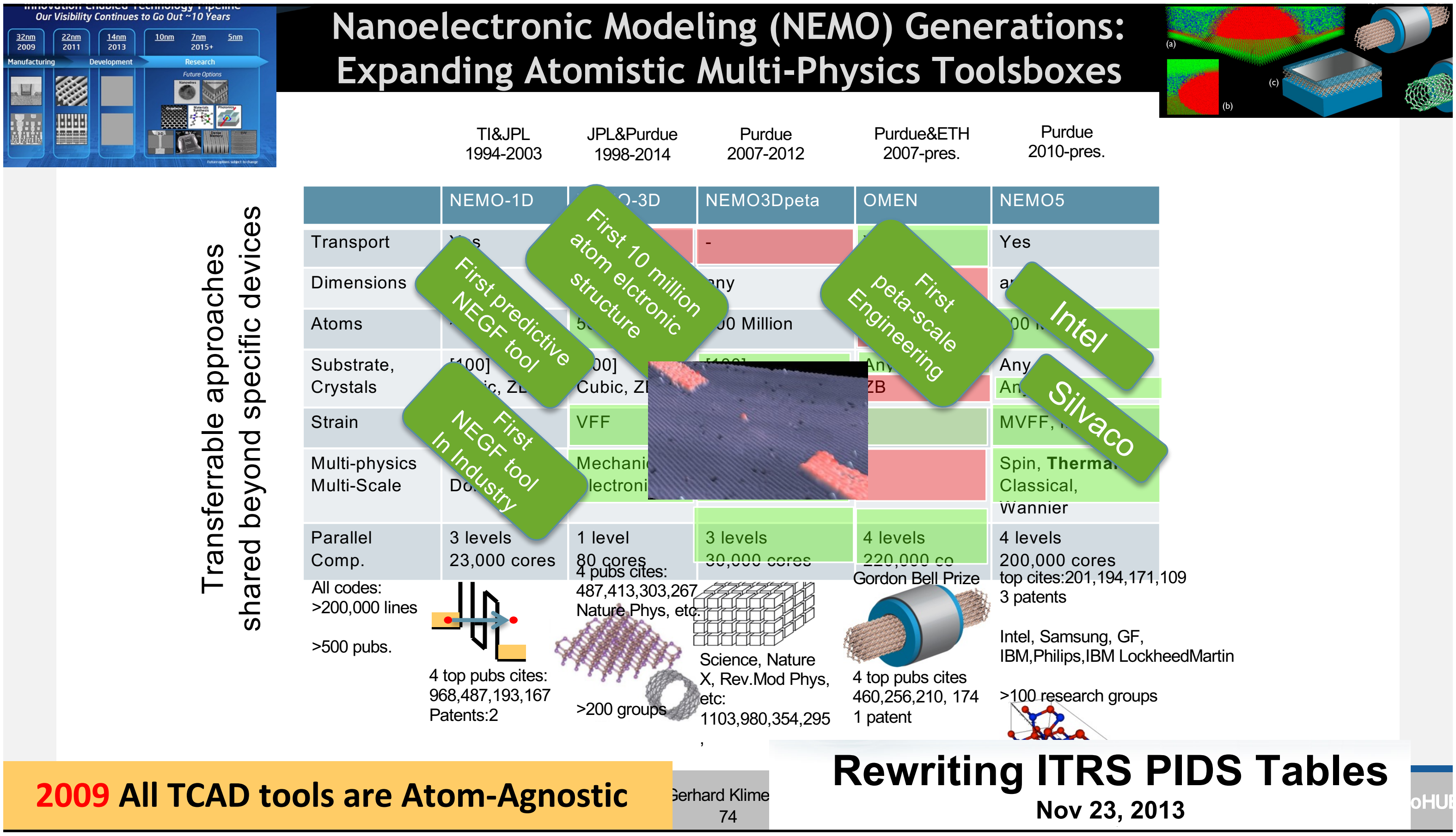


2009 All TCAD tools are Atom-Agnostic

Gerhard Klimec
73

Rewriting ITRS PIDS Tables

Nov 23, 2013



Nanoelectronic Modeling (NEMO) Generations: Expanding Atomistic Multi-Physics Toolsboxes

Transferable approaches shared beyond specific devices

	TI&JPL 1994-2003	JPL&Purdue 1998-2014	Purdue 2007-2012	Purdue&ETH 2007-pres.	Purdue 2010-pres.
	NEMO-1D	O-3D	NEMO3Dpeta	OMEN	NEMO5
Transport	s		-		Yes
Dimensions			ny		a
Atoms		5	0 Million		00
Substrate, Crystals	[100] ic, ZB	00] Cubic, Z		Any ZB	Any An
Strain		VFF			MVFF,
Multi-physics Multi-Scale	Do	Mechani lectroni			Spin, **Therma** Classical, Wannier
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co	4 levels 200,000 cores

All codes:
>200,000 lines

>500 pubs.

4 top pubs cites:
968,487,193,167
Patents:2

4 pubs cites:
487,413,303,267
Nature Phys, etc.

>200 groups

Science, Nature X, Rev.Mod Phys, etc:
1103,980,354,295
,

Gordon Bell Prize

4 top pubs cites
460,256,210, 174
1 patent

top cites:201,194,171,109
3 patents

Intel, Samsung, GF, IBM,Philips,IBM LockheedMartin

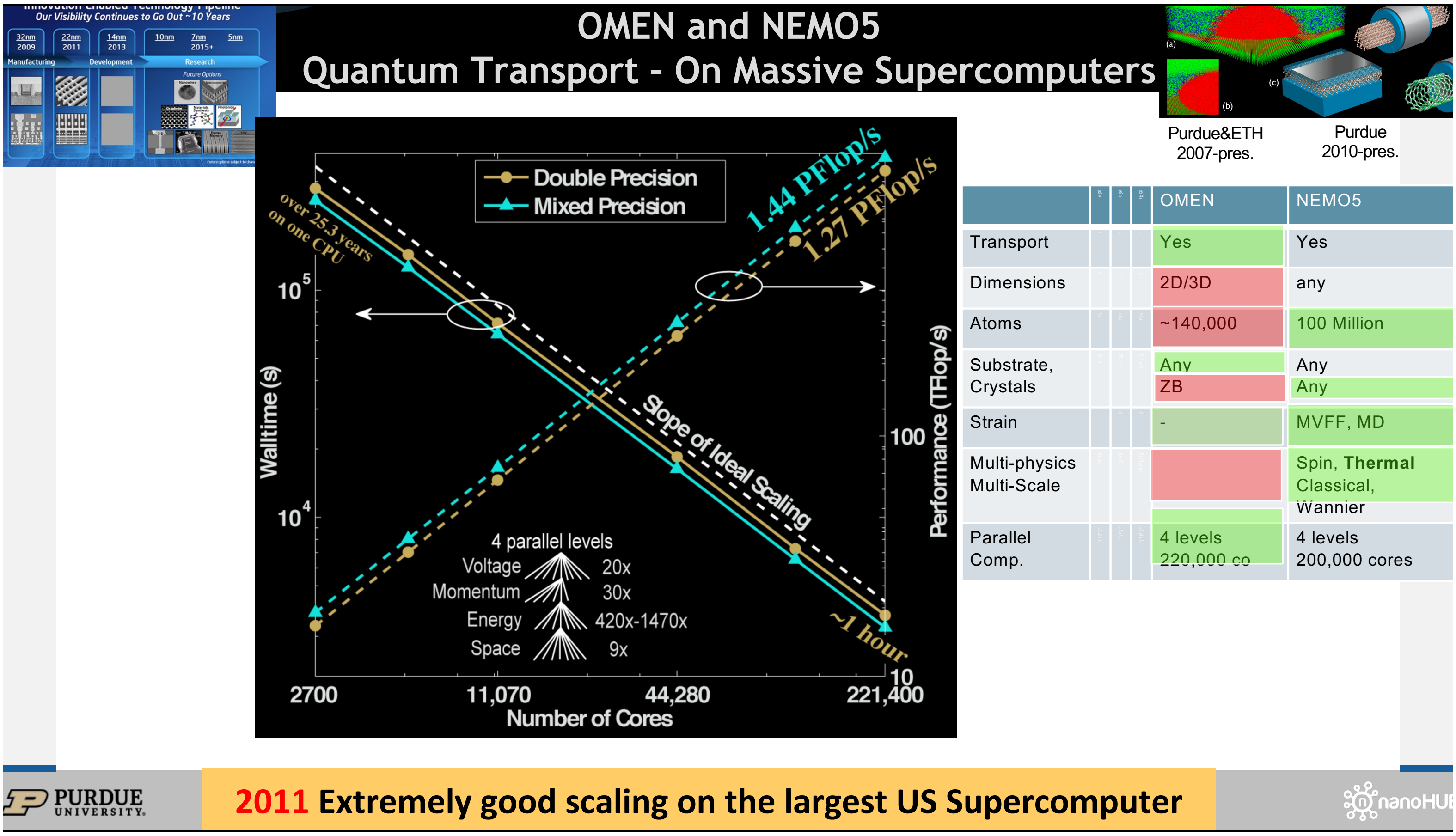
>100 research groups

2009 All TCAD tools are Atom-Agnostic

erhard Klime
74

Rewriting ITRS PIDS Tables
Nov 23, 2013

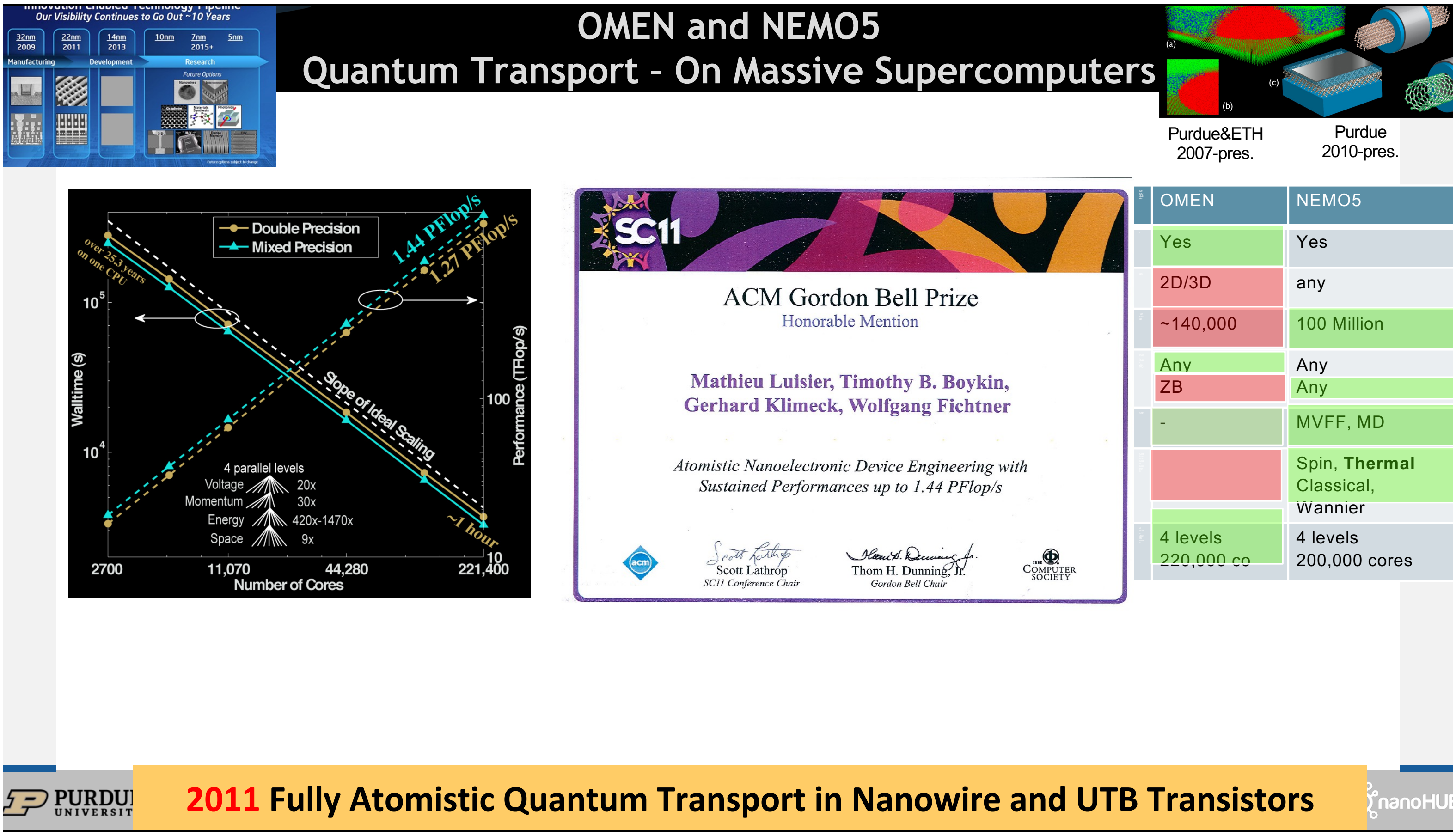
oHUE



OMEN and NEMO5
Quantum Transport - On Massive Supercomputers

	Purdue&ETH 2007-pres.	Purdue 2010-pres.
	OMEN	NEMO5
Transport	Yes	Yes
Dimensions	2D/3D	any
Atoms	~140,000	100 Million
Substrate, Crystals	Any ZB	Any Any
Strain	-	MVFF, MD
Multi-physics Multi-Scale		Spin, **Thermal** Classical, Wannier
Parallel Comp.	4 levels 220,000 co	4 levels 200,000 cores

2011 Extremely good scaling on the largest US Supercomputer



OMEN and NEMO5
Quantum Transport - On Massive Supercomputers

Purdue&ETH 2007-pres.	Purdue 2010-pres.

ACM Gordon Bell Prize
Honorable Mention

Mathieu Luisier, Timothy B. Boykin,
Gerhard Klimeck, Wolfgang Fichtner

Atomistic Nanoelectronic Device Engineering with
Sustained Performances up to 1.44 PFlop/s

Scott Lathrop
SC11 Conference Chair

Thom H. Dunning, Jr.
Gordon Bell Chair

IEEE Computer Society

	OMEN	NEMO5
[illegible]	Yes	Yes
[illegible]	2D/3D	any
[illegible]	~140,000	100 Million
[illegible]	Any ZB	Any Any
[illegible]	-	MVFF, MD
[illegible]		Spin, **Thermal** Classical, Wannier
[illegible]	4 levels 220,000 co	4 levels 200,000 cores

2011 Fully Atomistic Quantum Transport in Nanowire and UTB Transistors

---

OMEN
Quantum Transport - (

Intel® Parallel Computing Center

Collaborating on code modernization to enable the next leap in discovery.

Charles Wuischpard
Vice President, Data Center Group & General Manager, Workstation and High Performance Computing

Bob Burroughs
Director of Technical Computing Ecosystem Enabling

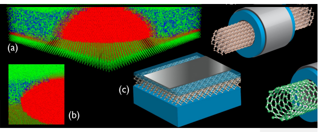
intel

In Recognition of
NEMO-5 Development
by the
Network for
Computational Nanotechnology
Purdue University

From
Process Technology Modeling Department
Intel Corporation
2013

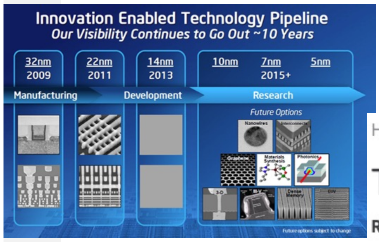
2011 Fully Atomistic Quantum Tr

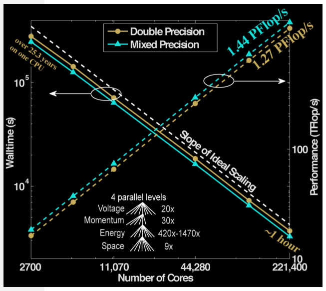
Intel Adoption of OMEN and NEMO5



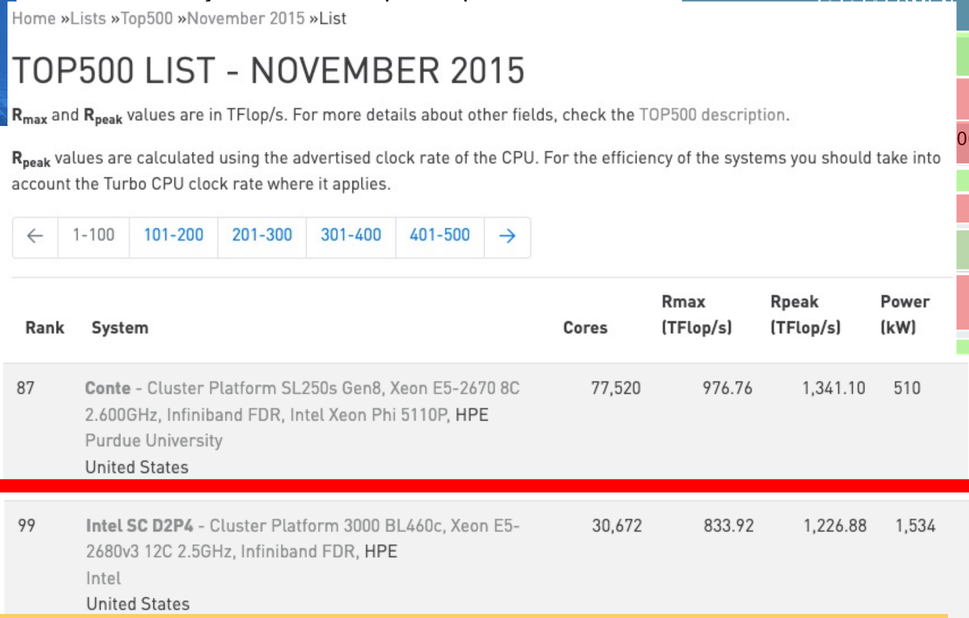
Purdue&ETH
2007-pres.

Purdue
2010-pres.





- 2009 initial engagement
- 2012-2017 co-development
- 2015 Intel buys a dedicated supercomputer to run



Home »Lists »Top500 »November 2015 »List

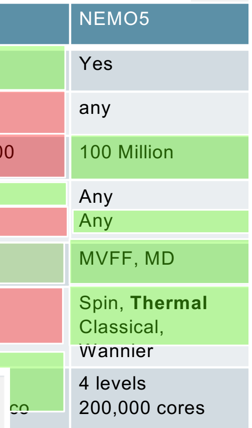
TOP500 LIST - NOVEMBER 2015

R_{max} and R_{peak} values are in TFlop/s. For more details about other fields, check the TOP500 description.

R_{peak} values are calculated using the advertised clock rate of the CPU. For the efficiency of the systems you should take into account the Turbo CPU clock rate where it applies.

← 1-100 101-200 201-300 301-400 401-500 →

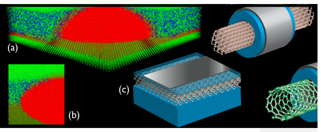
Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
87	**Conte** - Cluster Platform SL250s Gen8, Xeon E5-2670 8C 2.600GHz, Infiniband FDR, Intel Xeon Phi 5110P, HPE Purdue University United States	77,520	976.76	1,341.10	510
99	**Intel SC D2P4** - Cluster Platform 3000 BL460c, Xeon E5-2680v3 12C 2.5GHz, Infiniband FDR, HPE Intel United States	30,672	833.92	1,226.88	1,534



OMEN	NEMO5
	Yes
	any
00	100 Million
	Any Any
	MVFF, MD
	Spin, **Thermal** Classical, Wannier
co	4 levels 200,000 cores

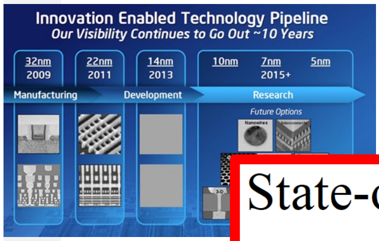
2015 Intel Embraces HPC to run Device Simulations

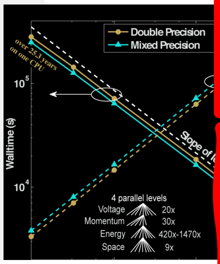
2019 Intel Publication at IEDM Announcing NEMO Integration



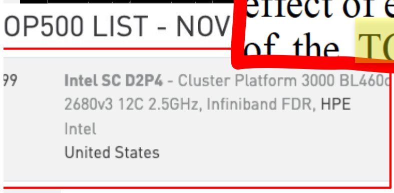
Purdue&ETH
2007-pres.

