A Single Atom Transistor: The Ultimate Scaling Limit – Entry into Quantum Computing

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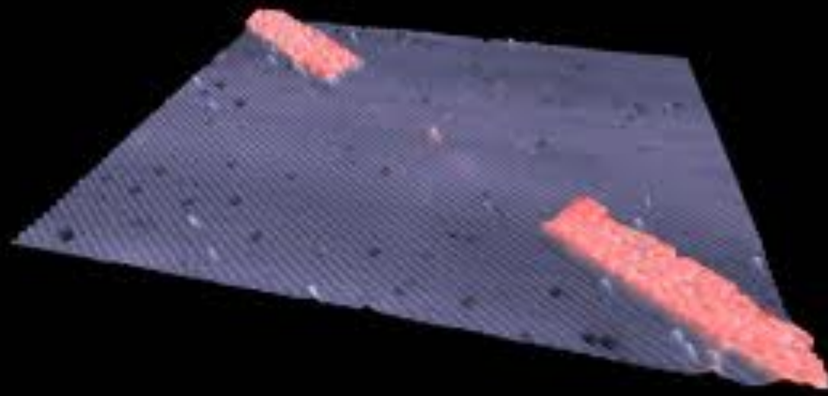
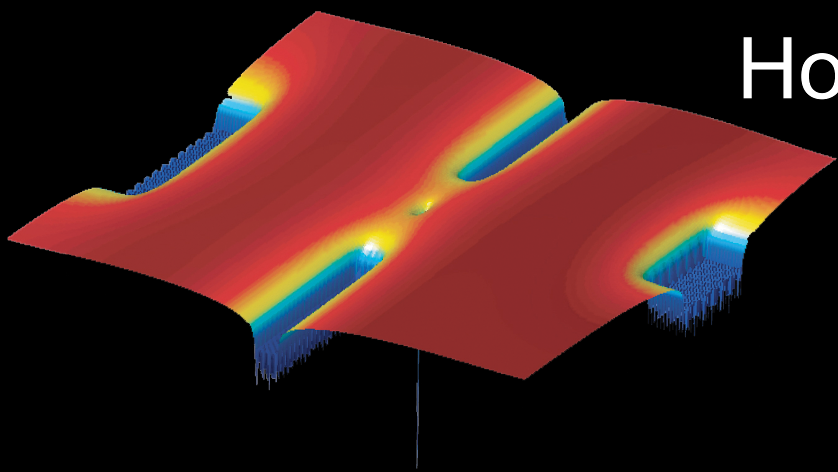
Inspired Modeling

Why?

What is it?



How to model this new world?



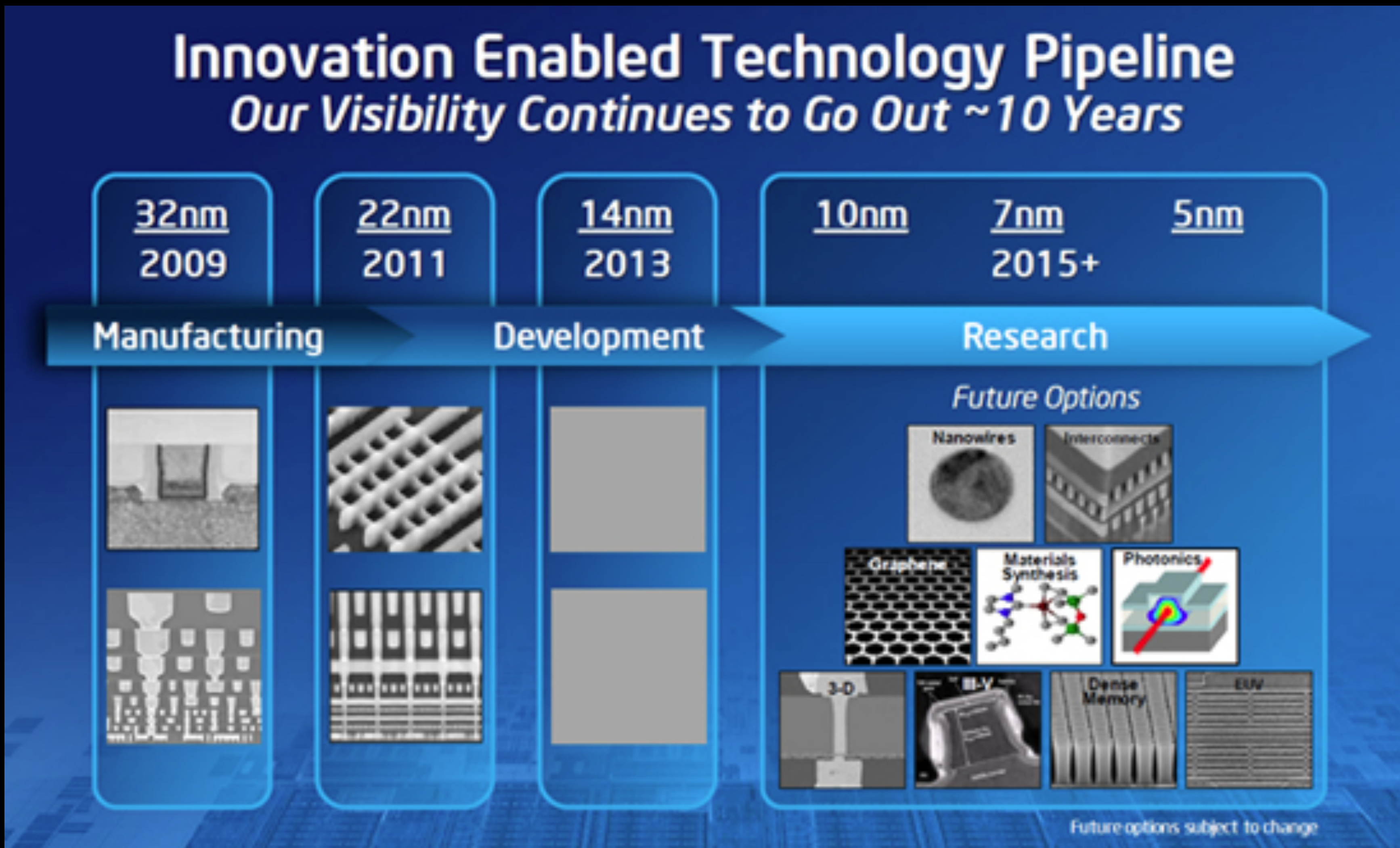
Where to study this?

Thanks to

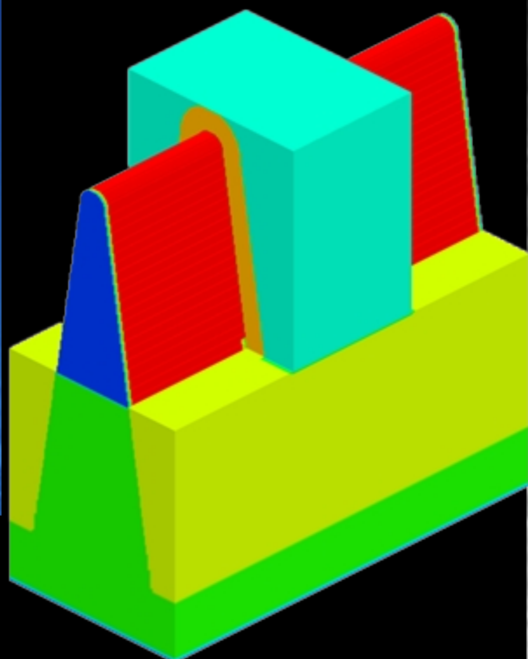
Research Group
@Purdue
@NASA JPL 1998-2003
@Texas Instruments 1994-1998