Purdue
2010-pres.



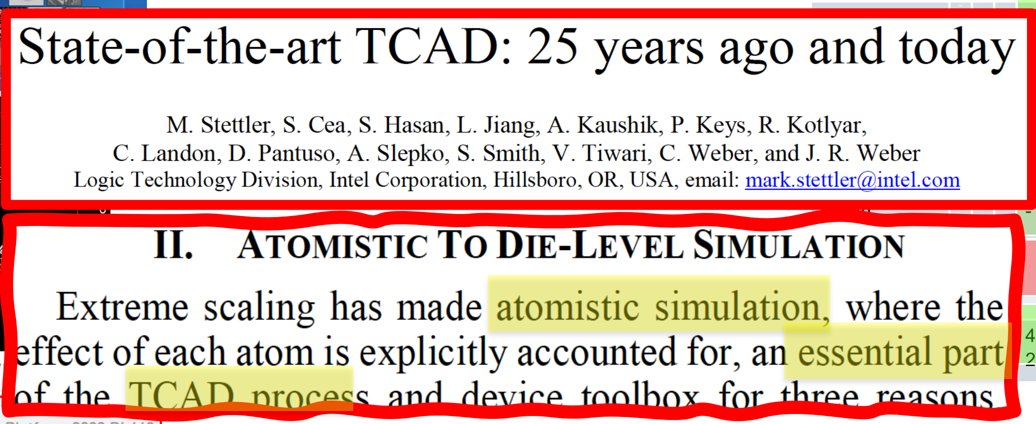


- 2009 initial engagement
- 2012-2017 co-development
- 2015 Intel buys a dedicated supercomputer to run NEMO



OP500 LIST - NOV

99	**Intel SC D2P4** - Cluster Platform 3000 BL460c 2680v3 12C 2.5GHz, Infiniband FDR, HPE Intel United States	

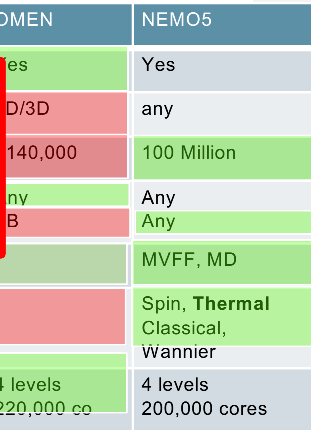


State-of-the-art TCAD: 25 years ago and today

M. Stettler, S. Cea, S. Hasan, L. Jiang, A. Kaushik, P. Keys, R. Kotlyar,
C. Landon, D. Pantuso, A. Slepko, S. Smith, V. Tiwari, C. Weber, and J. R. Weber
Logic Technology Division, Intel Corporation, Hillsboro, OR, USA, email: mark.stettler@intel.com

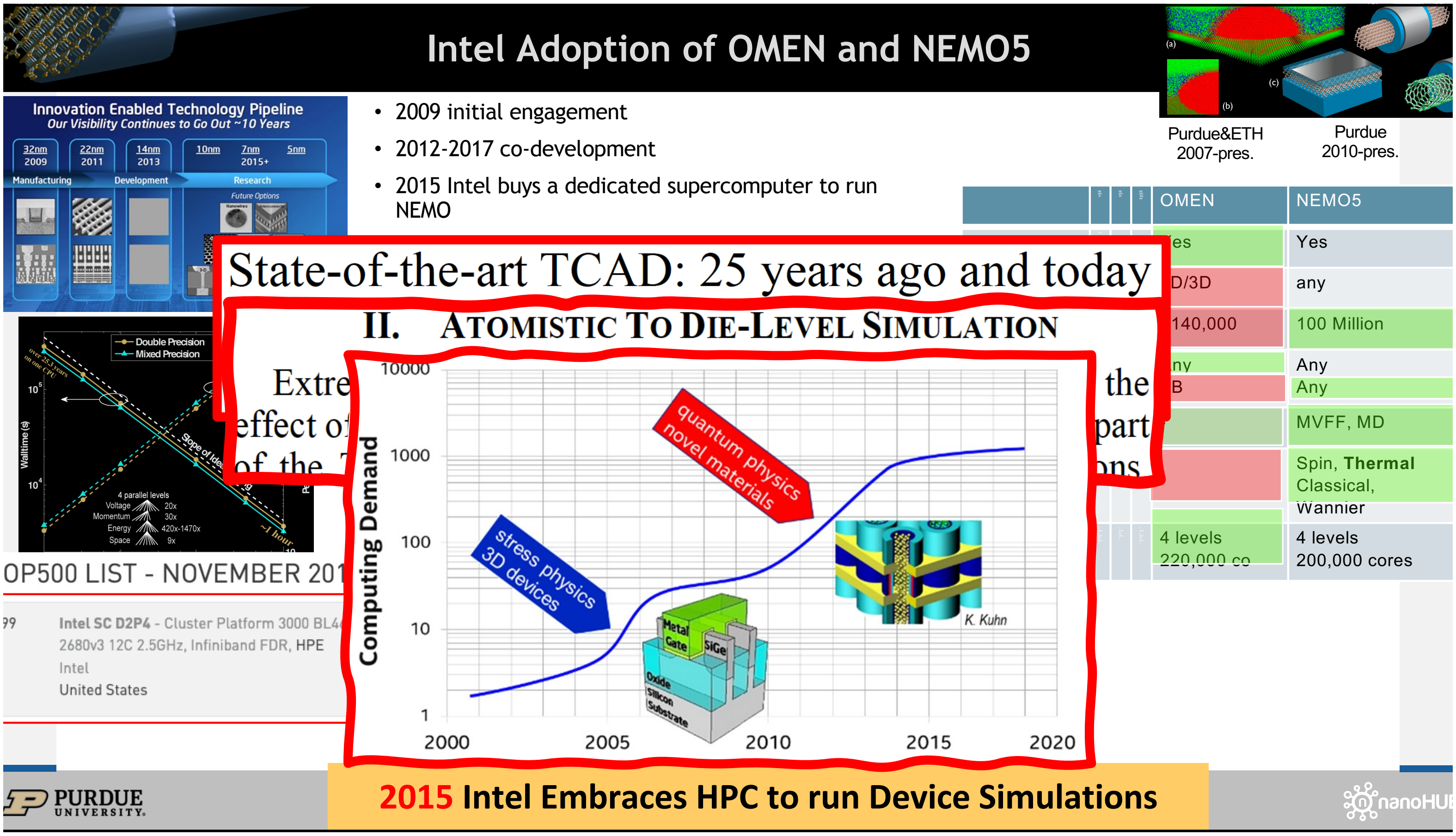
II. ATOMISTIC TO DIE-LEVEL SIMULATION

Extreme scaling has made atomistic simulation, where the effect of each atom is explicitly accounted for, an essential part of the TCAD process and device toolbox for three reasons



OMEN	NEMO5
es	Yes
D/3D	any
140,000	100 Million
ny B	Any Any
-	MVFF, MD
	Spin, **Thermal** Classical, Wannier
4 levels 220,000 co	4 levels 200,000 cores

2019 Intel Expresses Essential Need for Atomistic Simulations



Intel Adoption of OMEN and NEMO5

- 2009 initial engagement
- 2012-2017 co-development
- 2015 Intel buys a dedicated supercomputer to run NEMO

Purdue&ETH 2007-pres.

Purdue 2010-pres.

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OP500 LIST - NOVEMBER 201

99 Intel SC D2P4 - Cluster Platform 3000 BL4
2680v3 12C 2.5GHz, Infiniband FDR, HPE
Intel
United States

State-of-the-art TCAD: 25 years ago and today

II. ATOMISTIC TO DIE-LEVEL SIMULATION

Extre
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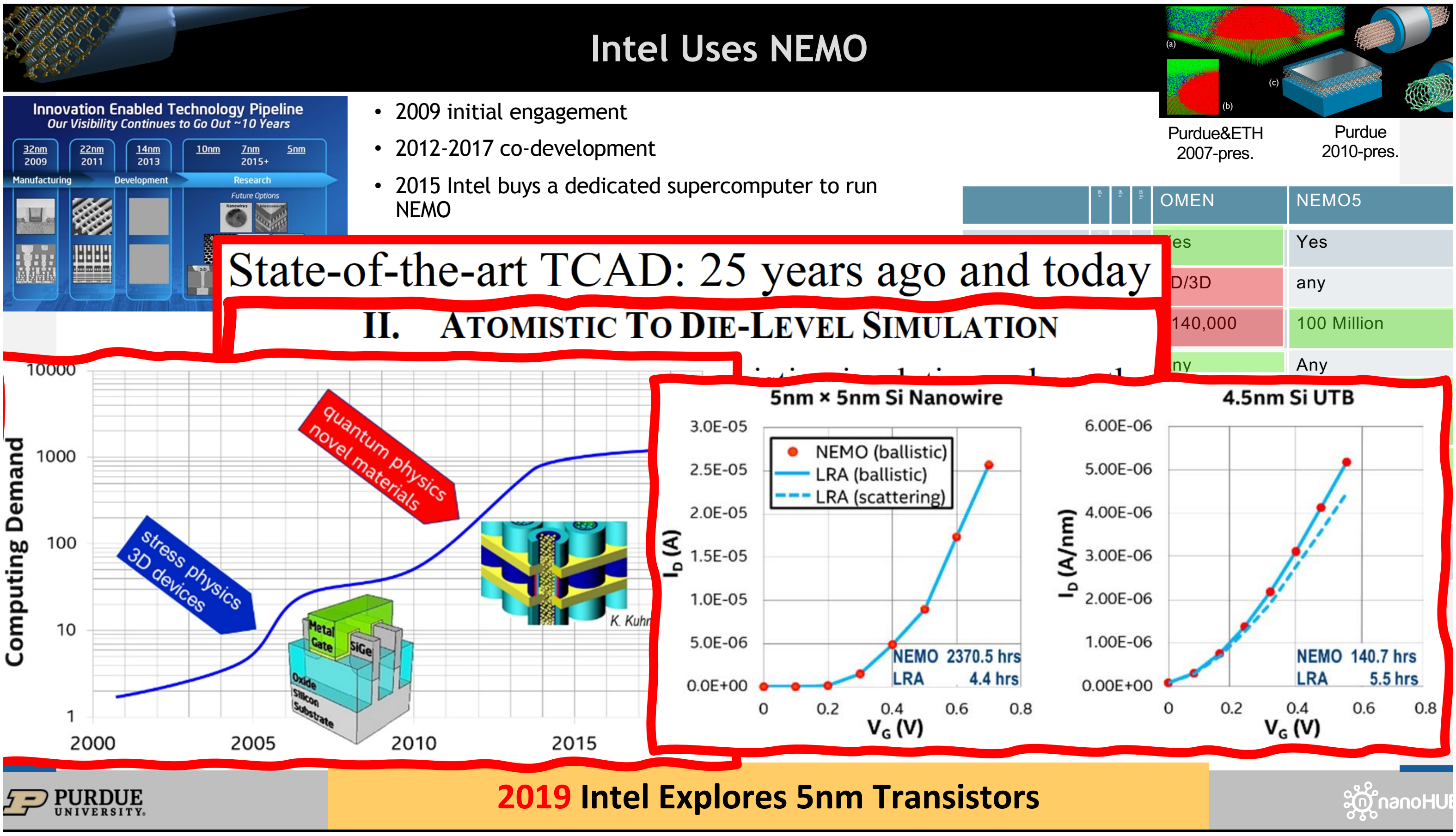


Intel Uses NEMO

- 2009 initial engagement
- 2012-2017 co-development
- 2015 Intel buys a dedicated supercomputer to run NEMO

Purdue&ETH 2007-pres.

Purdue 2010-pres.

OMEN	NEMO5
es	Yes
D/3D	any
140,000	100 Million
ny	Any

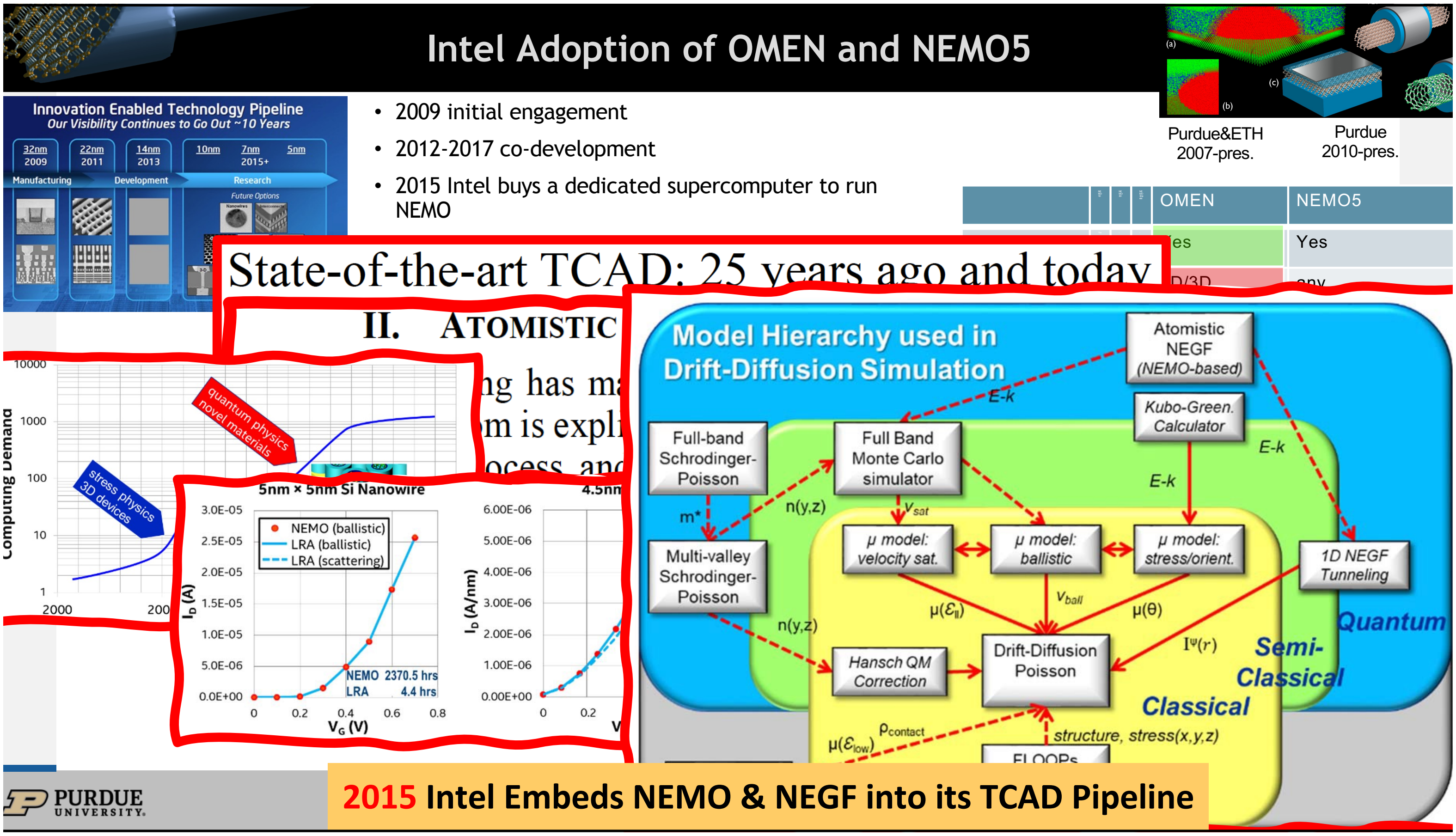
State-of-the-art TCAD: 25 years ago and today

II. ATOMISTIC TO DIE-LEVEL SIMULATION

NEMO	2370.5 hrs
LRA	4.4 hrs

NEMO	140.7 hrs
LRA	5.5 hrs

2019 Intel Explores 5nm Transistors



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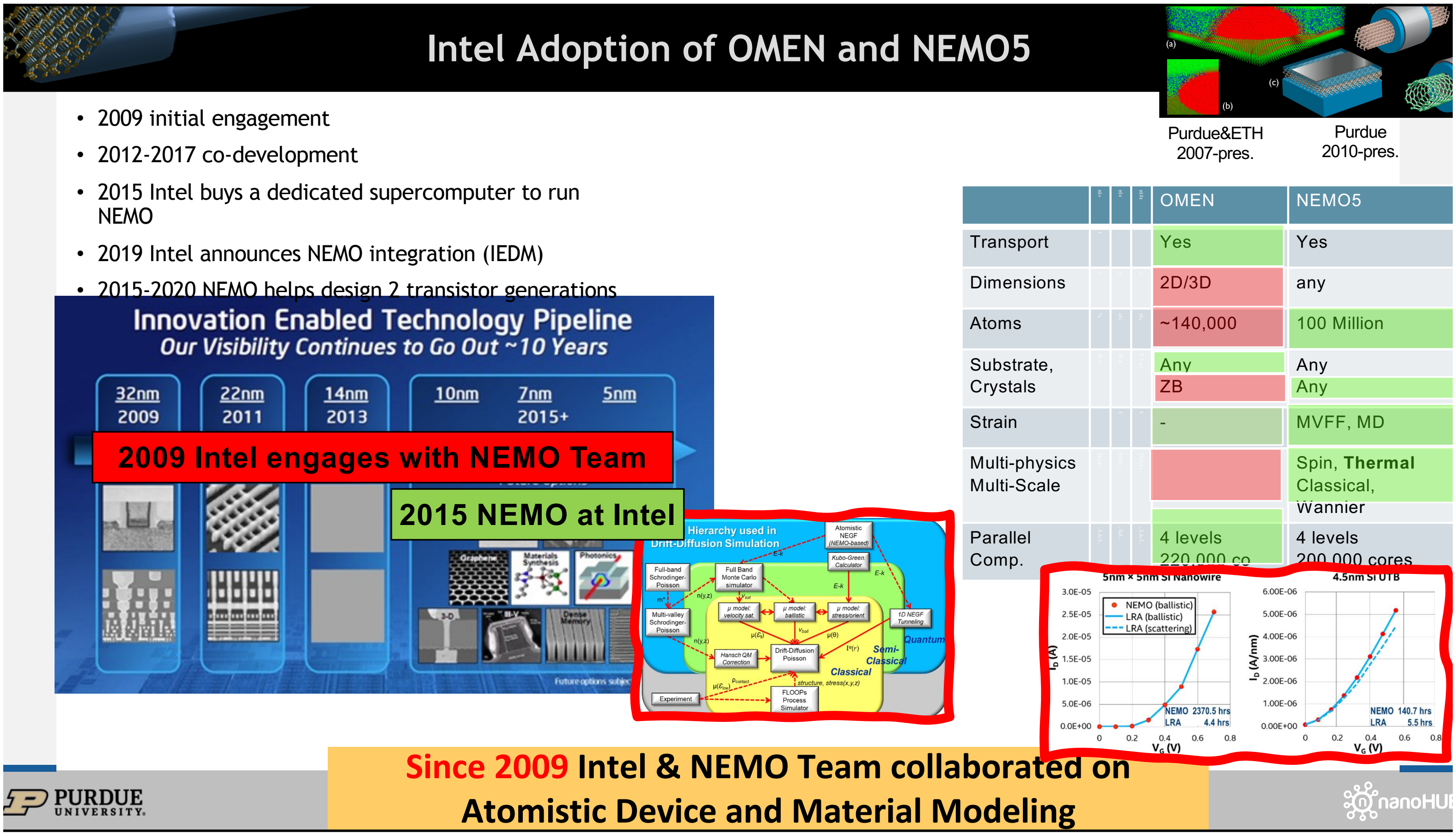
- 2015 Intel buys a dedicated supercomputer to run NEMO

2015 Intel Embeds NEMO & NEGF into its TCAD Pipeline



Intel Adoption of OMEN and NEMO5

- 2009 initial engagement
- 2012-2017 co-development
- 2015 Intel buys a dedicated supercomputer to run NEMO
- 2019 Intel announces NEMO integration (IEDM)
- 2015-2020 NEMO helps design 2 transistor generations

Purdue&ETH 2007-pres.

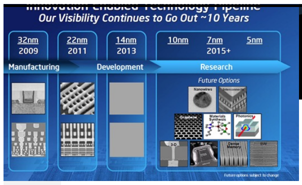
Purdue 2010-pres.

	OMEN	NEMO5
Transport	Yes	Yes
Dimensions	2D/3D	any
Atoms	~140,000	100 Million
Substrate, Crystals	Any ZB	Any Any
Strain	-	MVFF, MD
Multi-physics Multi-Scale		Spin, **Thermal** Classical, Wannier
Parallel Comp.	4 levels 220,000 co	4 levels 200,000 cores

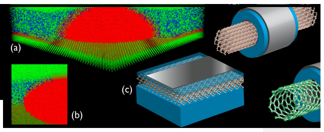
2009 Intel engages with NEMO Team

2015 NEMO at Intel

Since 2009 Intel & NEMO Team collaborated on Atomistic Device and Material Modeling



Usability of TCAD Tools on nanoHUB



Purdue&ETH
2007-pres.

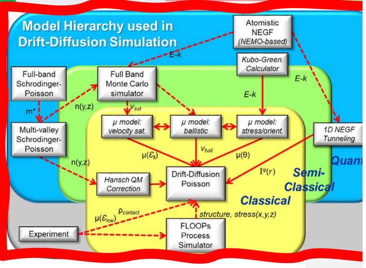
20

- Typical TCAD tools requirements:
  - Fundamental understanding of devices & processes
  - Significant operational training
  - Dedicated computational and license resources
  - ⇒Intended end-user: a designer and developer
- Typical semiconductor device of processing c
  - Teach fundamentals, not TCAD skills
  - Full schedule over a semester
  - ⇒Students do ~~NOT~~ use modeling and simulation
  - ⇒Apps wrapped around sophisticated tools!

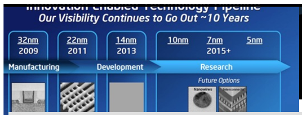
Research

Education

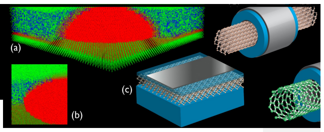
				OMEN	NEM
Transport				Yes	Yes
Dimensions				2D/3D	any
Atoms				~140,000	100
Substrate, Crystals				Any ZB	Any Any
Strain				-	MVF
Multi-physics Multi-Scale					Spin Clas



Since 2007 New Ways to Distribute Interactive TCAD Tools

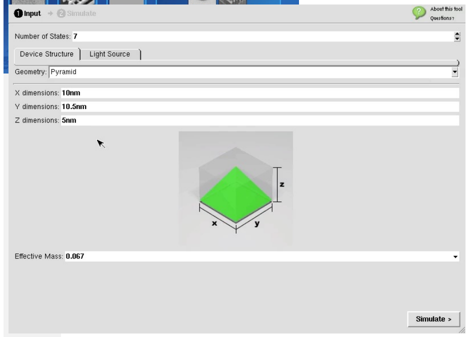


OMEN and NEMO5
Quantum Electronics on nanoHUB



Purdue&ETH
2007-pres.

20



Number of States: 7

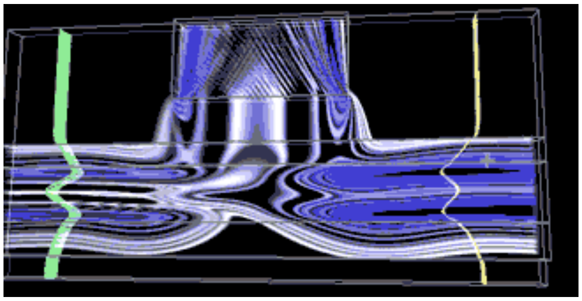
Geometry: Pyramid

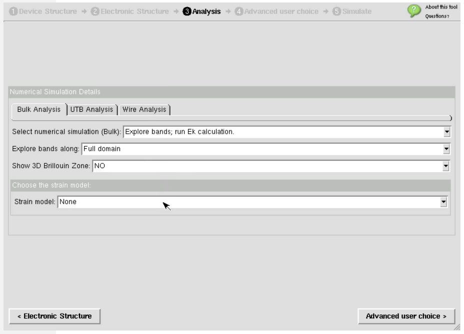
X dimensions: 10nm

Y dimensions: 10.5nm

Z dimensions: 5nm

Effective Mass: 0.067



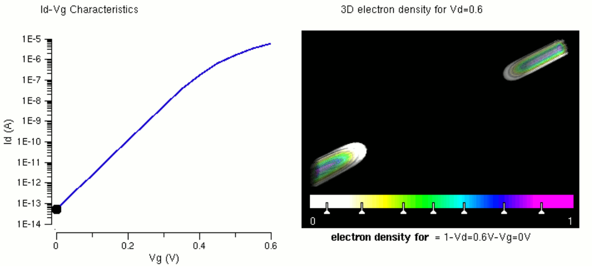


Select numerical simulation (Bulk): Explore bands; run Ek calculation.

Explore bands along: Full domain

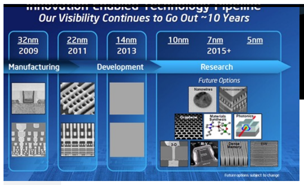
Show 3D Brillouin Zone: NO

Strain model: None

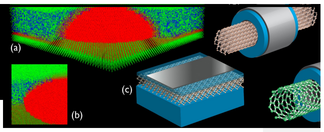


				OMEN	NEM
Transport				Yes	Yes
Dimensions				2D/3D	any
Atoms				~140,000	100
Substrate, Crystals				Any ZB	Any Any
Strain				-	MVF
Multi-physics Multi-Scale					Spin Clas Wan
Parallel Comp.				4 levels 220,000 co	4 lev 200,0

Since 2007 Atomistic tools on nanoHUB

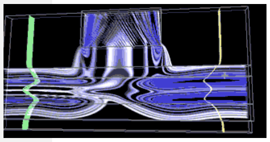


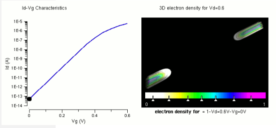
OMEN and NEMO5
Quantum Electronics on nanoHUB

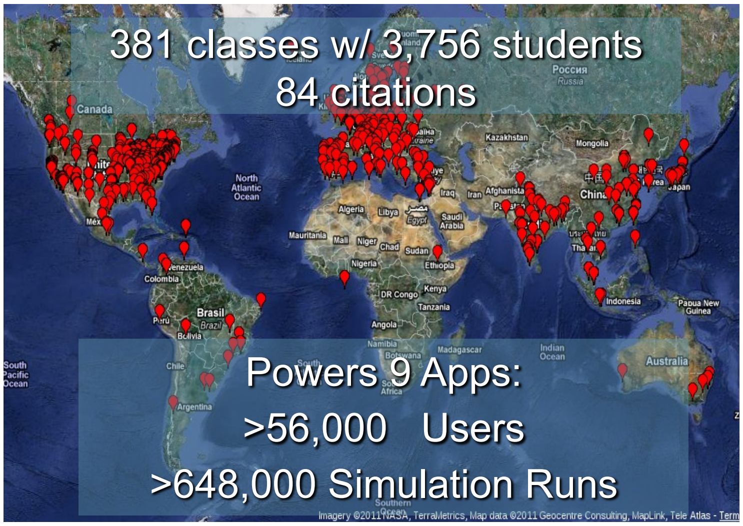


Purdue&ETH 2007-pres.

Purdue 2010-pres.







381 classes w/ 3,756 students
84 citations

Powers 9 Apps:
>56,000 Users
>648,000 Simulation Runs

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Strain				-	MVFF, MD
Multi-physics Multi-Scale					Spin, **Thermal** Classical, Wannier
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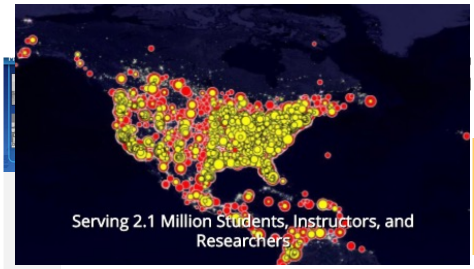

Serving 2.1 Million Students, Instructors, and Researchers

Semiconductor Education and Workforce Development. Simulation-Based Immersive Learning, Courses, Virtual Labs

Each Year over 8,000 students in classrooms use interactive Semiconductor modeling tools on nanoHUB

Who?
> 2.1 million users annually
> 2,400 contributors
- 172 countries
- Faculty
- Students
- Industry practitioners

What ?
> 700 nano-Apps in the cloud
> 6,500 lectures and tutorials
> 170 courses => MOOC

Cyberinfrastructure
24/7 operation with 99.4% uptime

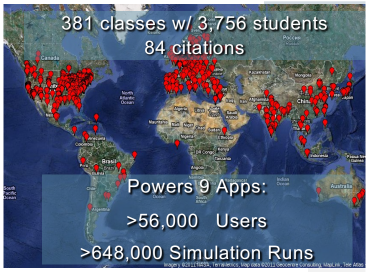
Educational Impact
- >89,730 students use tools in classrooms, >3,840 classes, 185 institutions
- Rapid curriculum change <6 months adoption rate

Research Impact:
- nanoHUB tools now listed in

WEB OF SCIENCE Google Scholar

- > 2,600 papers cite nanoHUB
- > 68,000 secondary citations
- h-index of 121

Transport
Dimension
Atoms
Substrate, Crystals
Strain
Multi-physi Multi-Scale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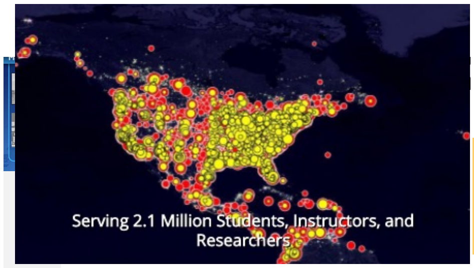
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Dimension
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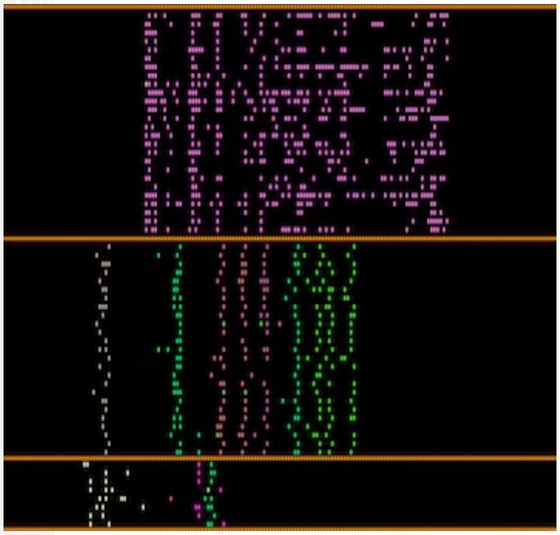

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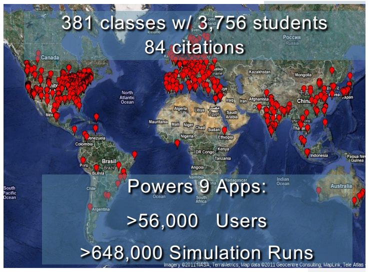
381 classes w/ 3,756 students
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Imagery ©2011 NASA, TerraMetrics, Map data ©2011 Geocentre Consulting, MapLink, Tele Atlas

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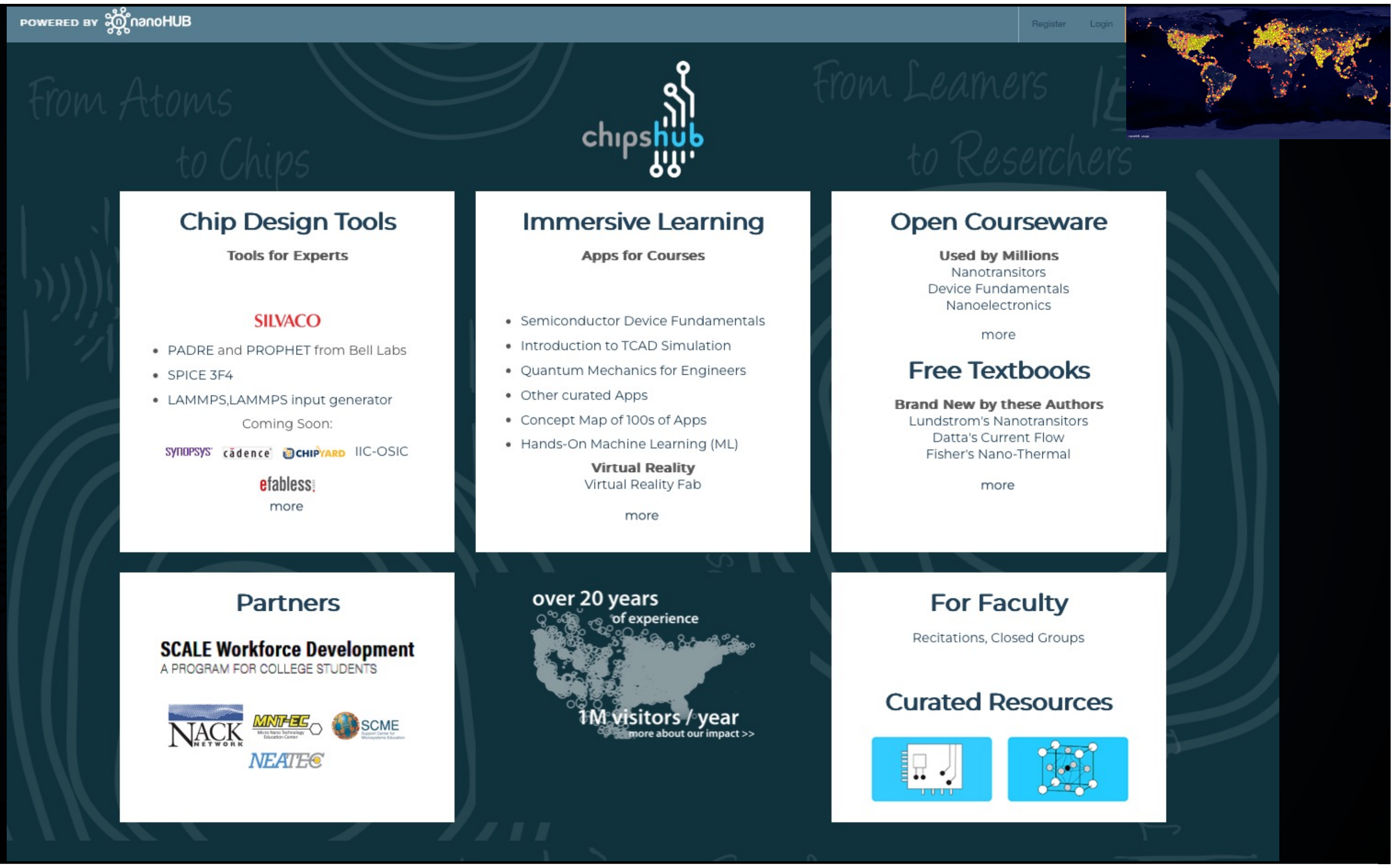
chipshub.org on nanoHUB
Simulation-Based Immersive Learning
Courses, Virtual Labs



Chip Design Tools

Tools for Experts

SILVACO
- PADRE and PROPHET from Bell Labs
- SPICE 3F4
- LAMMPS,LAMMPS input generator

Coming Soon:
SYNOPSYS cadence CHIPYARD IIC-OSIC
efabless
more

Immersive Learning

Apps for Courses

- Semiconductor Device Fundamentals
- Introduction to TCAD Simulation
- Quantum Mechanics for Engineers
- Other curated Apps
- Concept Map of 100s of Apps
- Hands-On Machine Learning (ML)

Virtual Reality
Virtual Reality Fab
more

Open Courseware

Used by Millions
Nanotransitors
Device Fundamentals
Nanoelectronics
more

Free Textbooks

Brand New by these Authors
Lundstrom's Nanotransitors
Datta's Current Flow
Fisher's Nano-Thermal
more

Partners

SCALE Workforce Development
A PROGRAM FOR COLLEGE STUDENTS
NACK NETWORK MNT-EC SCME NEATEC

over 20 years of experience
1M visitors / year
more about our impact >>

For Faculty

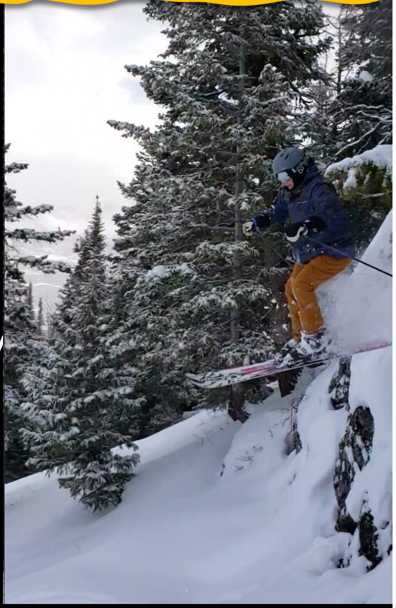
Recitations, Closed Groups

Curated Resources

Challenges at the Frontier of Modeling

I jumped off a cliff many times

- Modelling goals shared beyond specific devices
  - Qualitatively and quantitatively guide physics experiments
  - Design and engineer devices
  - Predictive not just “descriptive” or tightly calibrated
  - Realistically scaled and extended devices (beyond conceptual stick diagrams)
  - Transferrable approaches beyond a single device or material
- Transferrable approaches shared beyond specific dev
  - Multi-physics & multi-scale segmentation or partition
  - Smart choices of basis sets
  - Scalable compute times & accuracy (quick & dirty ⇔ detailed)
  - Usability and access to users (incl. computing hardware)



How did we get from Quantum Transport in RTDs to billions of chips with billions of nanotransistors?

Challenges at the Frontier of Modeling

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These Meta-Goals and Meta-Approaches define
The Frontiers of Modeling

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Thank you!
To my family!

If this does not work:
My plan B is ski teacher ☺

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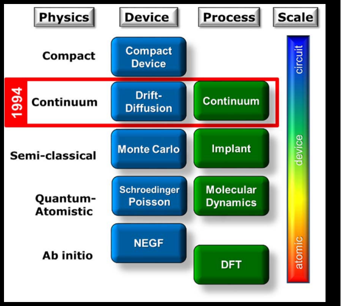
Challenges at the Frontier of Modeling

So What's Next????

Some opinionated opinions:

- NCFETs will give us maybe a few more generations
- TFETs are too hard
- The search for the next switch failed!