Collaborators:
Michelle Simmons, Sydney
Lloyd Hollenberg, Melbourne
Alan Seabaugh, Notre Dame

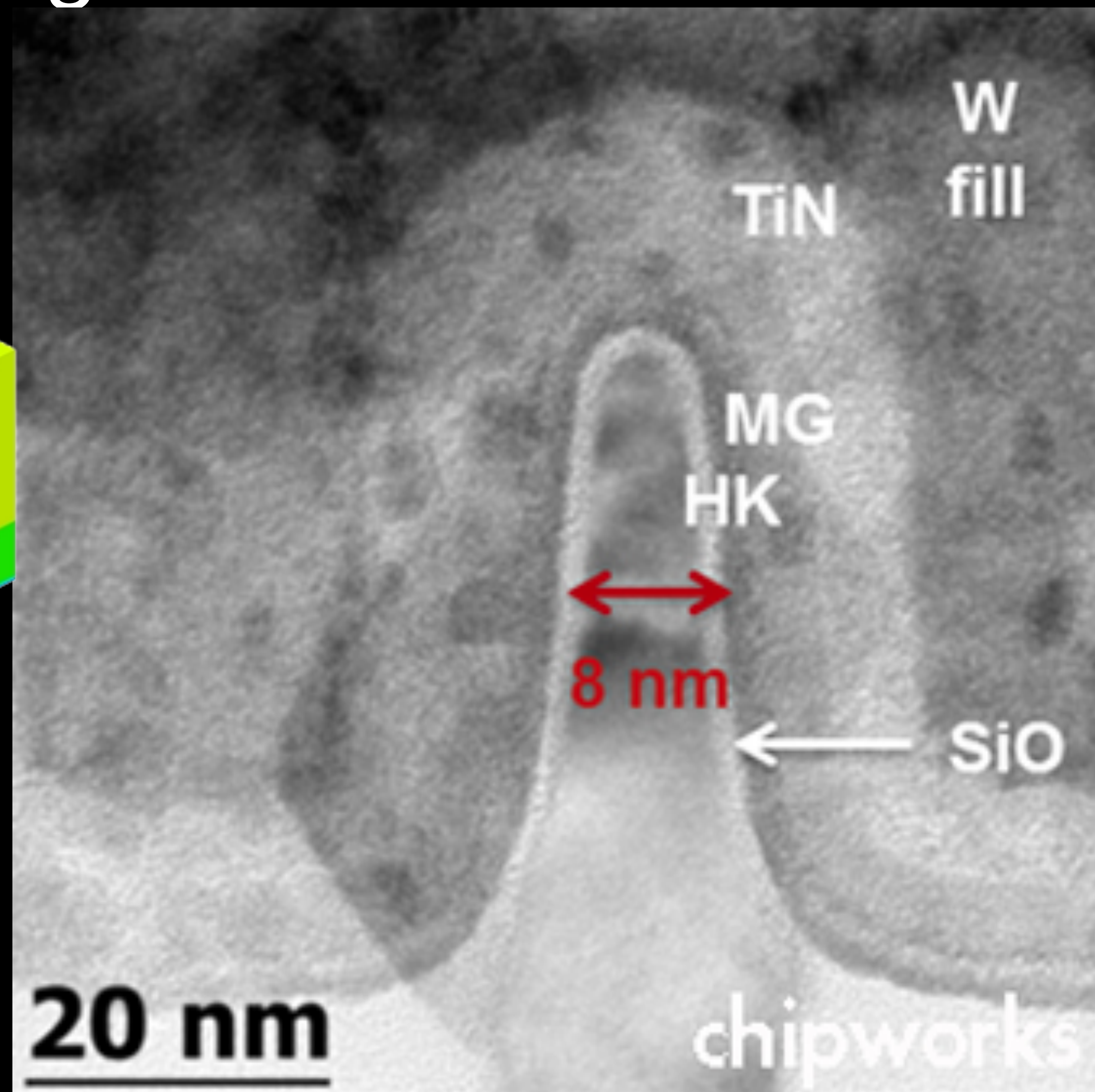
Intel Roadmap



Today: non-planar 3D devices
Better gate control!



Intel 22nm finFET



http://www.goldstandardsimulations.com/index.php/news/blog_search/simulation-analysis-of-the-intel-22nm-finfet/
http://www.chipworks.com/media/wpmu/uploads/blogs.dir/2/files/2012/08/Intel22nmPMOSfin.jpg

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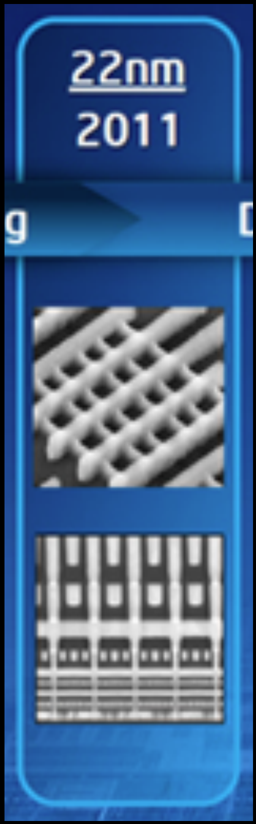
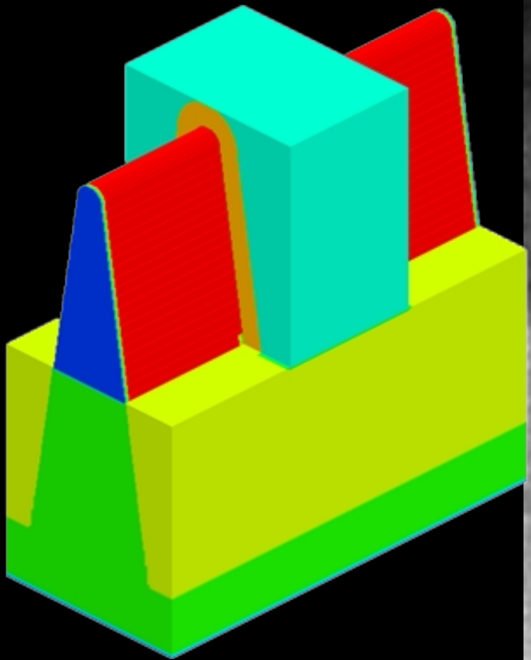
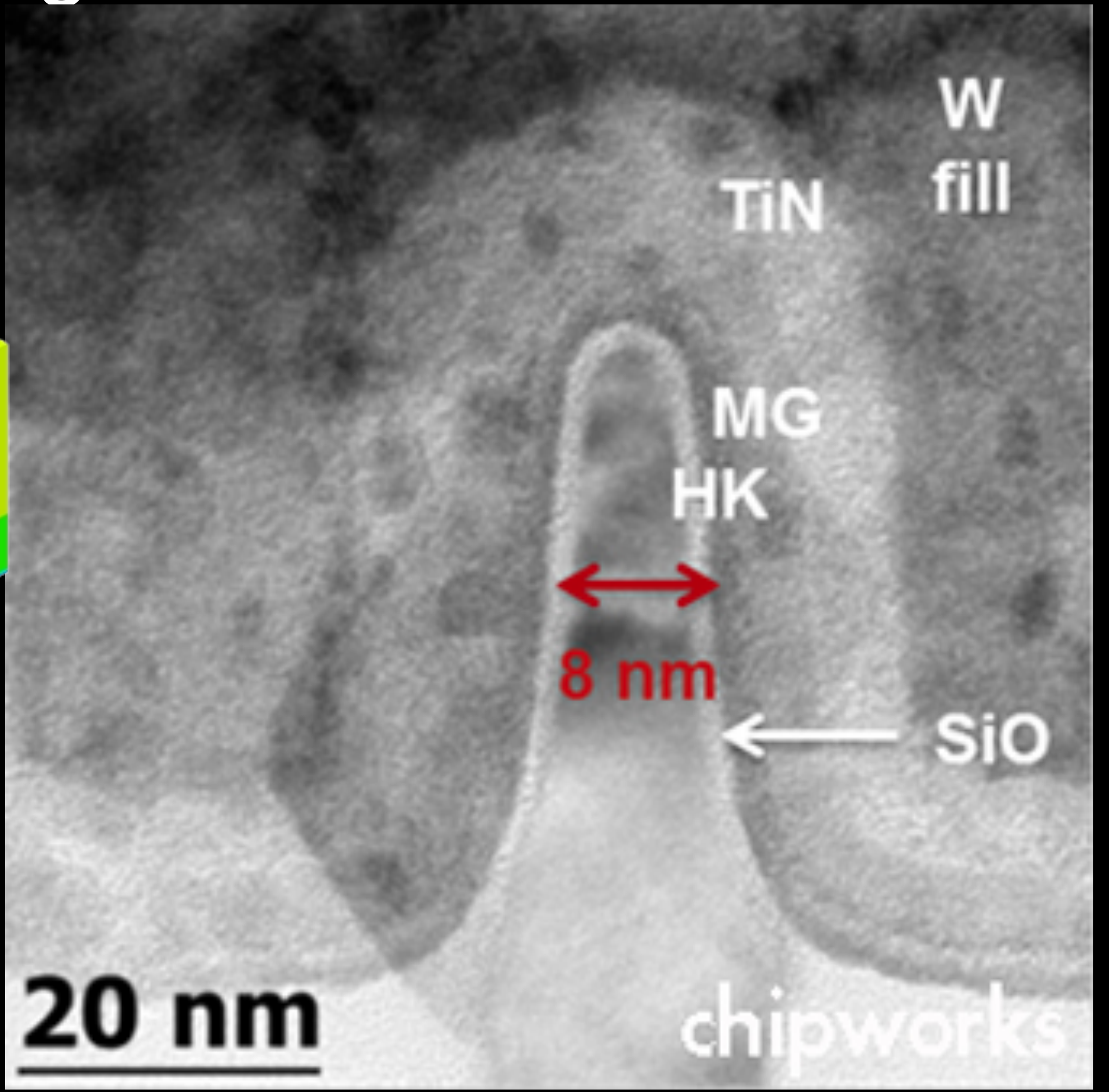