Si-CMOS is the end-game for logic (steel airplanes)



Physics	Device	Process
Compact	Compact Device	
Continuum	Drift-Diffusion	Continuum
Semi-classical	Monte Carlo	Implant
Quantum-Atomistic	Schroedinger Poisson	Molecular Dynamics
Ab initio	NEGF	DFT

Fundamental device research - curiosity driven

Application driven device research

Transition novel methods and insights to other fields

Nanoelectronics with user and machine learning

Novel devices to reduce circuit complexity - novel architectures

- Embrace the end of CMOS

Challenges at the Frontier of Modeling

So What's Next????

Si-CMOS is the end-game for logic (steel airplanes)

Fundamental device research - curiosity driven:

- 2D materials (maybe for memory, interconnect, or logic)

Application driven device research

- New materials in BEOL for 3D integration
- MEMs in new materials 2D and ferroelectric

Transition novel methods and insights to other fields

- Introduce OPEN systems to material science and chemistry

Nanoelectronics with user and machine learning

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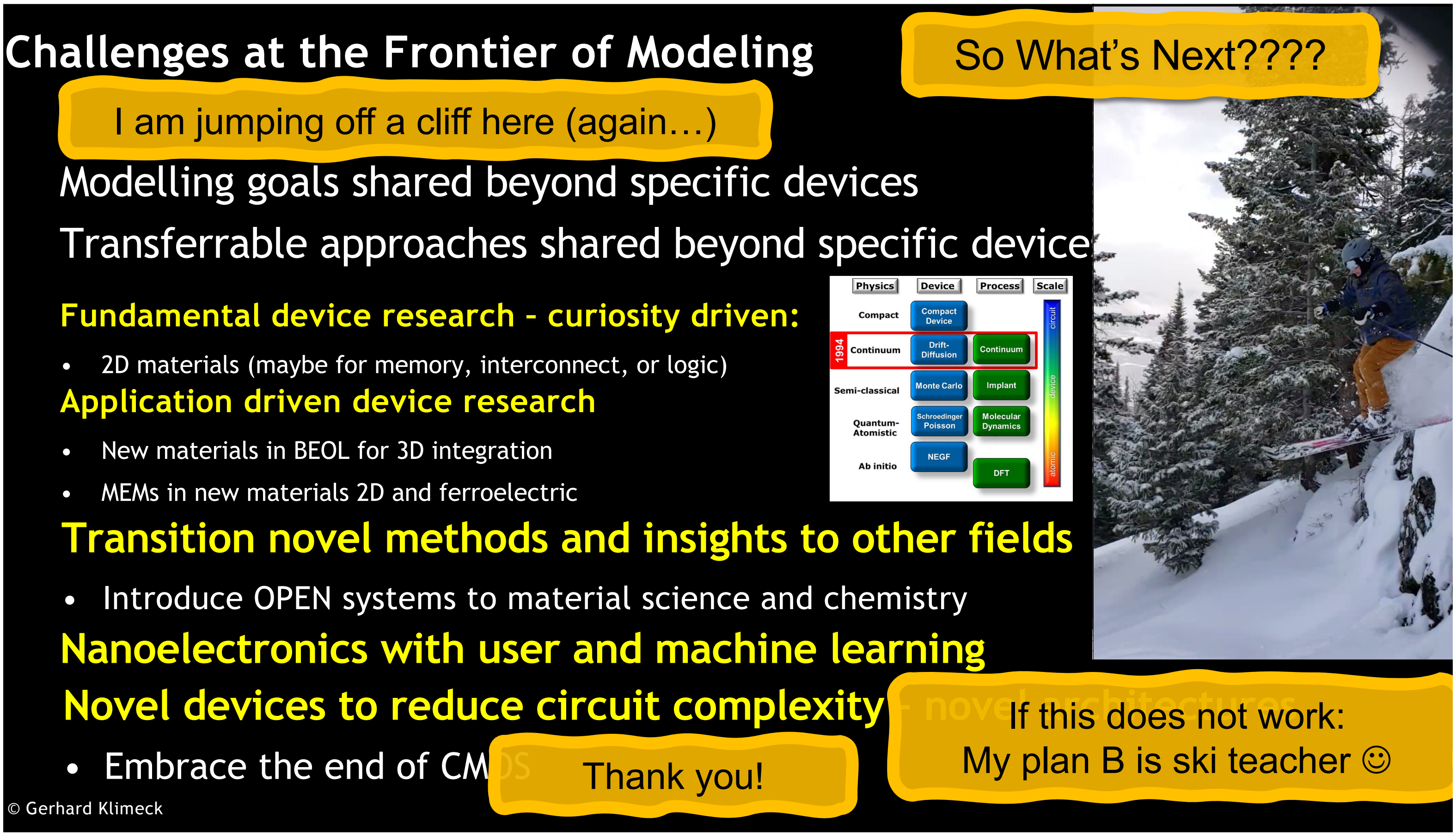

Challenges at the Frontier of Modeling

So What's Next????

I am jumping off a cliff here (again…)

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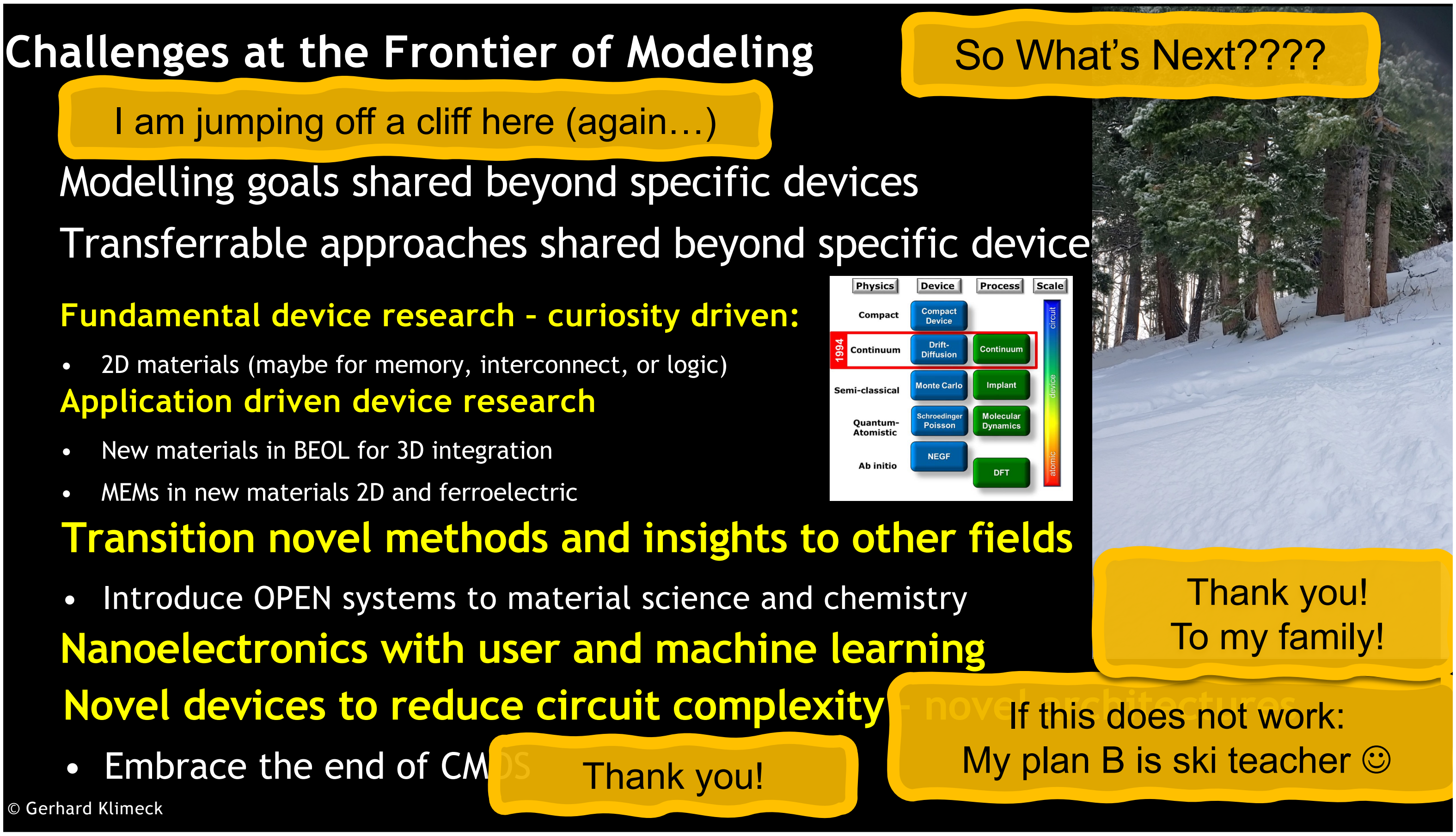
© Gerhard Klimeck



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My plan B is ski teacher ☺

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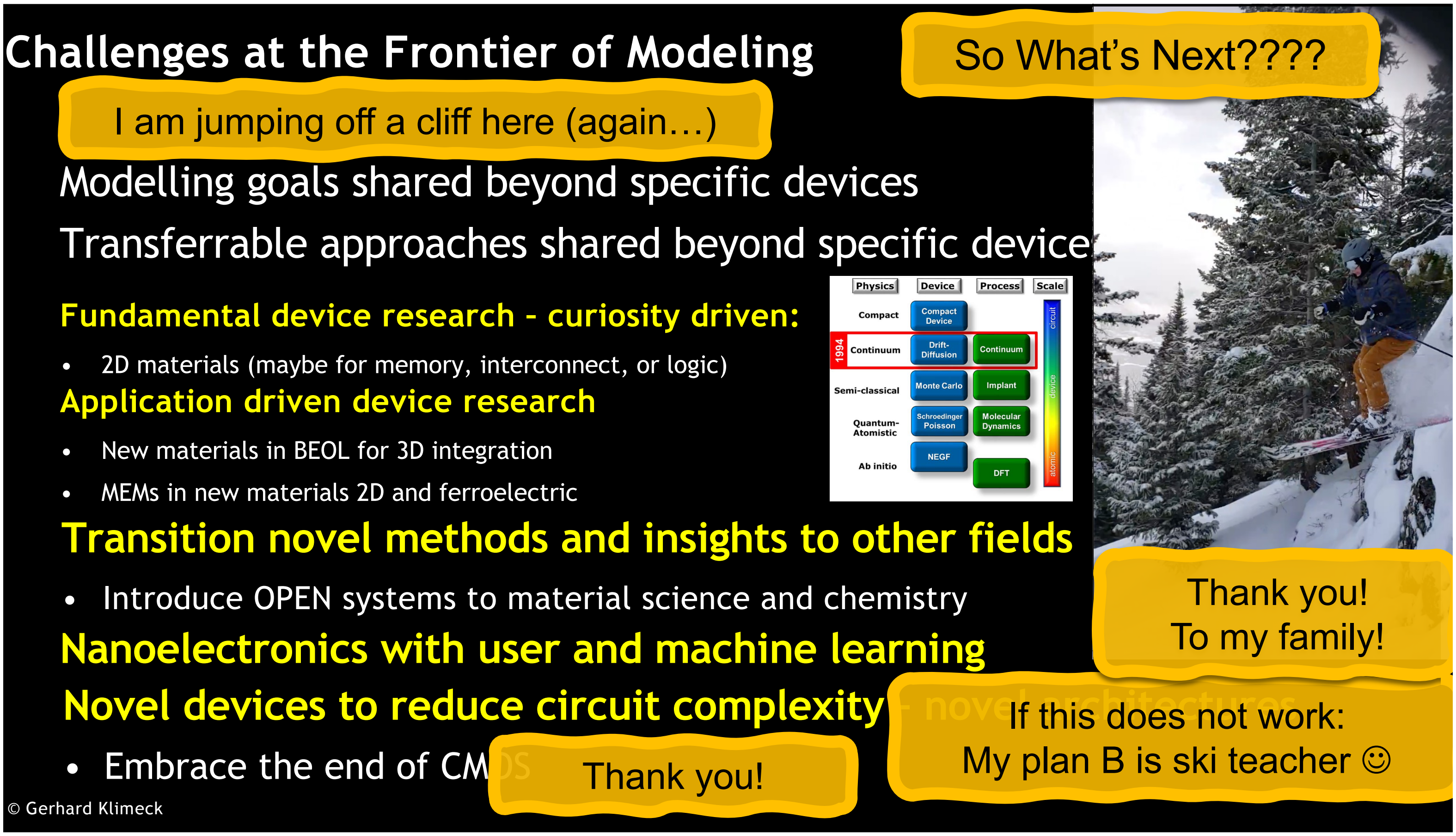

Challenges at the Frontier of Modeling

I am jumping off a cliff here (again…)

Modelling goals shared beyond specific devices

Transferrable approaches shared beyond specific device

Fundamental device research - curiosity driven:

- 2D materials (maybe for memory, interconnect, or logic)

Application driven device research

- New materials in BEOL for 3D integration
- MEMs in new materials 2D and ferroelectric

Transition novel methods and insights to other fields

- Introduce OPEN systems to material science and chemistry

Nanoelectronics with user and machine learning

Novel devices to reduce circuit complexity – novel architectures

- Embrace the end of CMOS

So What's Next????

Thank you!
To my family!

If this does not work:
My plan B is ski teacher ☺

Thank you!

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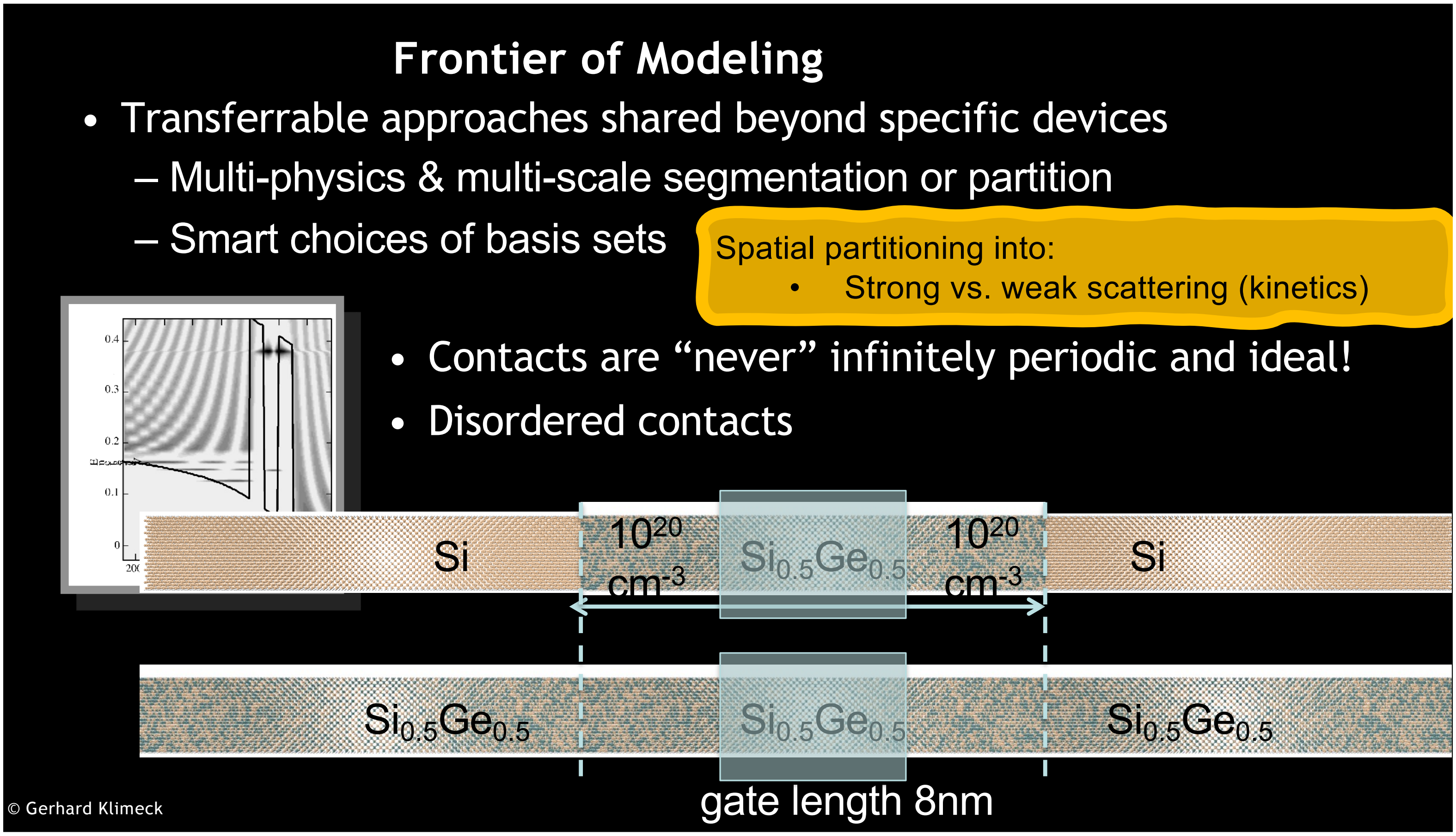

Frontier of Modeling

- Transferrable approaches shared beyond specific devices
  - – Multi-physics & multi-scale segmentation or partition
  - – Smart choices of basis sets

Spatial partitioning into:
- Strong vs. weak scattering (kinetics)

- Contacts are "never" infinitely periodic and ideal!
- Disordered contacts

gate length 8nm

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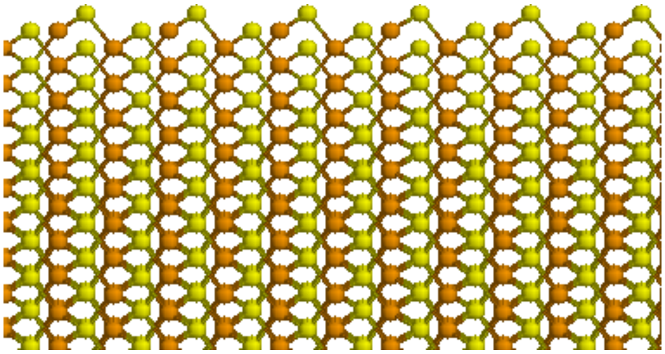
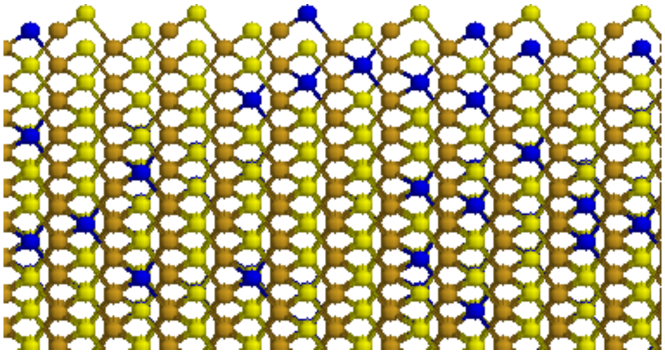
AlGaAs alloy nanowire
Adding Al into GaAs



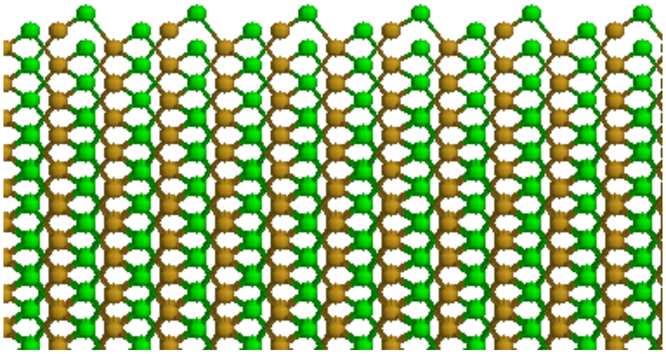
Ordered nanowire
-perfect GaAs

Insert
Al



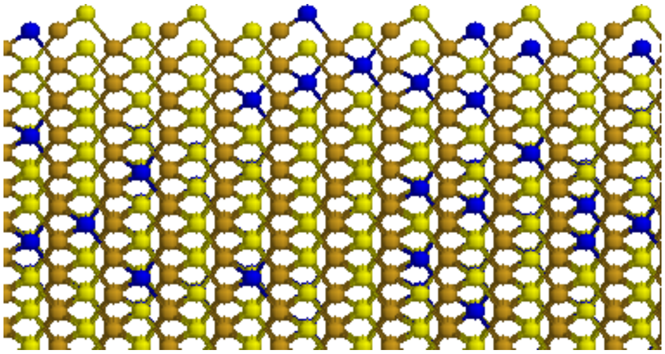
Alloyed nanowire
-locally disordered
-Not periodic

AlGaAs alloy nanowire
VCA Average



Alloyed nanowire
-Average Al and Ga
-locally ordered
-Periodic

Typical
Approach:
VCA



Alloyed nanowire
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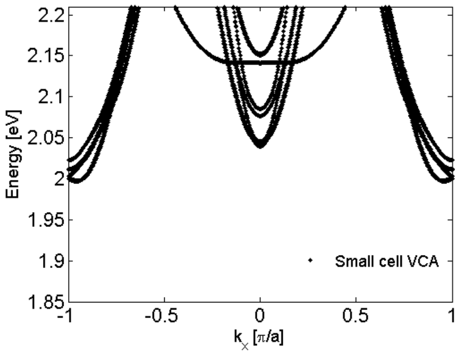
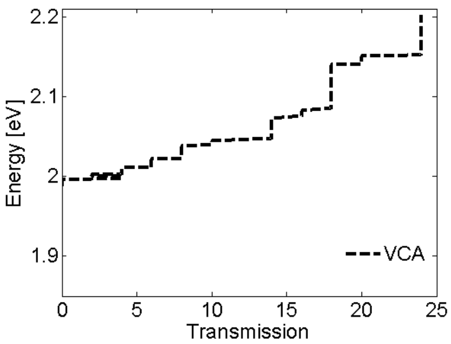
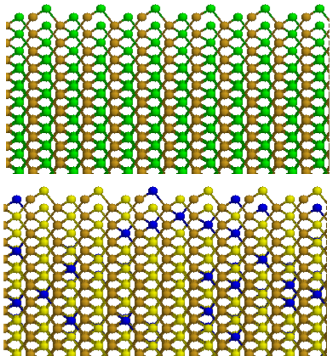
Bandstructure and transmission of VCA AlGaAs alloy nanowire





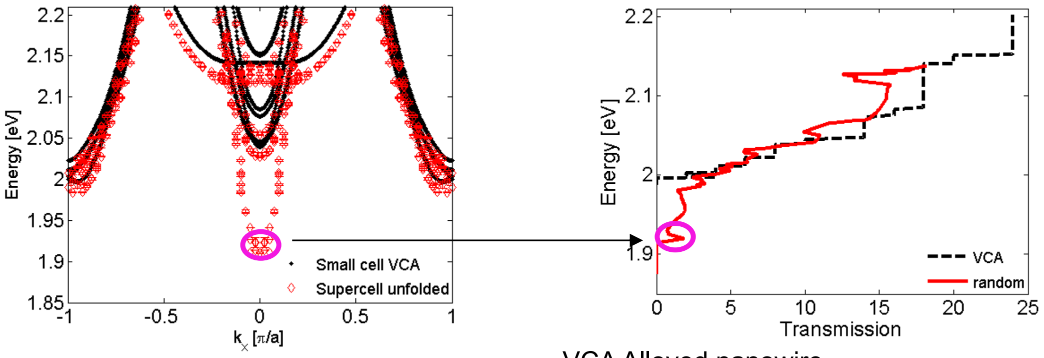


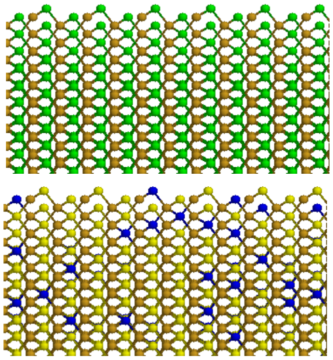
?

VCA Alloyed nanowire
-Average over Al and Ga
-locally ordered
-periodic
-every band has step transmission

Truly Alloyed nanowire
-locally disordered
-Not periodic

Bandstructure and transmission of VCA AlGaAs alloy nanowire





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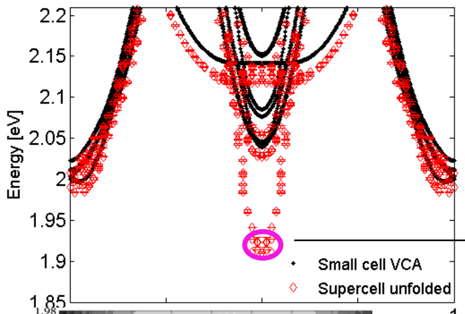
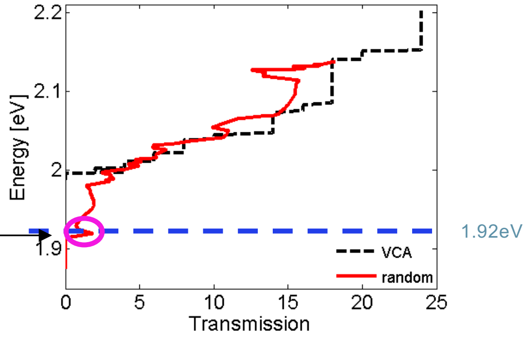
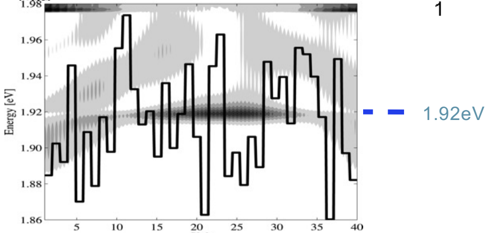
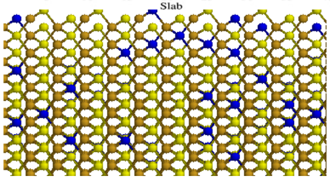
-Approximate bandstructure - lower bandgap
-Transmission - no steps - resonance features

Bandstructure and transmission of VCA AlGaAs alloy nanowire









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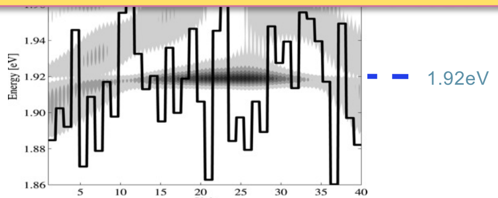
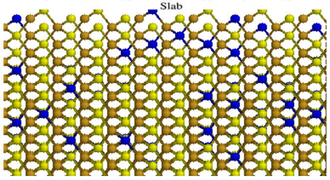
- Transmission - no steps - resonance features
- Localized states - resonant tunneling

Achievements:
true atomistic electronic structure model
Transport with real disordered alloy
Localization of states emerges naturally

Short-Comings:
No true strain model
Contacts are smooth
No I-V
No Phonon Scattering





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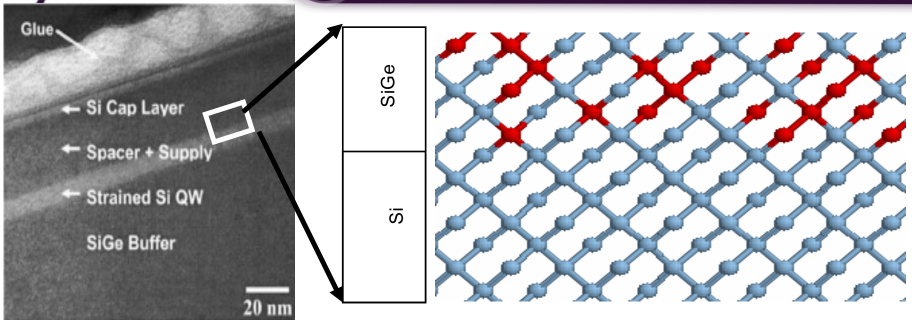
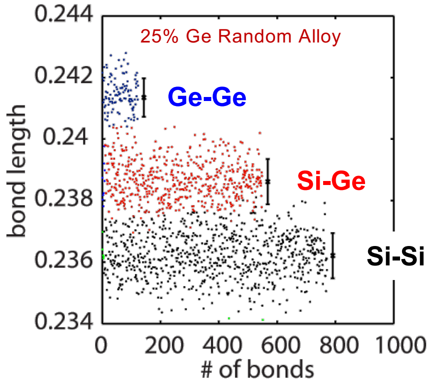
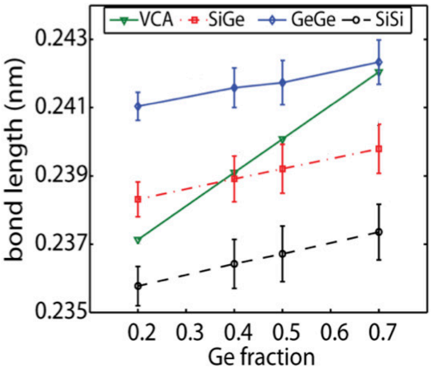
Atomistic Disorder in SiGe



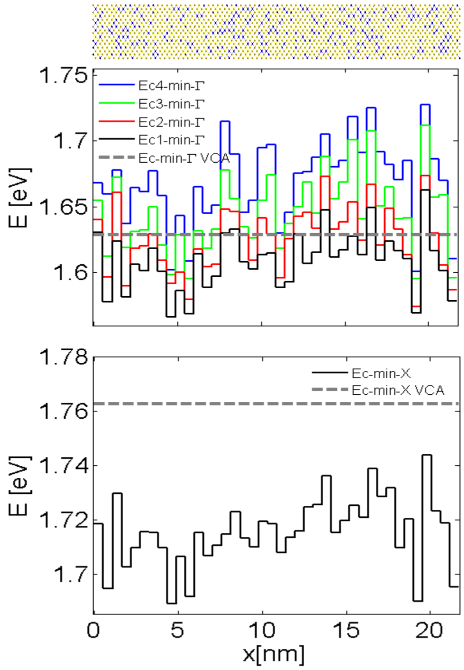
Alloy disorder
- Atom Type
- Bond Length





Atom Positions Fluctuate! => NOT a homogeneous crystal

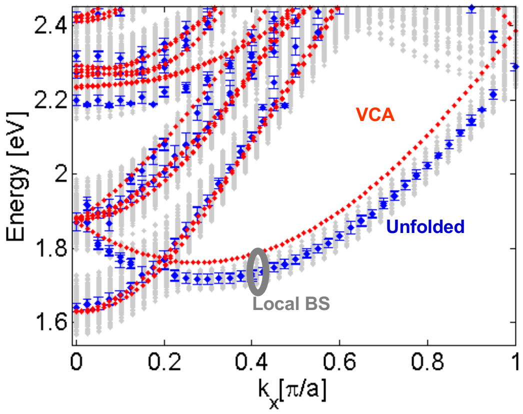
SiGe nanowire



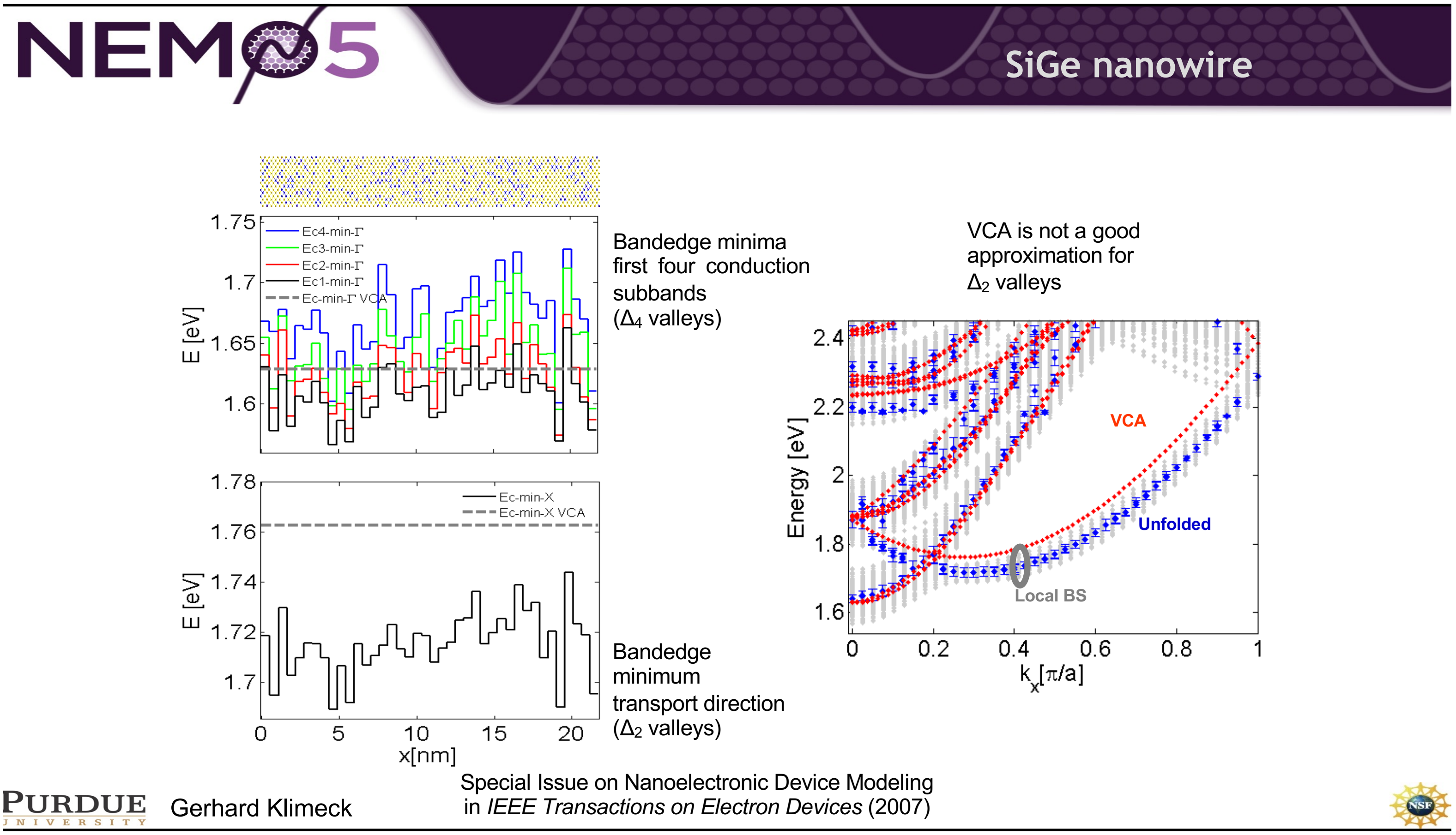
Bandedge minima first four conduction subbands (Δ_4 valleys)

Bandedge minimum transport direction (Δ_2 valleys)

VCA is not a good approximation for Δ_2 valleys



Special Issue on Nanoelectronic Device Modeling in *IEEE Transactions on Electron Devices* (2007)



SiGe nanowire

Bandedge minima first four conduction subbands (Δ_4 valleys)

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Gerhard Klimeck

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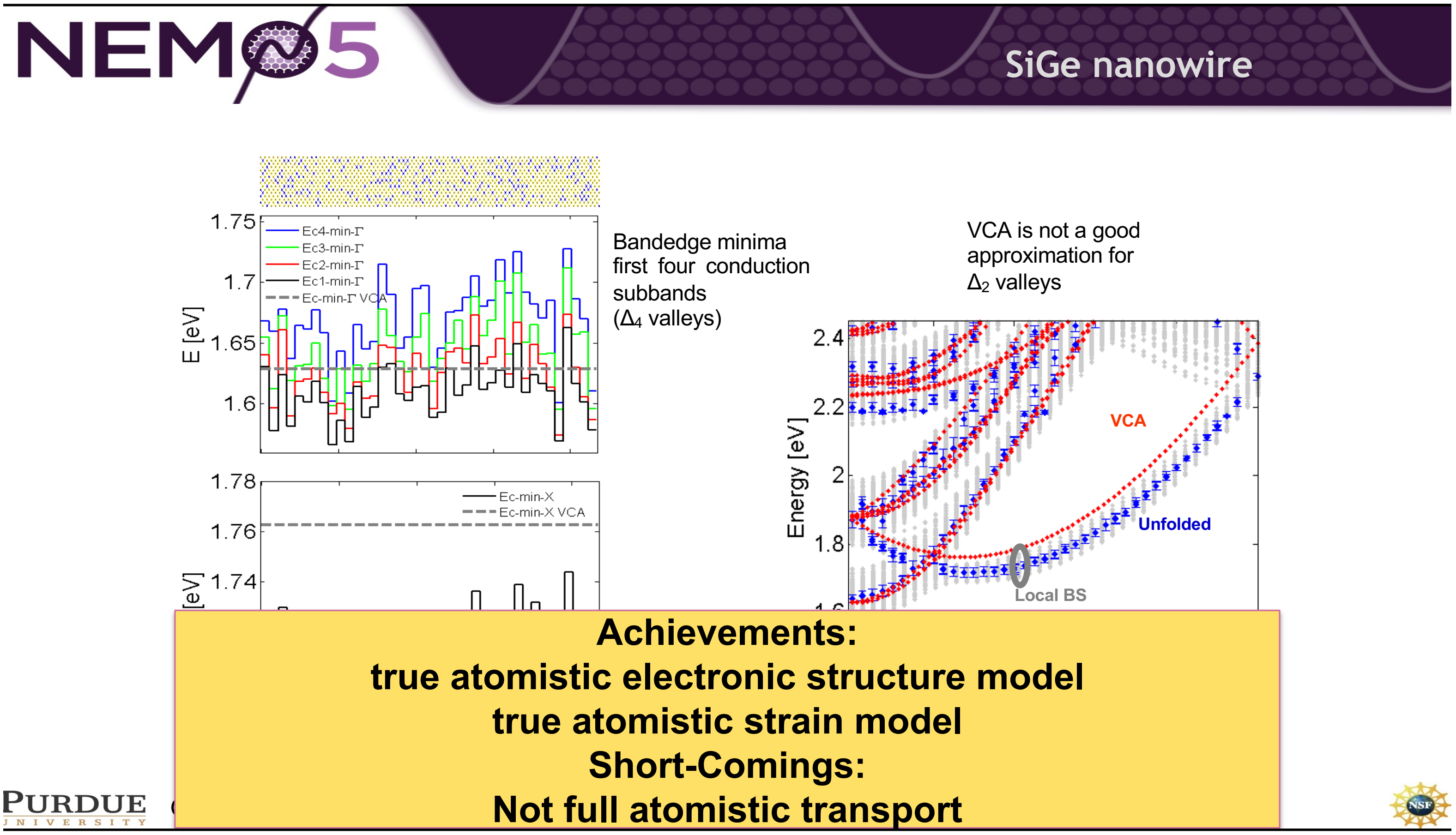


SiGe nanowire

Bandedge minima first four conduction subbands (Δ_4 valleys)

VCA is not a good approximation for Δ_2 valleys

Achievements:
true atomistic electronic structure model
true atomistic strain model
Short-Comings:
Not full atomistic transport