22nm = 176 atoms

8nm = 64 atoms



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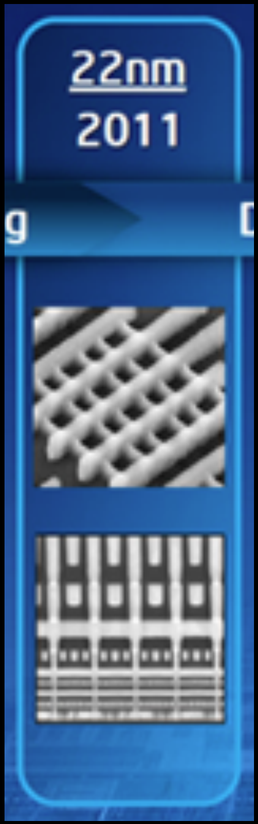
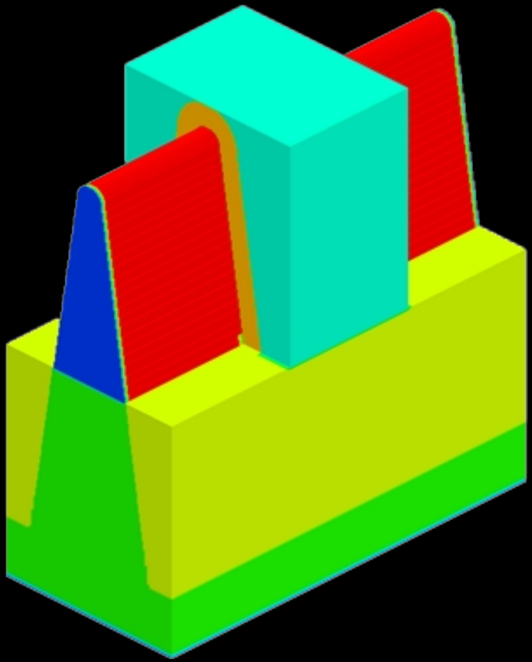
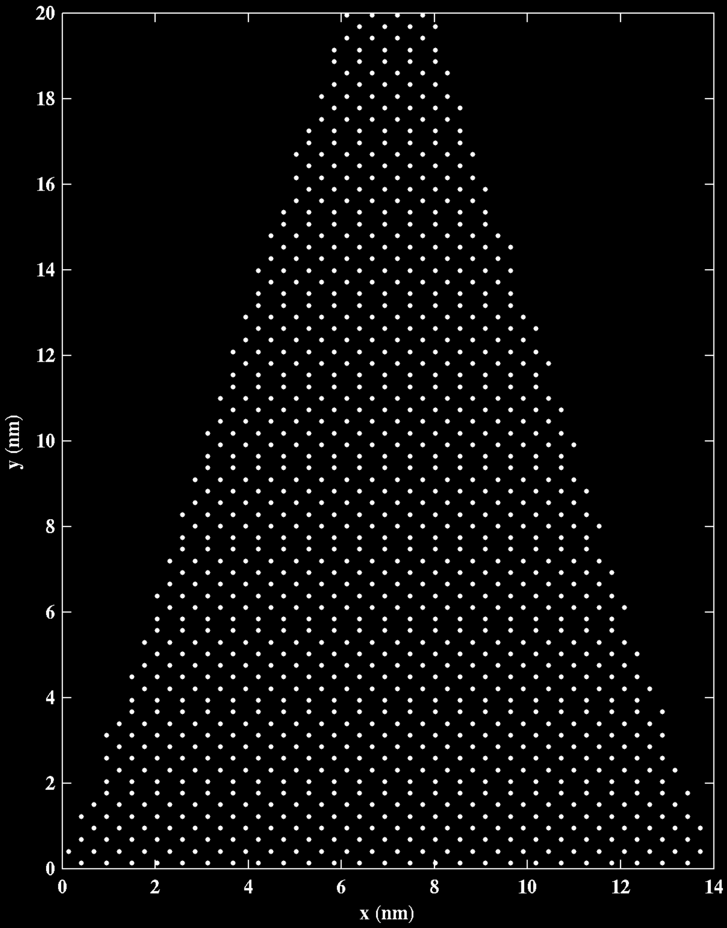