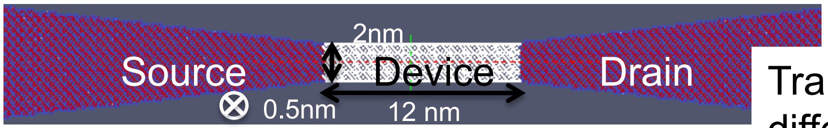
NEMO5 Complex Lead structures

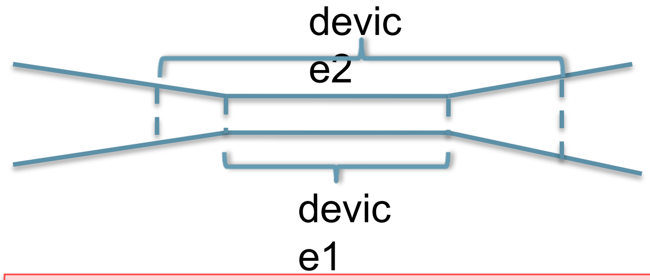
Motivation:
Complex lead geometries are substantial to many state of the art devices
Existing lead algorithms require the full solution of the total lead
but
Lead sections in high distance are not relevant for the device performance

Lead algorithm in NEMO5:
Divide lead into segments
Apply unidirectional RGF on lead surface Green's function
Add smooth damping potential as a function of the lead/device distance

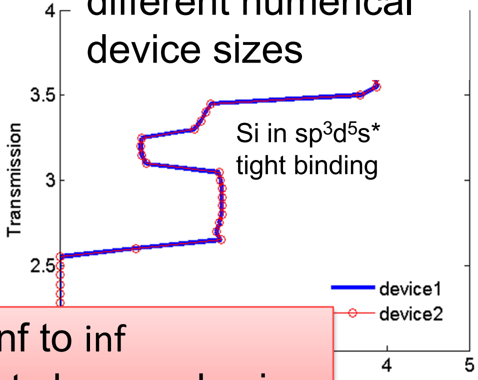
NEMO5 Complex Lead structures

Application: trumpet shaped leads
Fabrication of leads is rarely a perfect rectangular shape
No known algorithm can handle this lead type

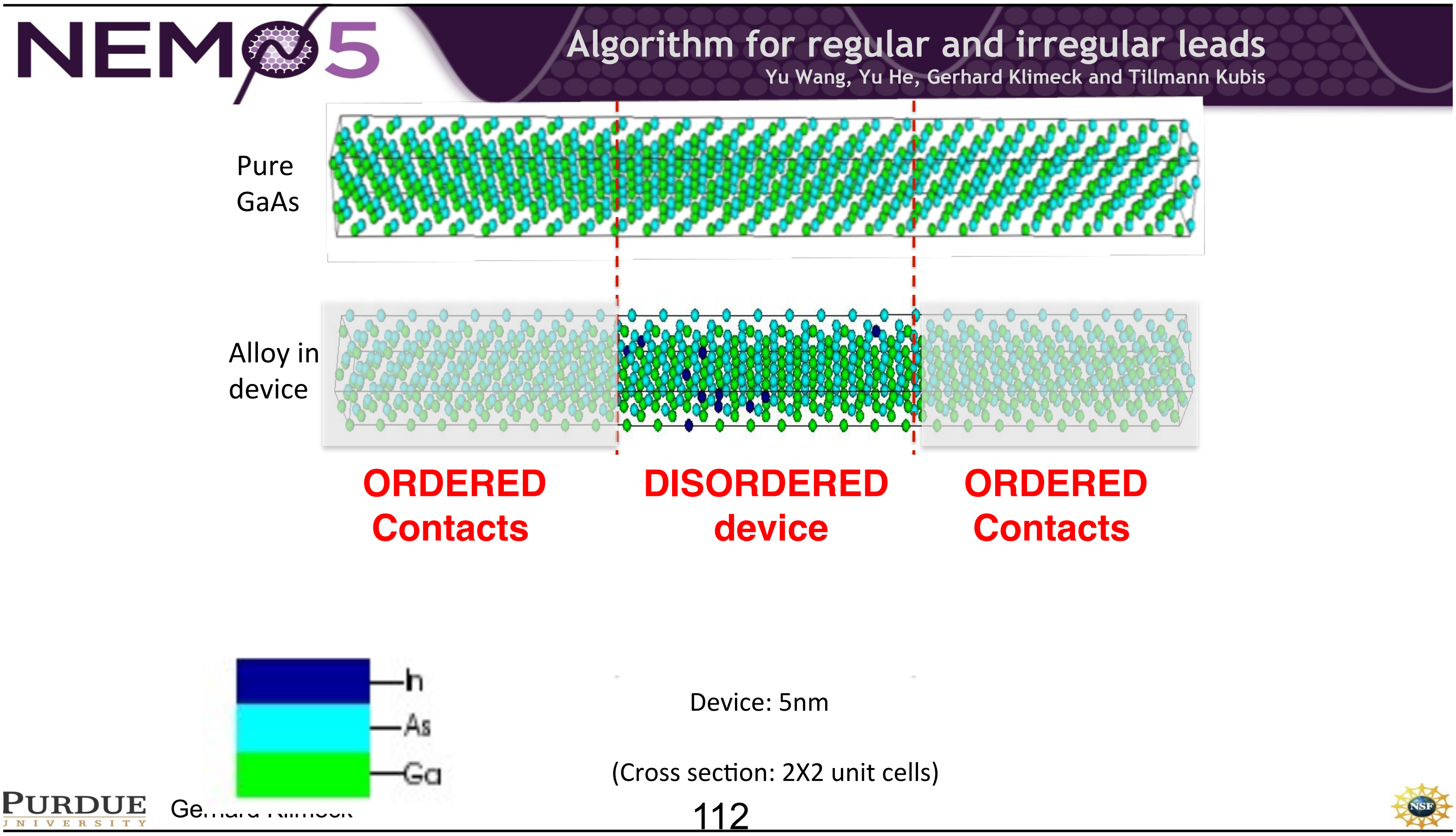




Transmission for different numerical device sizes



Transport: electrons propagate from –inf to inf
✓ Increasing numerical device does not change physics
✓ Algorithm correctly describes general leads



NEMO5

Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis

Pure GaAs

Alloy in device

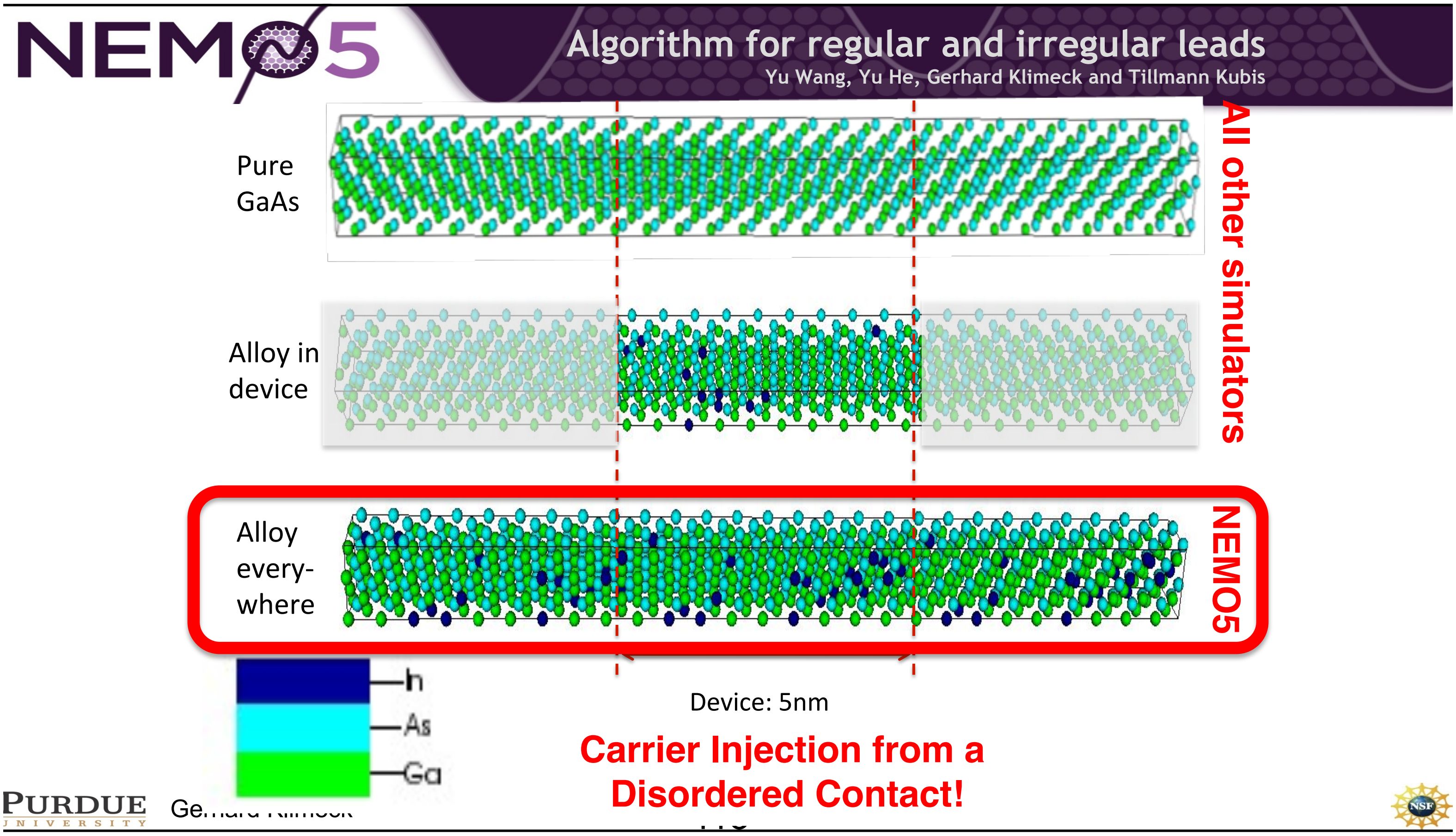
ORDERED Contacts

DISORDERED device

ORDERED Contacts

Device: 5nm

(Cross section: 2X2 unit cells)



NEMO5

Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis

Pure GaAs

Alloy in device

All other simulators

Alloy every-where

NEMO5

Device: 5nm

Carrier Injection from a Disordered Contact!

Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis

Comparison with transer matrix method in regular leads.

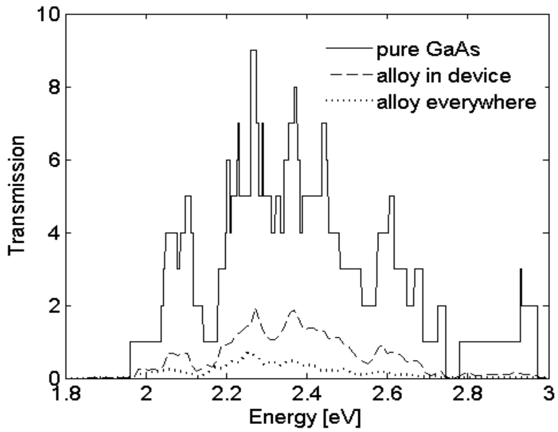
A GaAs nanowire with alloy structures:

2 unit cells

2 unit cells

Device: 5nm

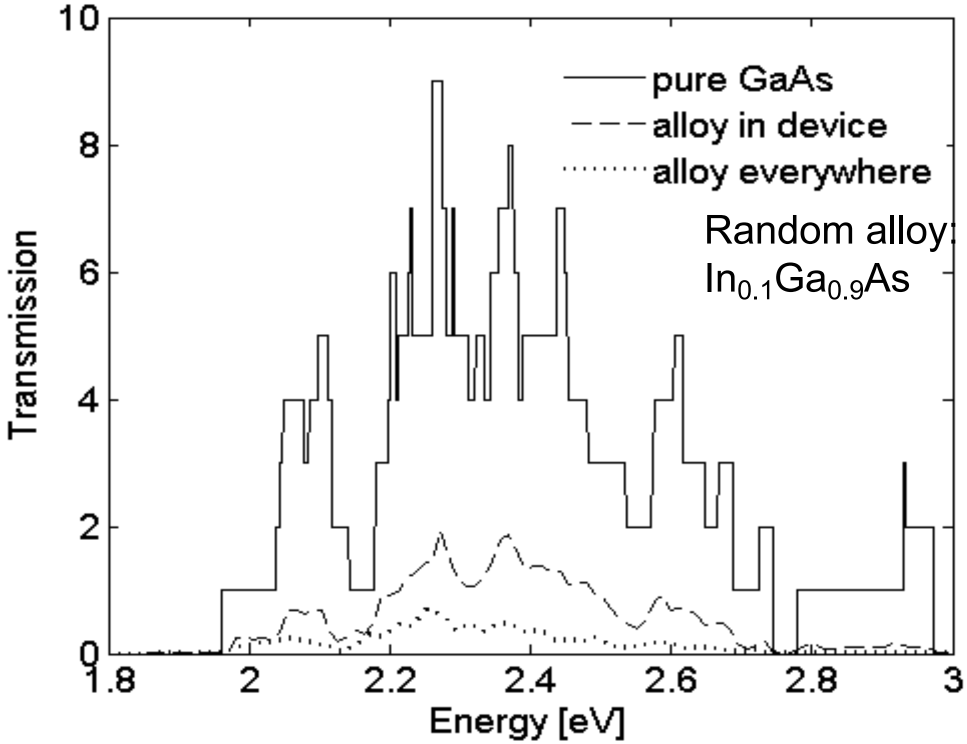
Random alloy: $In_{0.1}Ga_{0.9}As$



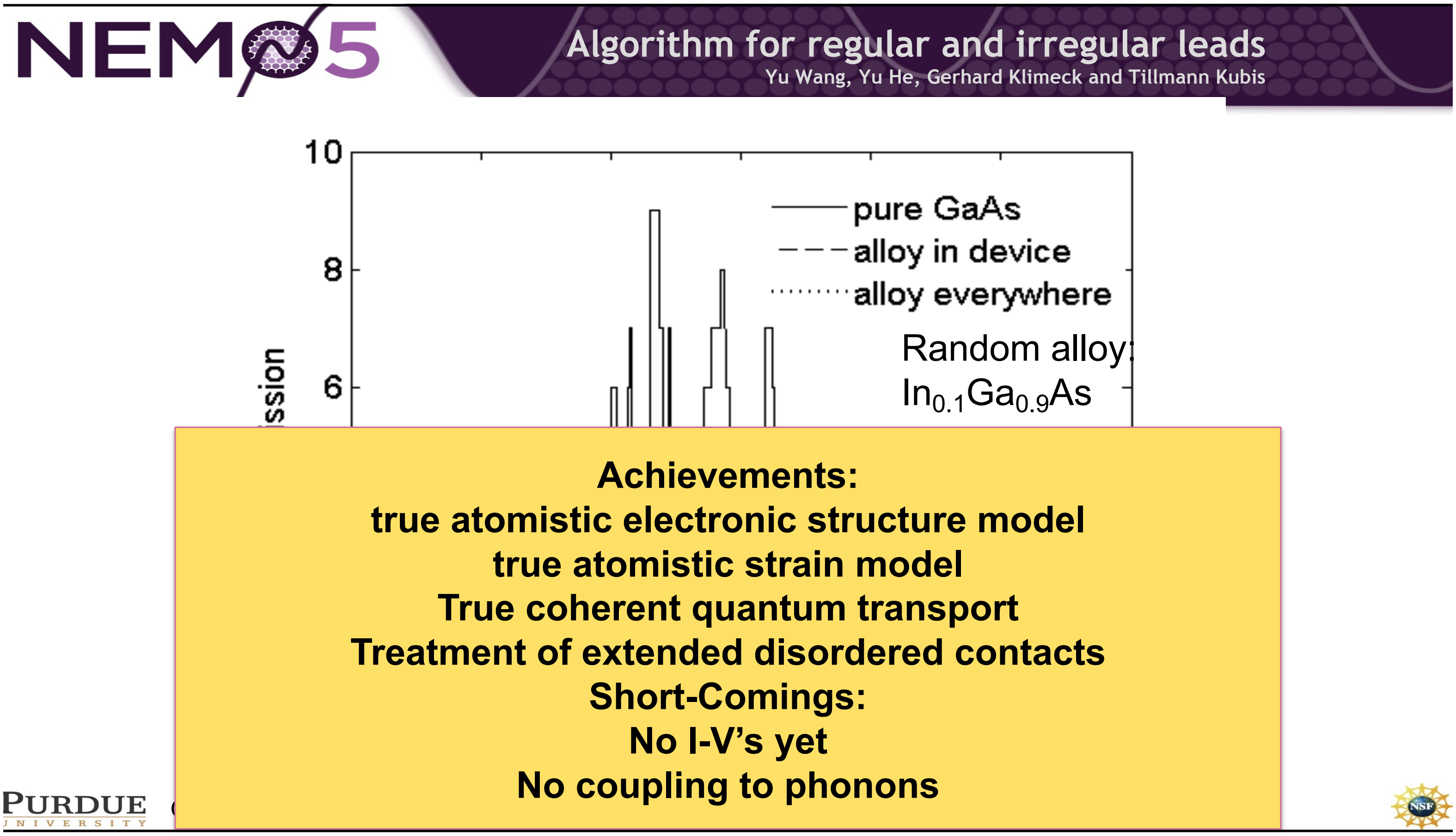
Application in random alloy structures.

Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis



Random alloy: $In_{0.1}Ga_{0.9}As$

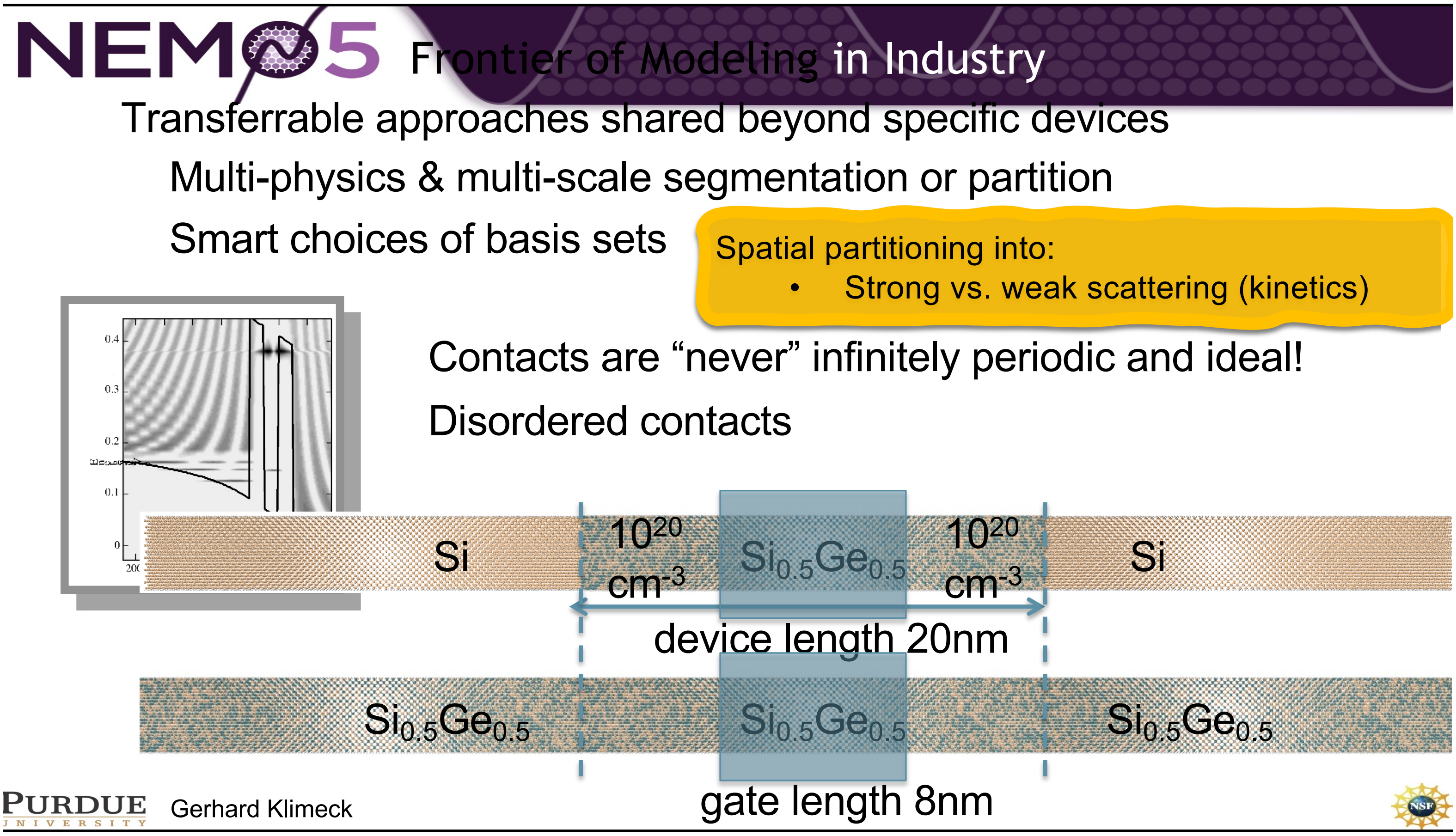


Algorithm for regular and irregular leads

Yu Wang, Yu He, Gerhard Klimeck and Tillmann Kubis

Random alloy: $In_{0.1}Ga_{0.9}As$

Achievements:
true atomistic electronic structure model
true atomistic strain model
True coherent quantum transport
Treatment of extended disordered contacts
Short-Comings:
No I-V's yet
No coupling to phonons



Frontier of Modeling in Industry

Transferrable approaches shared beyond specific devices

Multi-physics & multi-scale segmentation or partition

Smart choices of basis sets

Spatial partitioning into:
- Strong vs. weak scattering (kinetics)

Contacts are “never” infinitely periodic and ideal!