1,085 atoms



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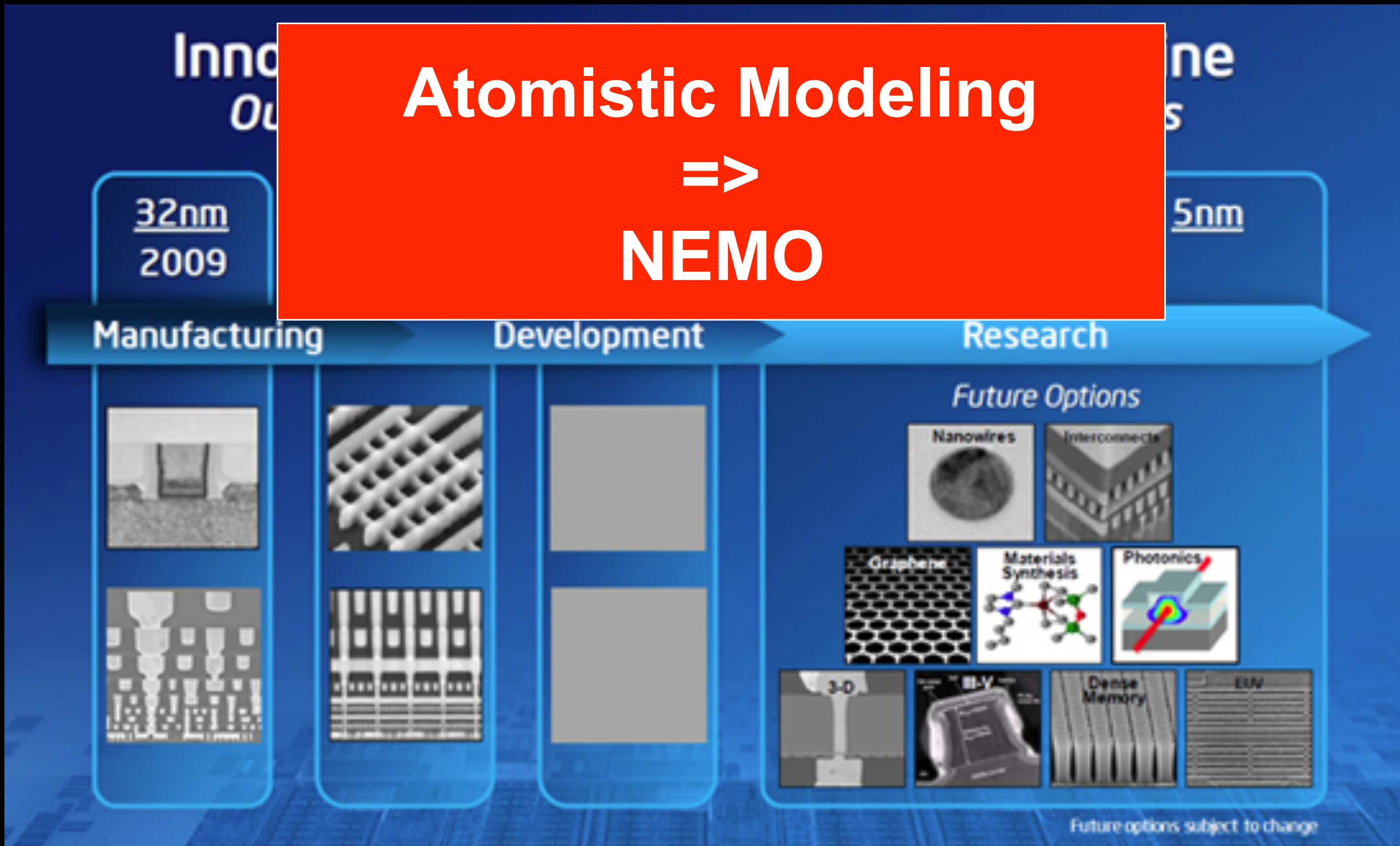
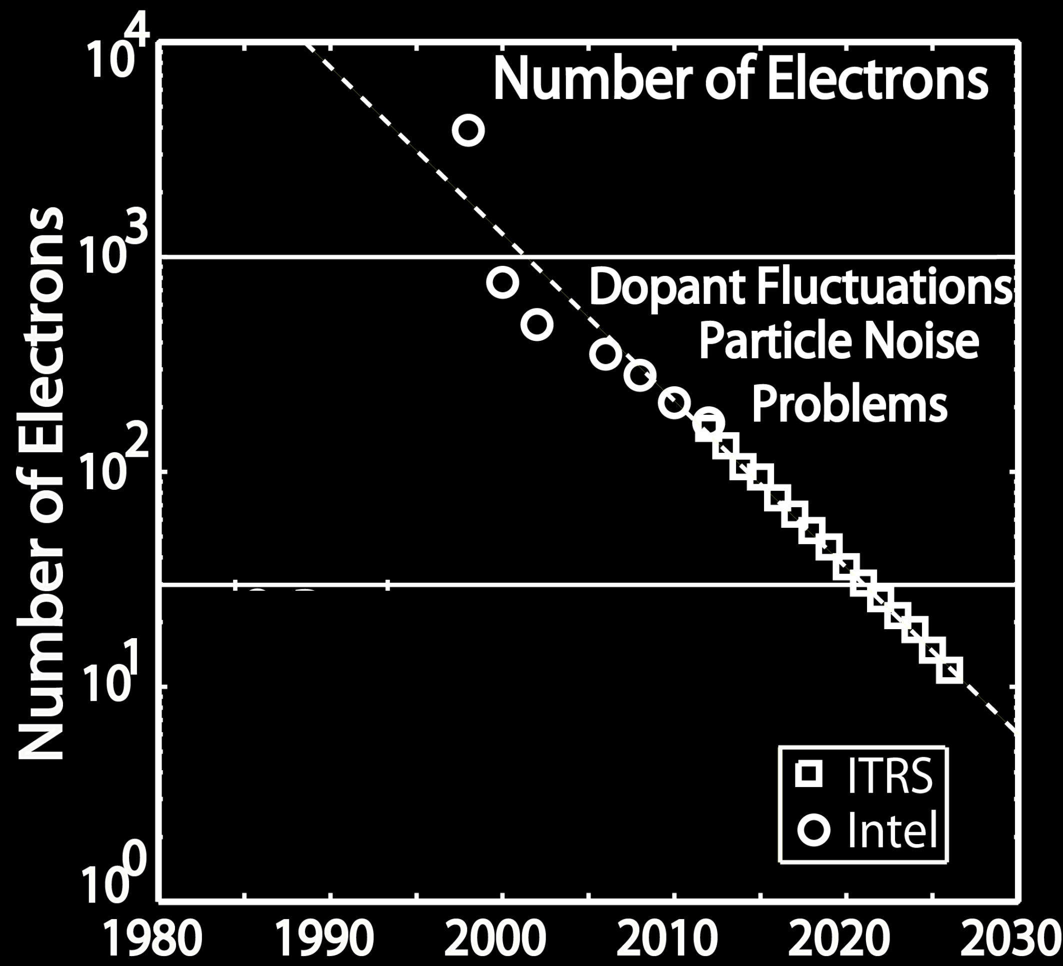
Roadmap of finite atoms!



Atomistic Modeling
=>
NEMO

nm Node	22	14	10	7	5
Node atoms	176	122	80	56	40
Critical atoms	64	44(?)	29(?)	20(?)	14(?)
Electrons	160-190	64-80	30-38	18-23	11-15

Roadmap of finite electrons!



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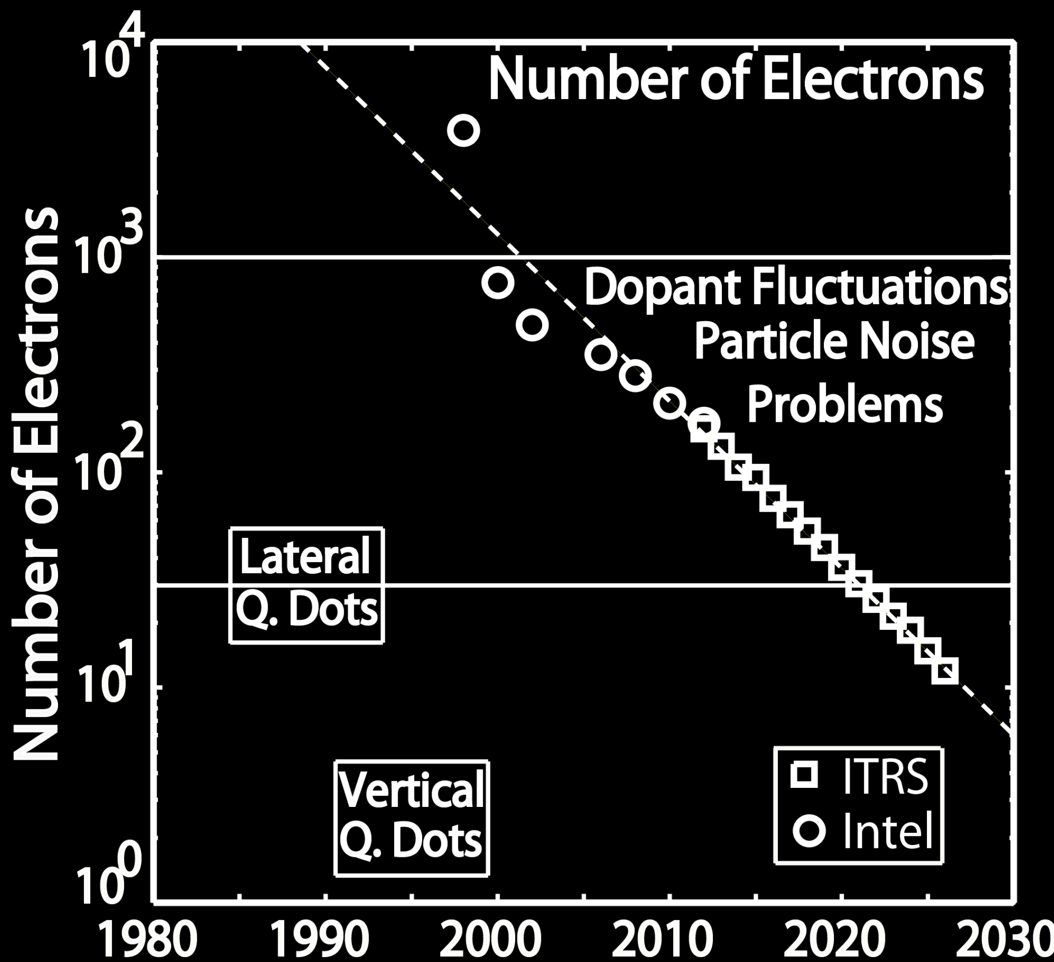
Quantum Dot Research



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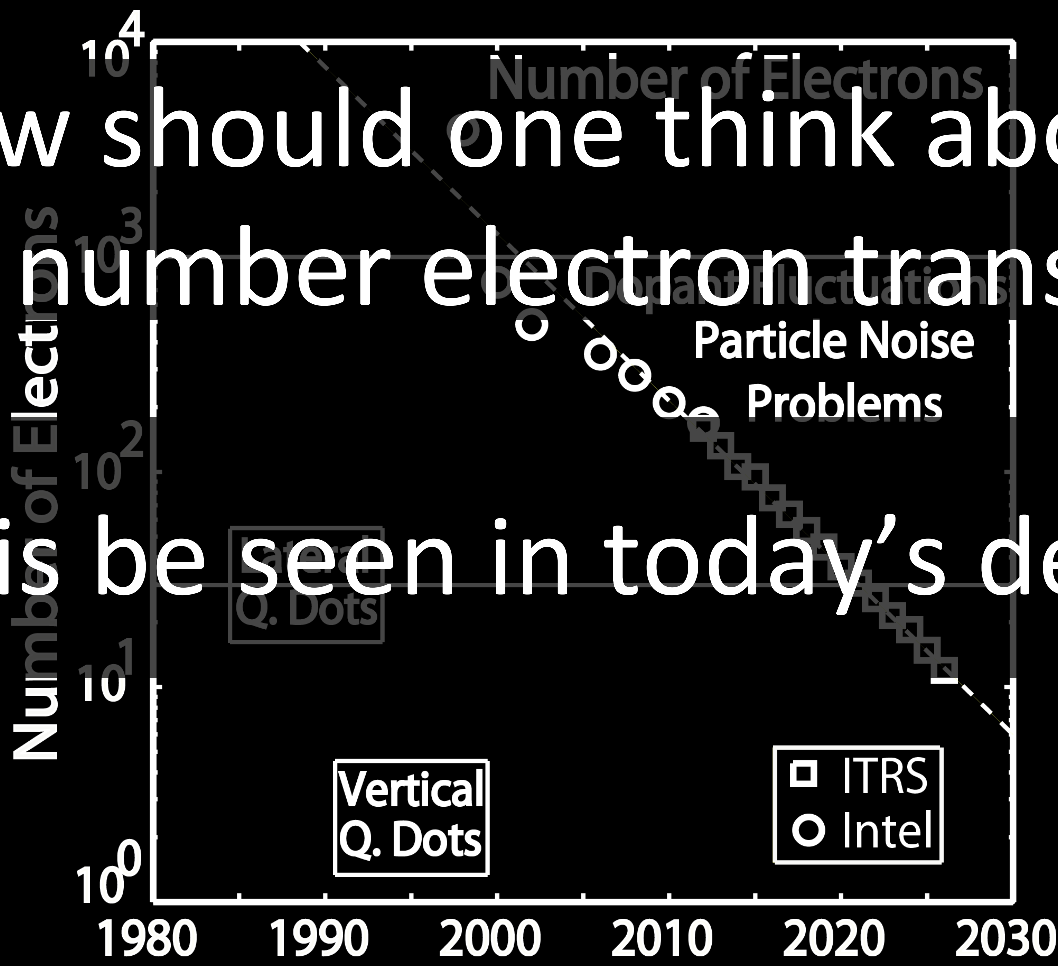

How should one think about finite number electron transport?

Can this be seen in today's devices?