Disordered contacts

Gerhard Klimeck

Frontier of Modeling

- Transferrable approaches shared beyond specific devices
  - Multi-physics & multi-scale segmentation or partition
  - Smart choices of basis sets

Spatial partitioning into:
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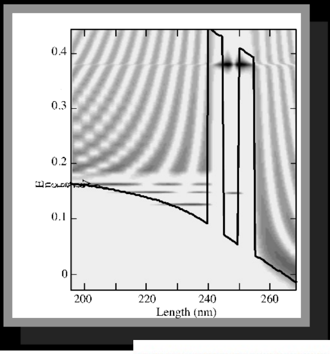
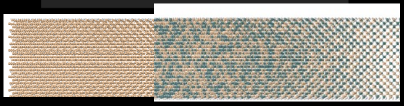
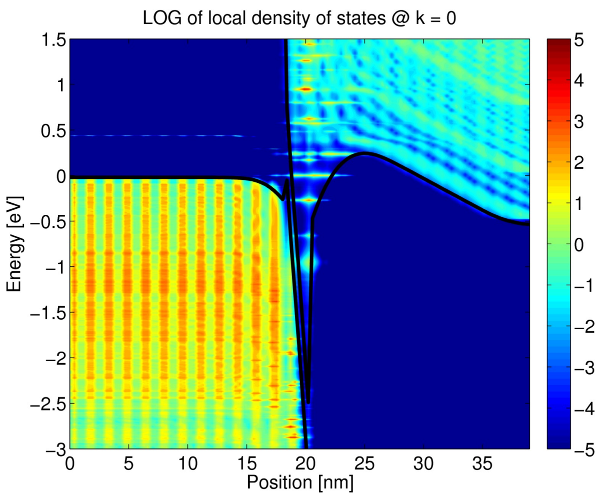




- Contacts are “never” infinitely periodic and ideal!
- Disordered contacts
- Tunnel FETs



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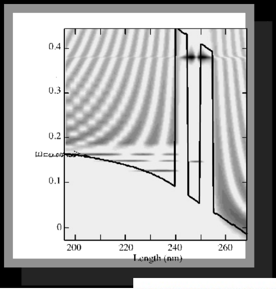
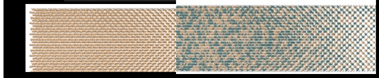
Frontier of Modeling

- Transferrable approaches shared beyond specific devices
  - Multi-physics &
  - Smart choices c





- Cc
- Di
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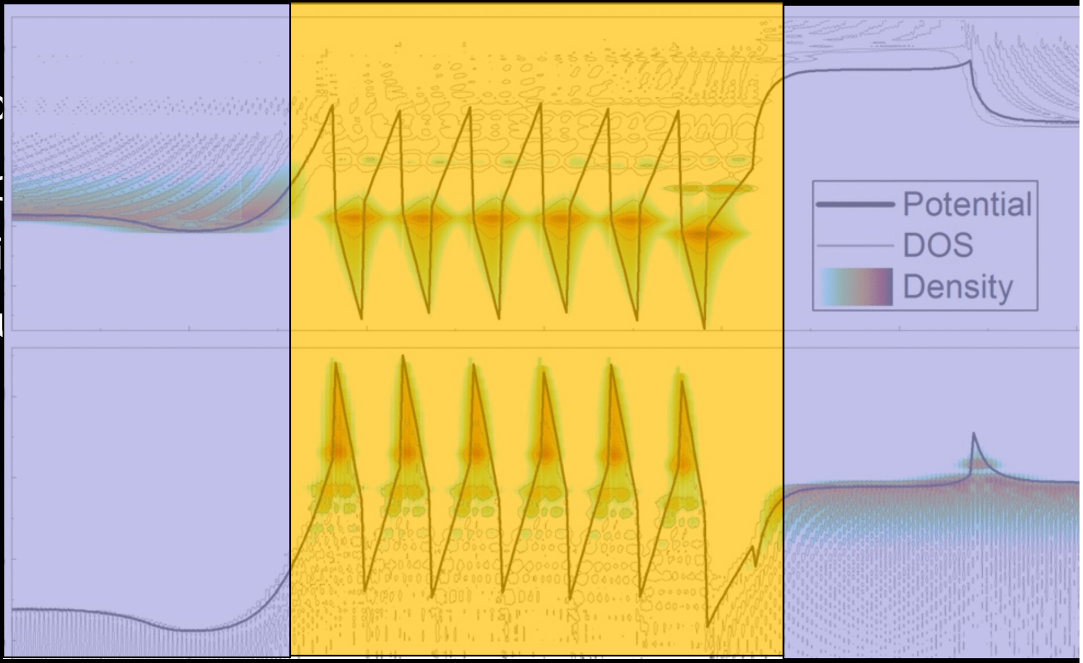
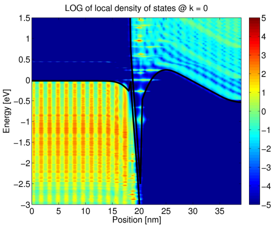




- Superlattice LEDs

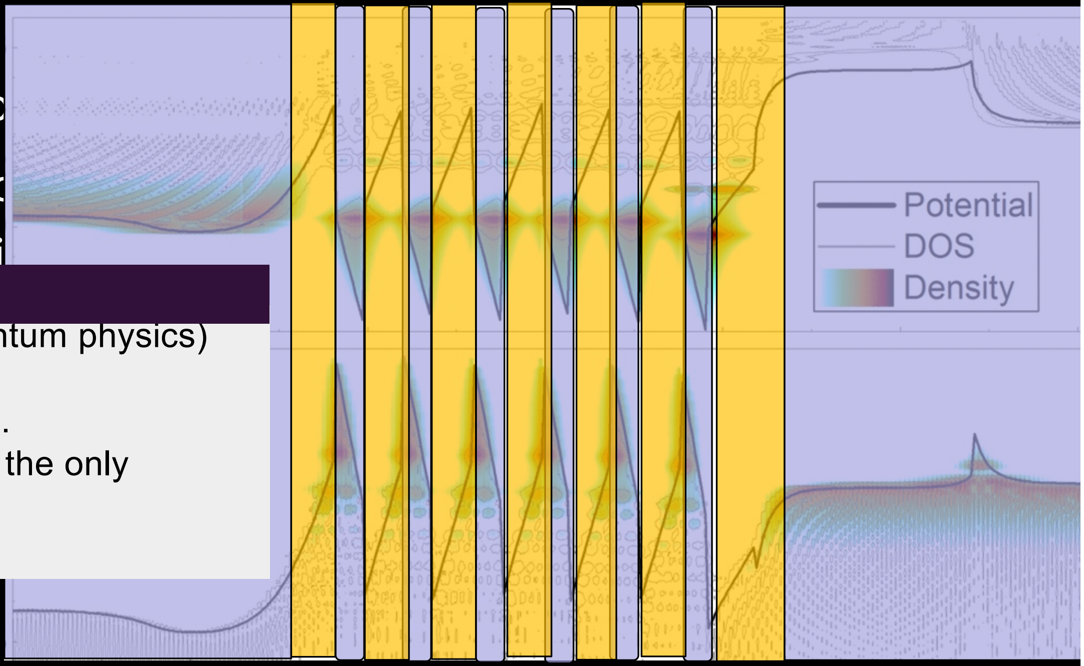
© Gerhard Klimec

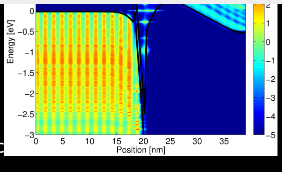
Frontier of Modeling

- Transferrable approaches shared beyond specific devices
  - Multi-physics &
  - Smart choices c

- Co
- Di

Multi Eq Neq NEGF
- Carriers are wave like. (Quantum physics)
- Optimized for QWs
- Eq and Neq regions required.
- Eq: complete thermalization, the only occurrence of recombination





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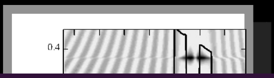

- Contacts are “never” infinitely periodic and ideal!

Multi Eq Neq NEGF
- Carriers are wave like. (Quantum physics)
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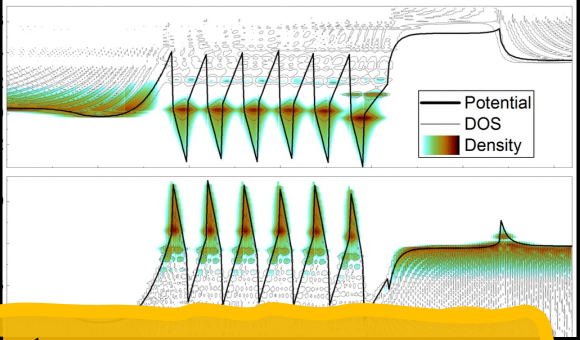
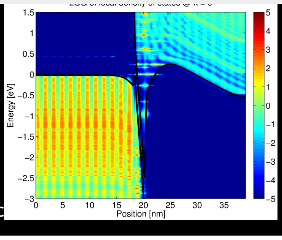
acts

Ds





Spatial partitioning into:
- Strong vs. weak scattering (kinetics)

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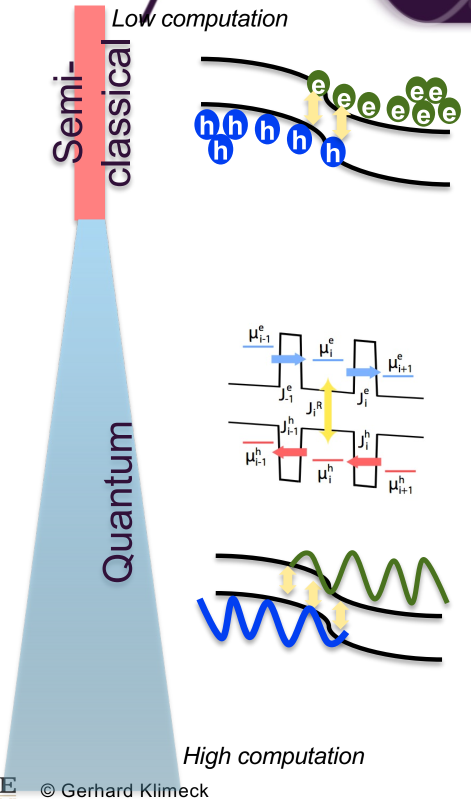
Methods on the Market



Drift-diffusion

- Current continuity Eqn. (Spatially continuous RG)
- Carriers are particle like.(Newton physics)
- Quasi-fermi levels(Efn,Efp) assumed.
- Quantum correction with artificial B.C.

Ballistic NEGF

- Recombination/scattering processes missing.

Multi Eq Neq NEGF

- Carriers are wave like. (Quantum physics)
- Optimized for QWs
- Eq and Neq regions required.
- Eq: complete thermalization, the only occurrence of recombination

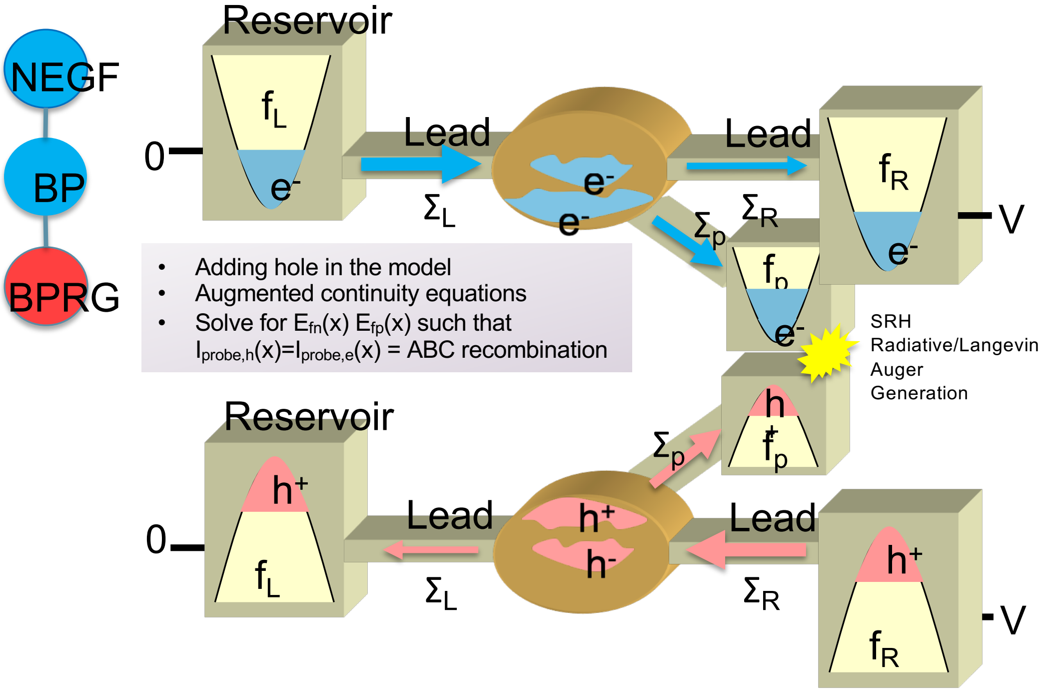
BPRG NEGF

- ✓ Carriers are wave like. (Quantum physics)
- ✓ Recombination/Generation considered
- ✓ Scattering considered
- ✓ Non-equilibrium everywhere

Self-consistent Born approximation NEGF

- High computation for e-e interaction.

NEGF + Büttiker Probe + Recombination

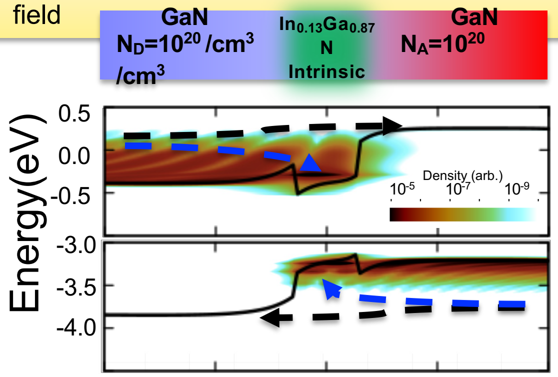


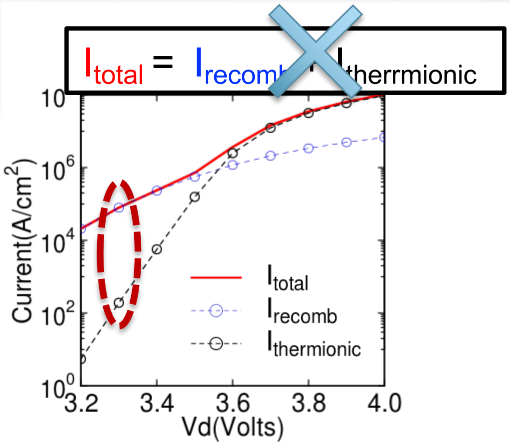
- Adding hole in the model
- Augmented continuity equations
- Solve for $E_{fn}(x)$ $E_{fp}(x)$ such that $I_{probe,h}(x)=I_{probe,e}(x)$ = ABC recombination

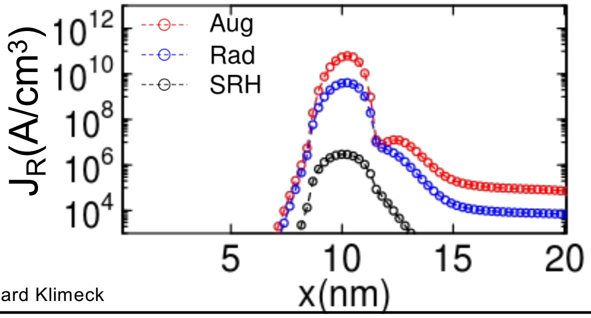
Tillmann Kubis

NEGF can include recombination and resistive losses!

- Hamiltonian: 2 band TB model + VCA
- Self-consistently solved with Poisson with piezo-electric field



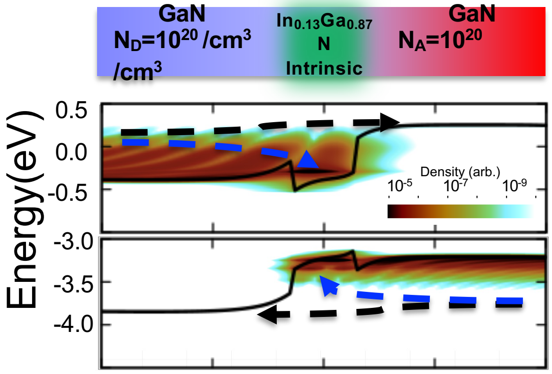




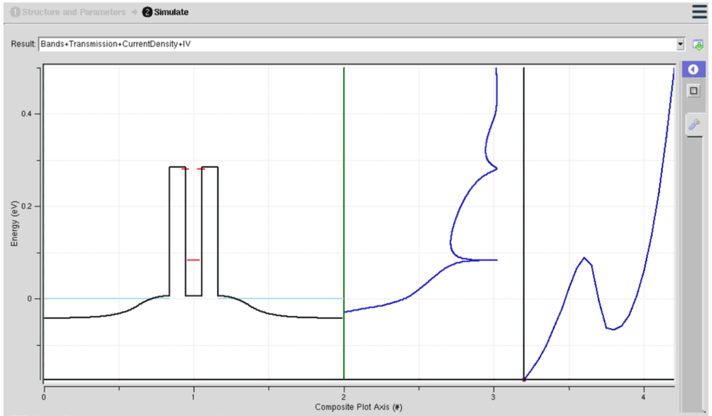
At low bias:

- Recombination current dominates.
- Recombination enhanced in QW region.

NEGF meets fundamental Device Modeling Requirements



Resistor! / PN Diode



Result: Bands+Transmission+CurrentDensity+IV

Bands+Transmission+CurrentDensity+IV = 1_Bias=0V

True Quantum Device

Klimeck Challenge:
“Here is the bar for other theories to model real quantum devices:
If you can quantitatively model and simulate many realistic RTDs and Ohmic Losses then you have a good start for a quantum transport theory.