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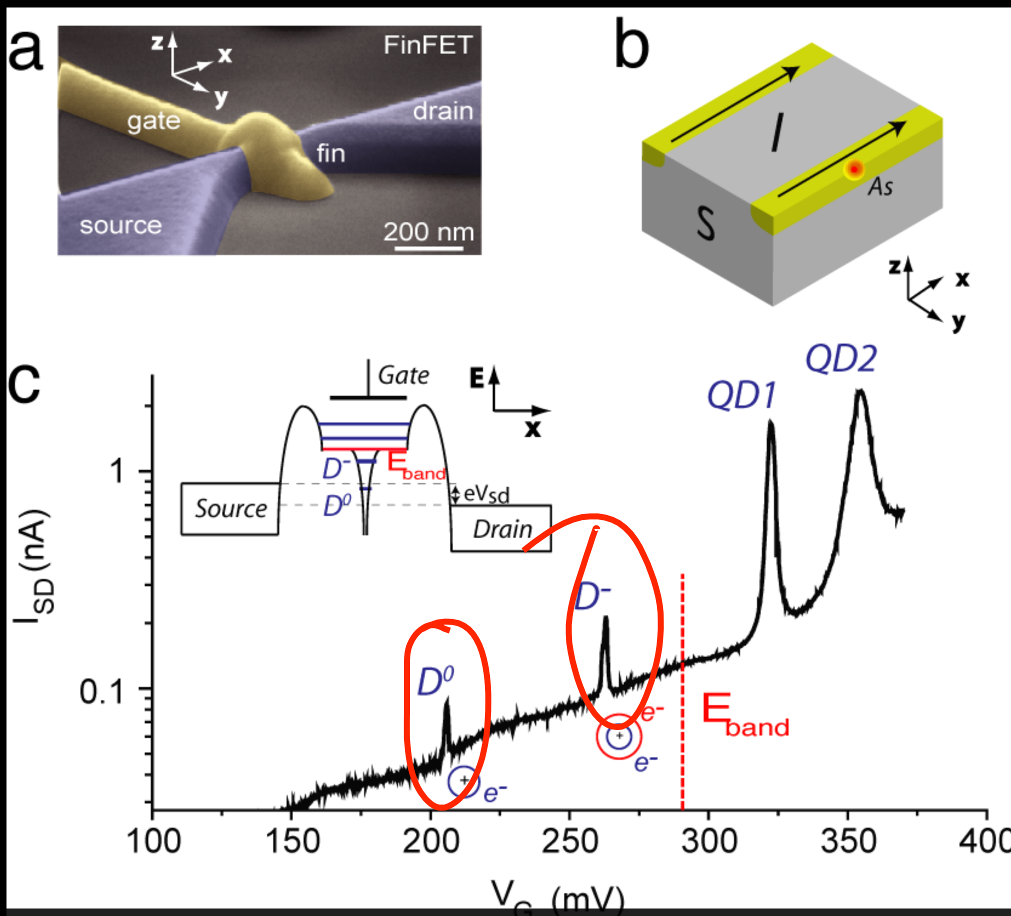
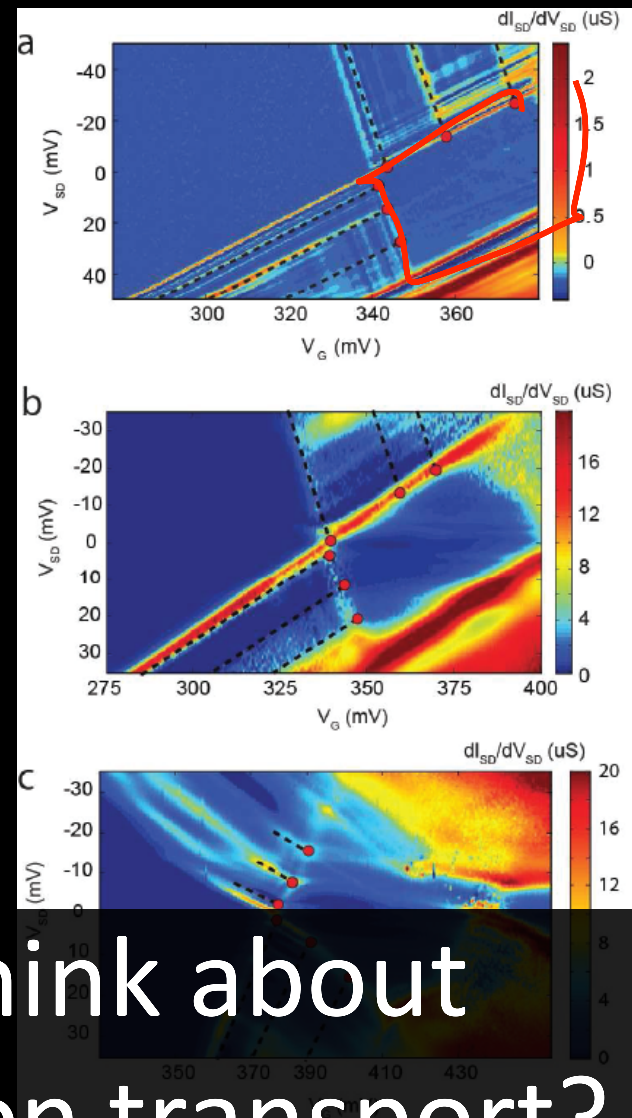
FinFETs with finite electrons

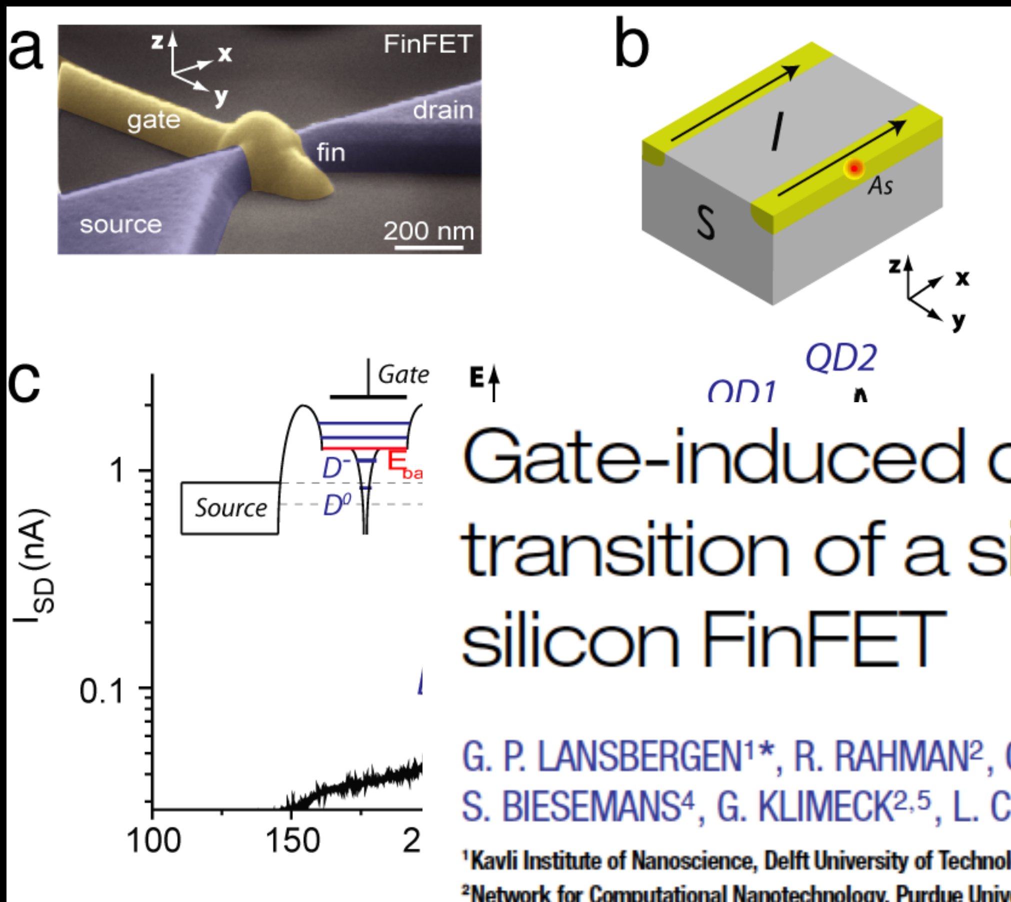


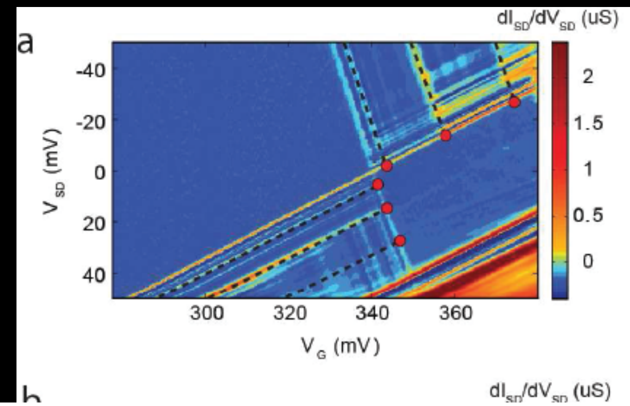


How should one think about finite number electron transport?

- IMEC & Delft & Purdue & Melbourne Nature Physics (2008)
- Single impurity / electron effects
- Each device has a specific fingerprint => Metrology of As vs P impurities

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

- IMEC & Delft
  Nature Physic

How

finite number electron

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

The single-atom transistor

Presentation Outline

- Why?
  - Continuum invalid
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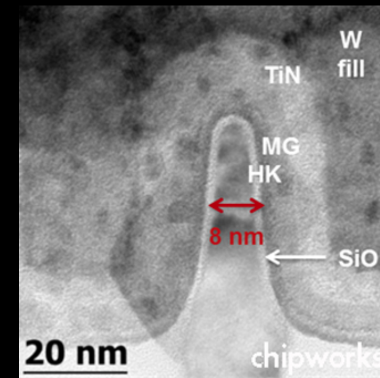
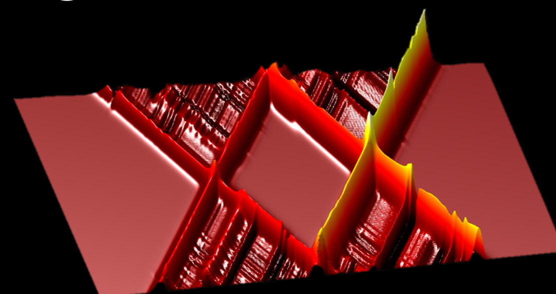
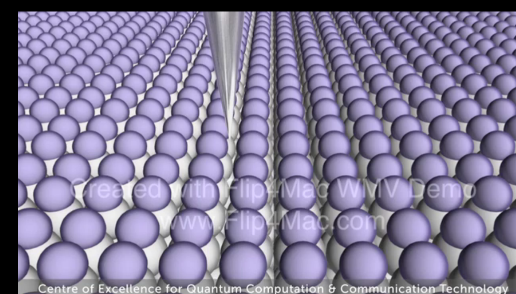
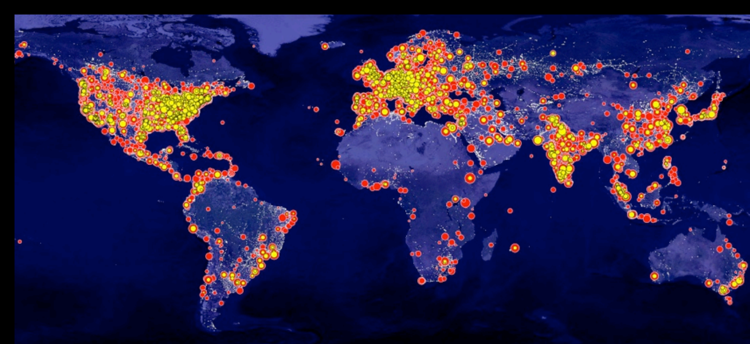
- What is it?
  - Coulomb diamond
  - How is it built?
  - Results
- How to model this?
  - NEMO
- Where to study this?
  - nanoHUB.org