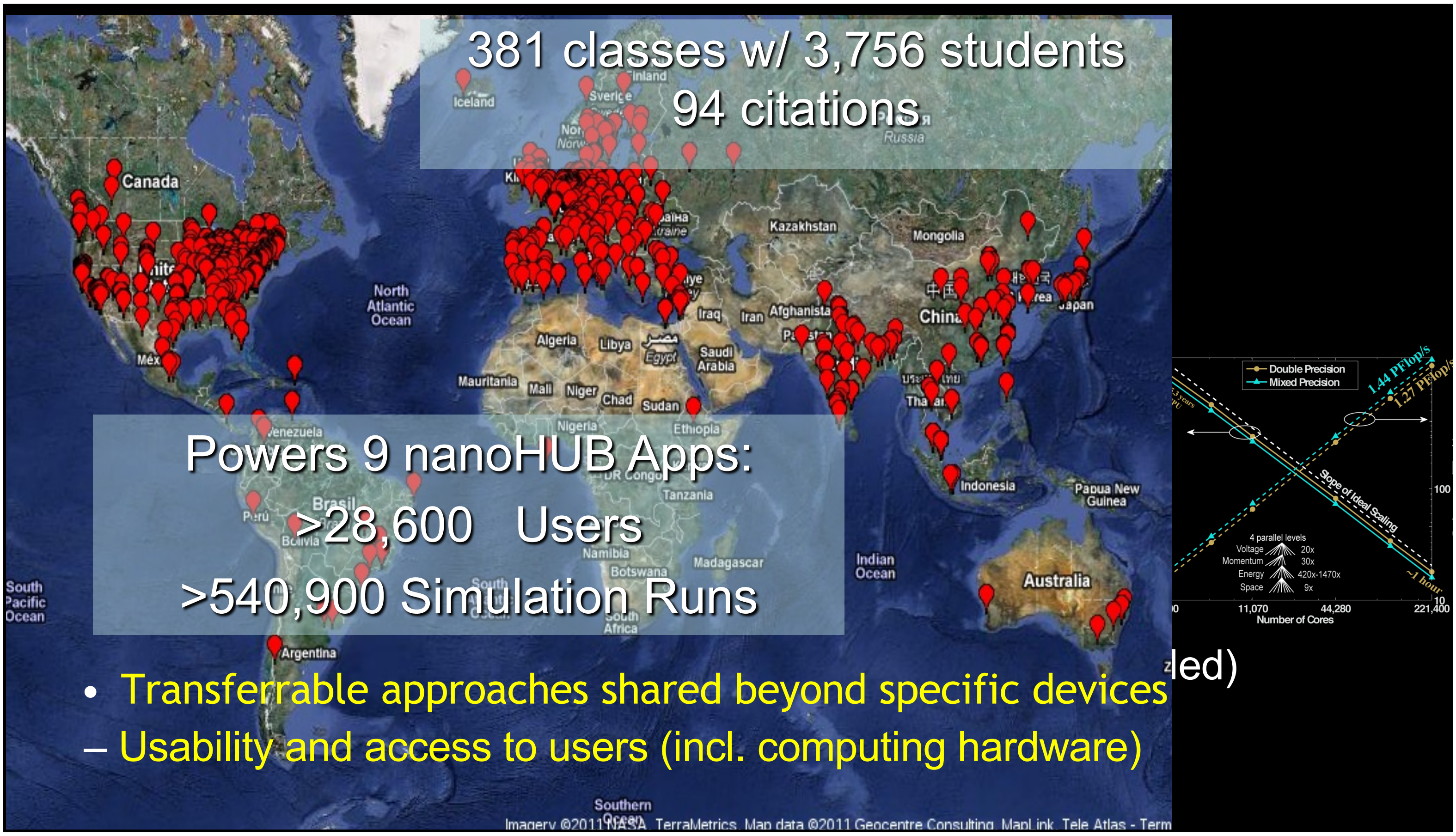
NEGF enables:
Fundamental Quantum Transport
(critical)

Fundamental, Hamiltonian-based treatment of carrier scattering
=> intellectually interesting, but non-essential for most real devices

Atomistic, local basis beyond envelope functions
=> critical

Spatial partitioning in OPEN systems
=> Couple to empirical scattering, and DD, CRITICAL
=> This is THE MOST UNDERAPPRECIATED FEATURE!

Klimeck Challenge:
“Here is the bar for other theories to model real quantum devices:
If you can quantitatively model and simulate many realistic RTDs and Ohmic Losses
then you have a good start for a quantum transport theory.



381 classes w/ 3,756 students
94 citations

Powers 9 nanoHUB Apps:
>28,600 Users
>540,900 Simulation Runs

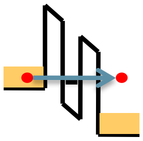
led)

- Transferrable approaches shared beyond specific devices
  – Usability and access to users (incl. computing hardware)

A 25-Year Journey Through Nanoelectronics Tools NEMO and OMEN

Transferrable approaches shared beyond specific devices

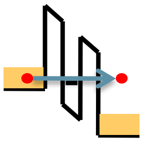
	NEMO-1D
Transport	Yes
Dimensions	1D
Atoms	~1,000
Substrate, Crystals	[100] Cubic, ZB
Strain	-
Multi-physics Multi-Scale	Scattering Domains
Parallel Comp.	3 levels 23,000 cores

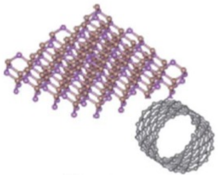


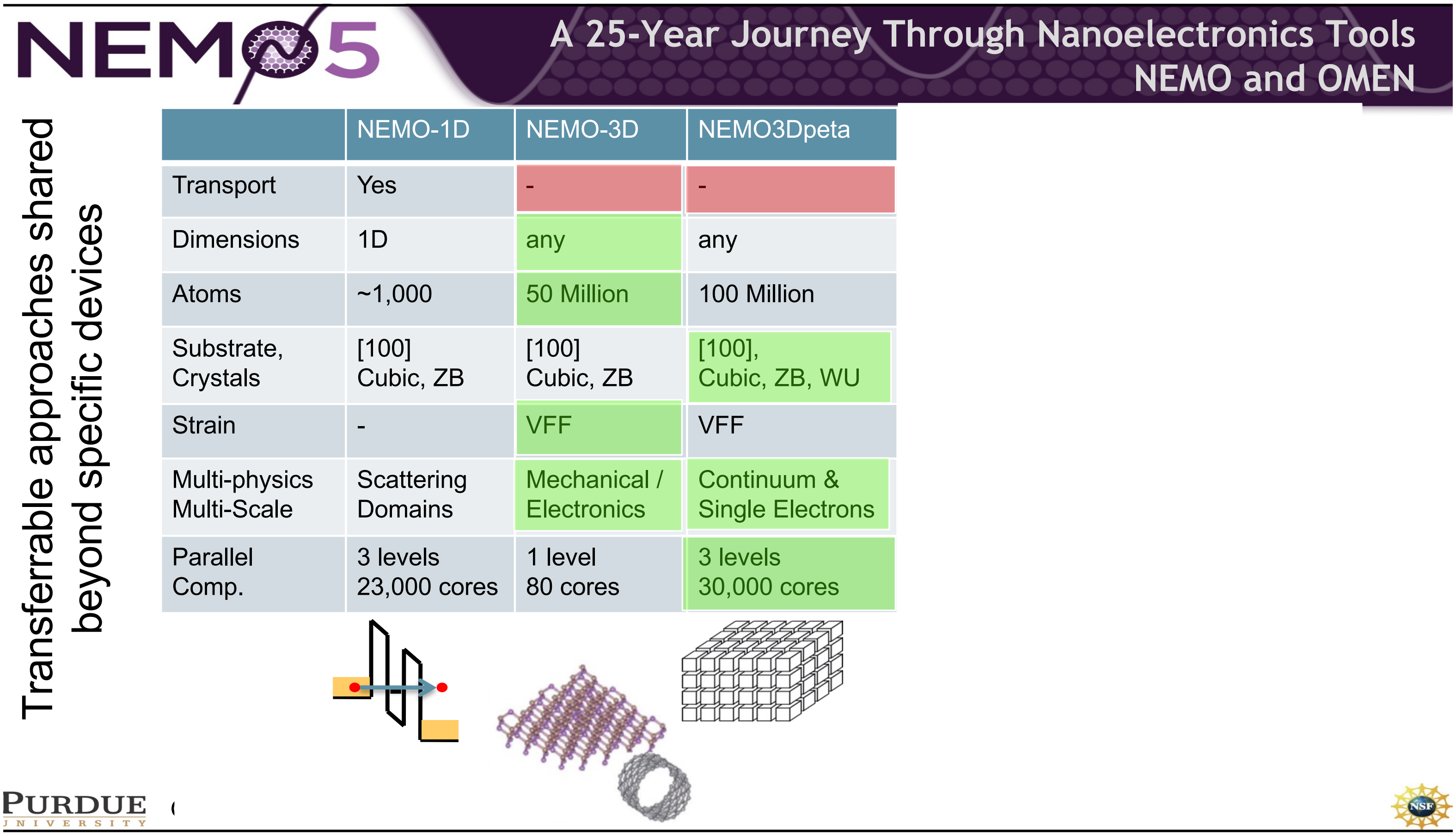
A 25-Year Journey Through Nanoelectronics Tools NEMO and OMEN

Transferrable approaches shared beyond specific devices

	NEMO-1D	NEMO-3D
Transport	Yes	-
Dimensions	1D	any
Atoms	~1,000	50 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB
Strain	-	VFF
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores







NEMO5

A 25-Year Journey Through Nanoelectronics Tools NEMO and OMEN

Transferrable approaches shared beyond specific devices

	NEMO-1D	NEMO-3D	NEMO3Dpeta
Transport	Yes	-	-
Dimensions	1D	any	any
Atoms	~1,000	50 Million	100 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic, ZB, WU
Strain	-	VFF	VFF
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics	Continuum & Single Electrons
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores

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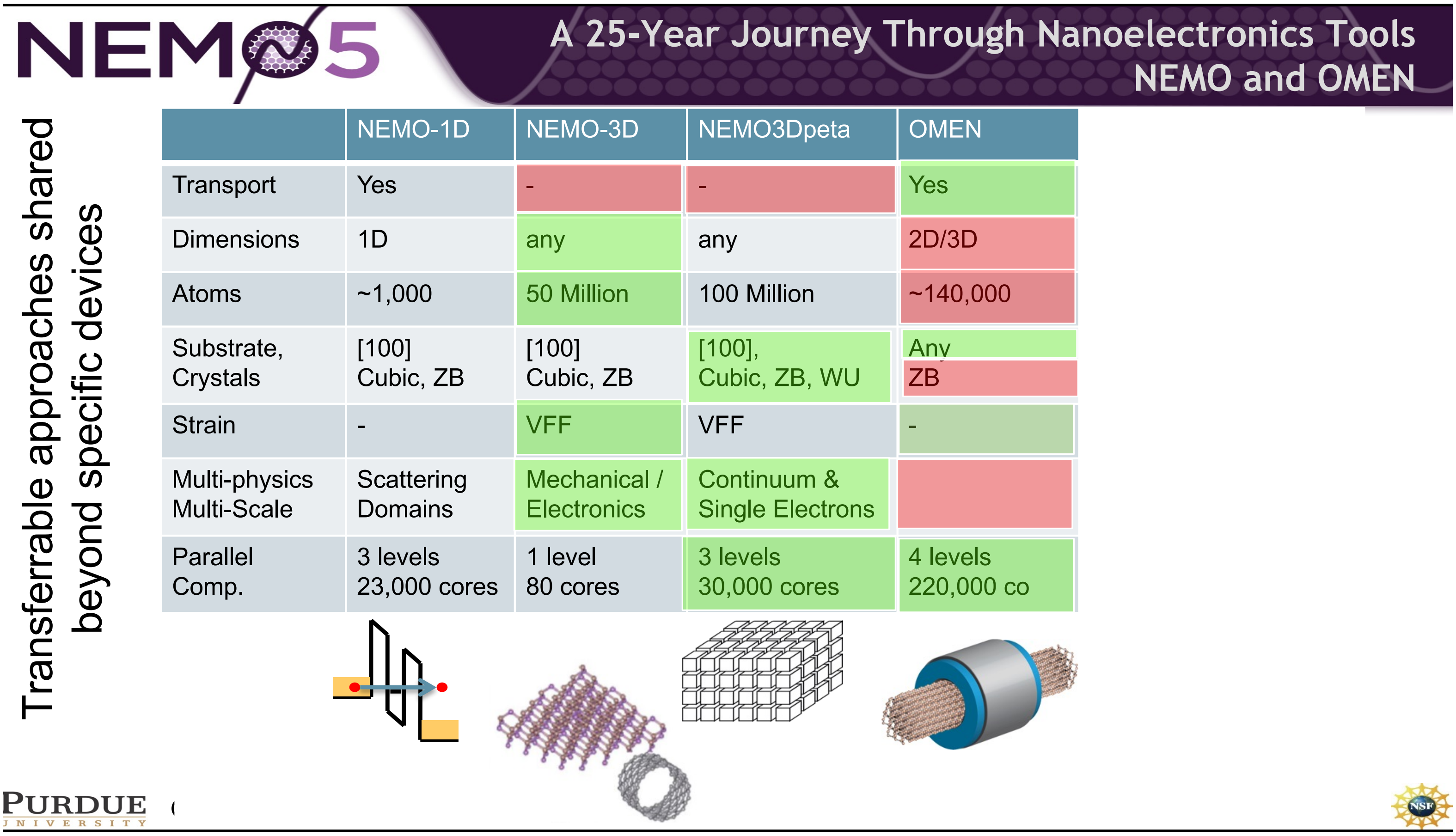

NEMO5

A 25-Year Journey Through Nanoelectronics Tools NEMO and OMEN

Transferrable approaches shared beyond specific devices

	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN
Transport	Yes	-	-	Yes
Dimensions	1D	any	any	2D/3D
Atoms	~1,000	50 Million	100 Million	~140,000
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic, ZB, WU	Any ZB
Strain	-	VFF	VFF	-
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics	Continuum & Single Electrons	
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co

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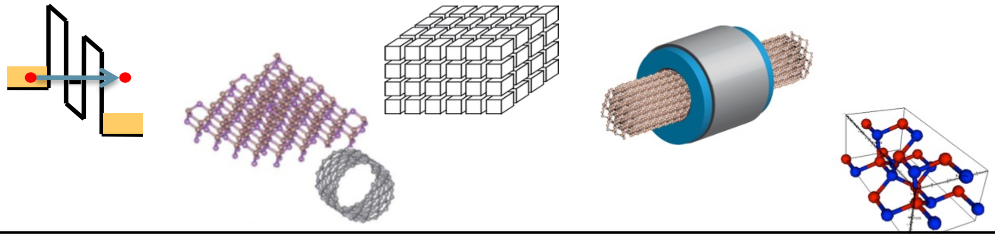
A 25-Year Journey Through Nanoelectronics Tools
NEMO and OMEN

Transferrable approaches shared beyond specific devices

	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN	NEMO5
Transport	Yes	-	-	Yes	Yes
Dimensions	1D	any	any	2D/3D	any
Atoms	~1,000	50 Million	100 Million	~140,000	100 Million
Substrate, Crystals	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic, ZB, WU	Any ZB	Any Any
Strain	-	VFF	VFF	-	MVFF, MD
Multi-physics Multi-Scale	Scattering Domains	Mechanical / Electronics	Continuum & Single Electrons		Spin, **Thermal** Classical, Wannier
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co	4 levels 200,000 cores



A 25-Year Journey Through Nanoelectronics Tools
NEMO and OMEN

Transferrable approaches shared beyond specific devices

	NEMO-1D	O-3D	NEMO3Dpeta	OMEN	NEMO5
Transport	Y s		-		Yes
Dimensions			ny		a
Atoms		5	00 Million		00 M
Substrate, Crystals	[100] ic, ZB	00] Cubic, Z		Any ZB	Any An
Strain		VFF			MVFF,
Multi-physics Multi-Scale	Do	Mechani lectroni			Spin, **Therma** Classical, Wannier
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co	4 levels 200,000 cores

First predictive NEGF tool

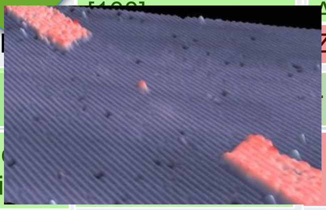
First 10 million atom elctronic structure

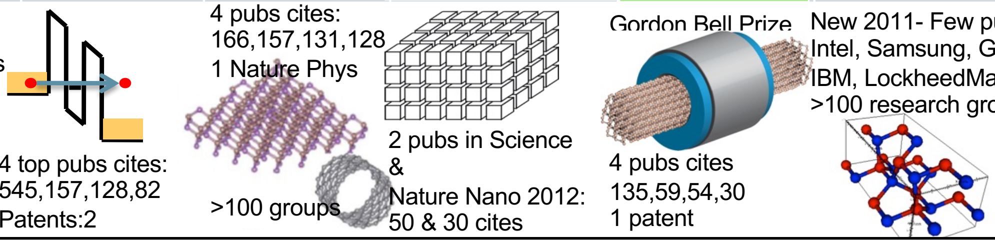
First peta-scale Engineering

Intel

Silvaco

First NEGF tool In Industry





All codes:
>100,000 lines

>500 papers

4 top pubs cites:
545,157,128,82
Patents:2

4 pubs cites:
166,157,131,128
1 Nature Phys

>100 groups

2 pubs in Science
&
Nature Nano 2012:
50 & 30 cites

Gordon Bell Prize

4 pubs cites
135,59,54,30
1 patent

New 2011- Few publ.
Intel, Samsung, GF,
IBM, LockheedMartin
>100 research groups

NEMO5

Core Code / Theory Development

Transferrable approaches shared beyond specific devices

- NEMO-1D (Texas Instruments ‘94-’98, JPL ‘98-’03)
  - »Roger Lake, R. Chris Bowen
- NEMO3D (NASA JPL, Purdue, ’98-’07)
  - »R. Chris Bowen, Fabiano Oyafuso, Seungwon Lee
- NEMO3D-peta (Purdue, ’06-’11)
  - »Hoon Ryu, Sunhee Lee
- OMEN (ETH, Purdue, ‘06-’11)
  - »Mathieu Luisier
- NEMO5 (Purdue, ‘09-’21)
  - »8 professionals: T. Kubis, M. Povolotsky, J. Fonseca, B. Novakovic, R. Rahman, A. Ajoy, H-H Park, S. Steiger
  - 30+ students: Tarek Ameen, James Charles, Junzhe Geng, Kaspar Haume, Yu He, Ganesh Hegde, Yuling Hsueh, Hesam Ilatikhameneh, Zhengping Jiang, SungGeun Kim, Daniel Lemus, Daniel Mejia, Kai Miao, Samik Mukherjee, Seung Hyun Park, Ahmed Reza, Mehdi Salmani, Parijat Sengupta, Saima Sharmin, Yaohua Tan, Archana Tankasala, Daniel Valencia, Evan Wilson,

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Challenges at the Frontier of Modeling

So What’s Next????

Moore’s Law driving TCAD Evolution

- 1994: classical continuum devices and carrier distributions,
- 2019: Quantum transport (NEGF) w/ atomic resolution

Intel Adoption of NEMO:

- 2009 initial Intel engagement
- **2015 Intel buys a dedicated supercomputer (within top 100) to run NEMO**
- 2019 Intel announces NEMO integration
- 2015-2020 NEMO helps design 2 transistor generations

SILVACO licenses NEMO (2018)

State-of-the-art TCAD:
25 years ago and today,
Mark Stettler et al, IEDM 2019