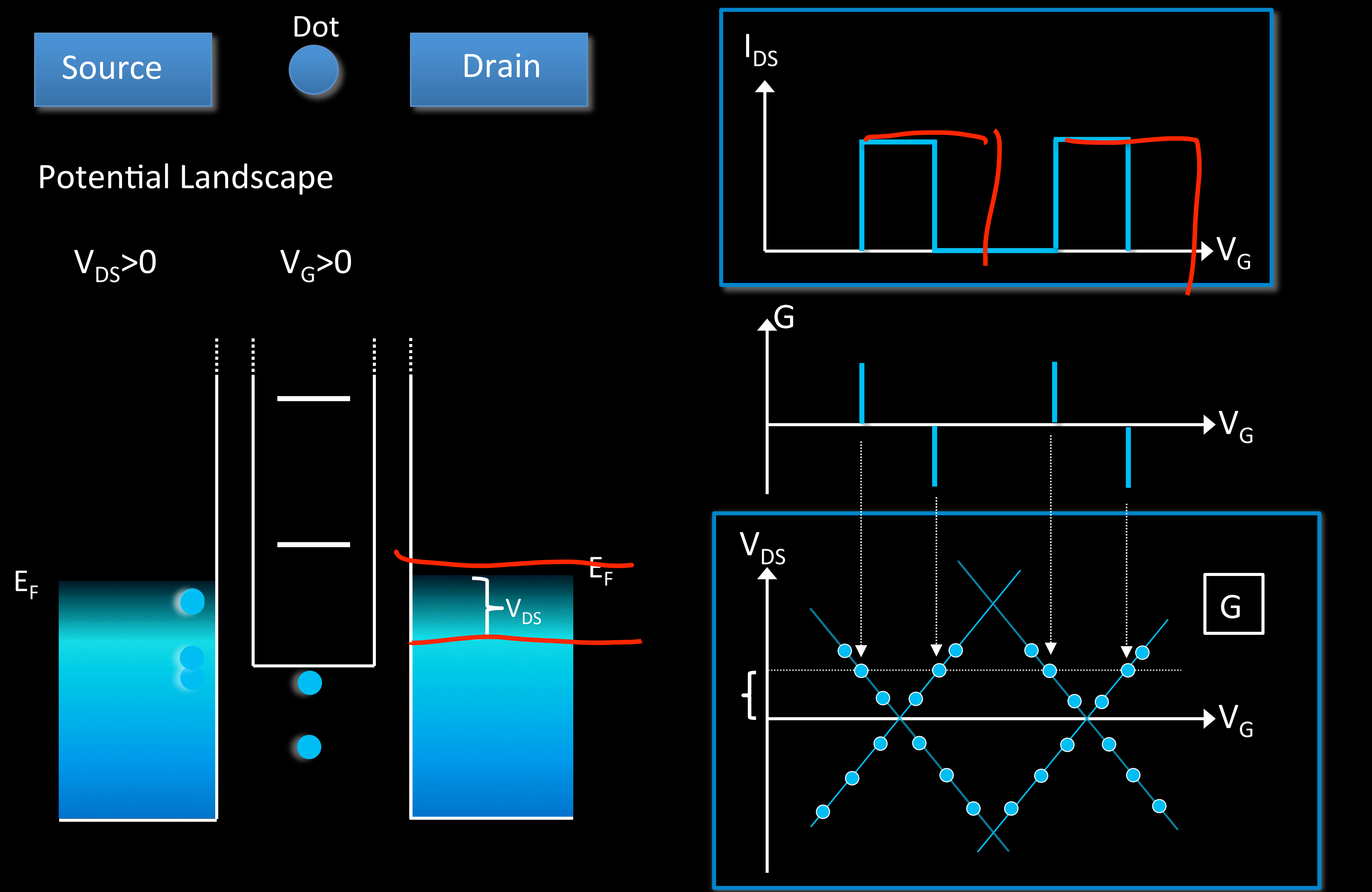


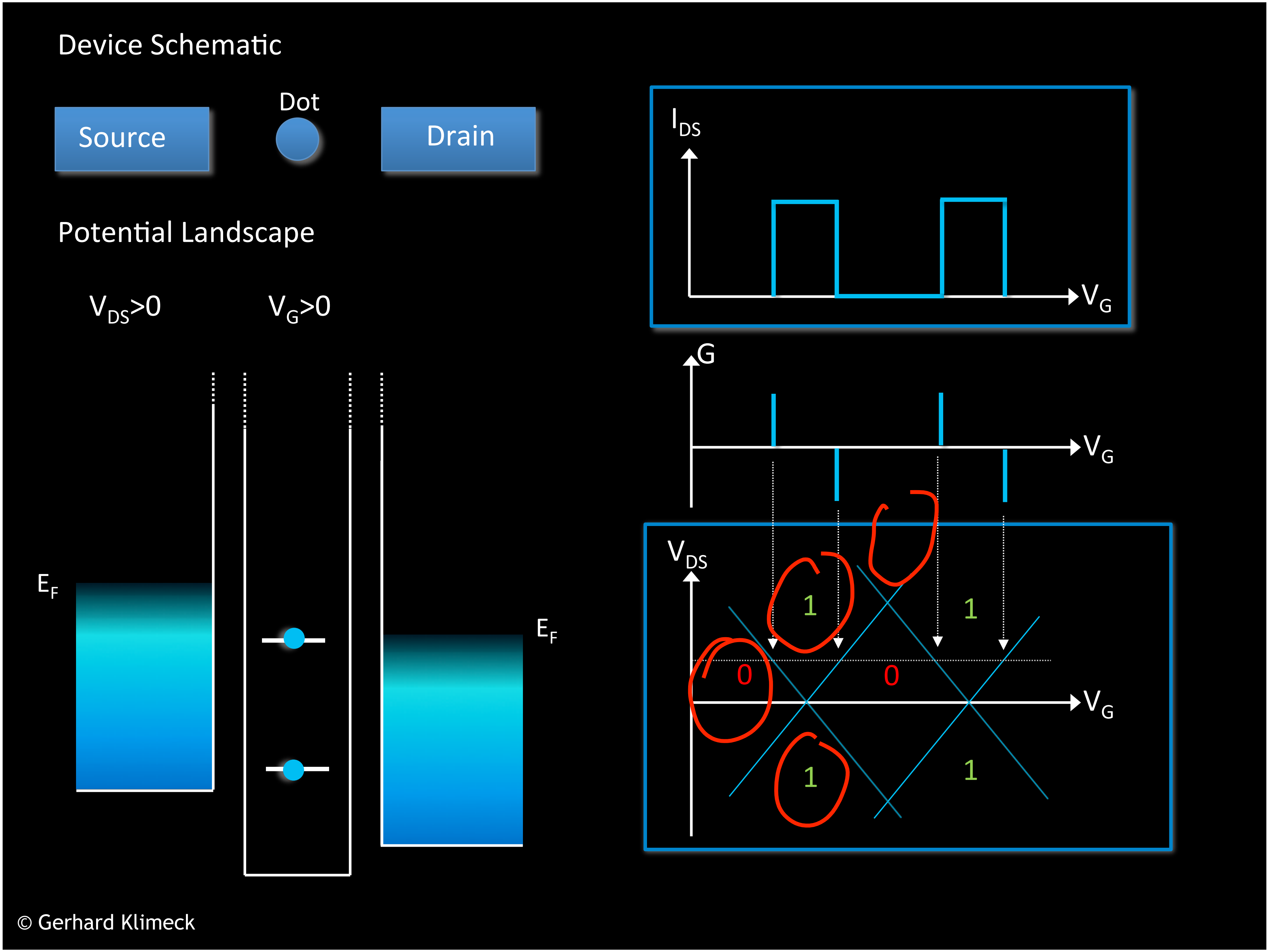




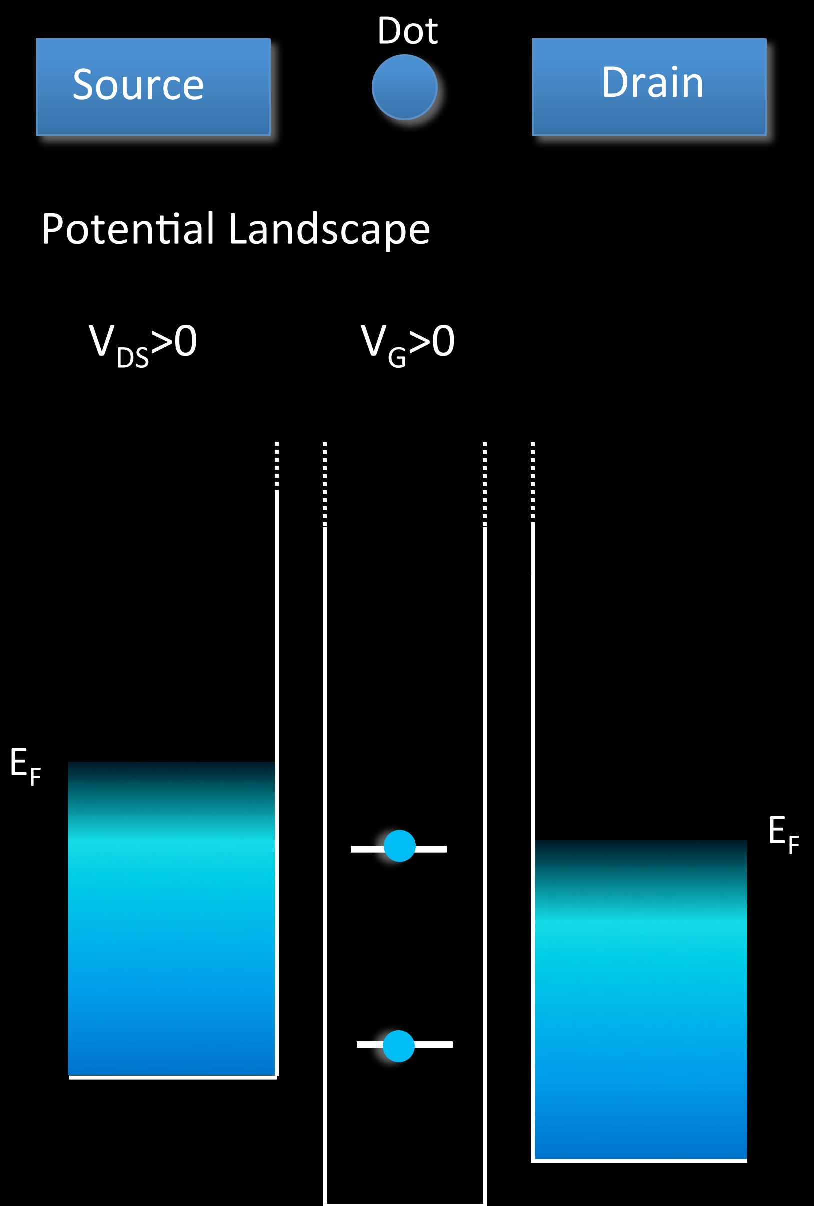


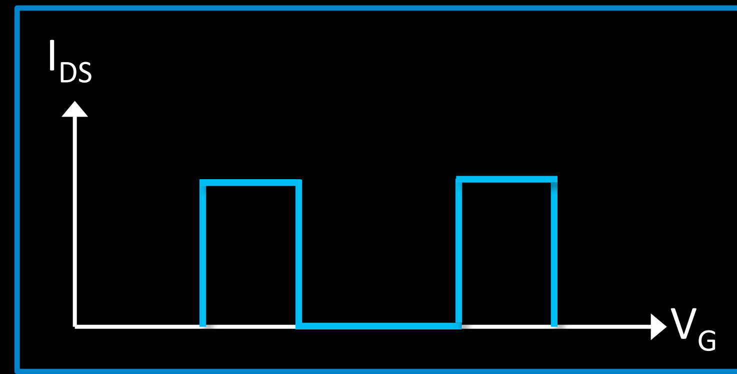
Single Electron Transport




Device Schematic
Source
Dot
Drain
Potential Landscape
$V_{DS}>0$
$V_G>0$
E_F
E_F
I_{DS}
V_G
G
V_G
V_{DS}
1
1
0
0
V_G
1
1
© Gerhard Klimeck

“The I-V curve of atomic transistors”

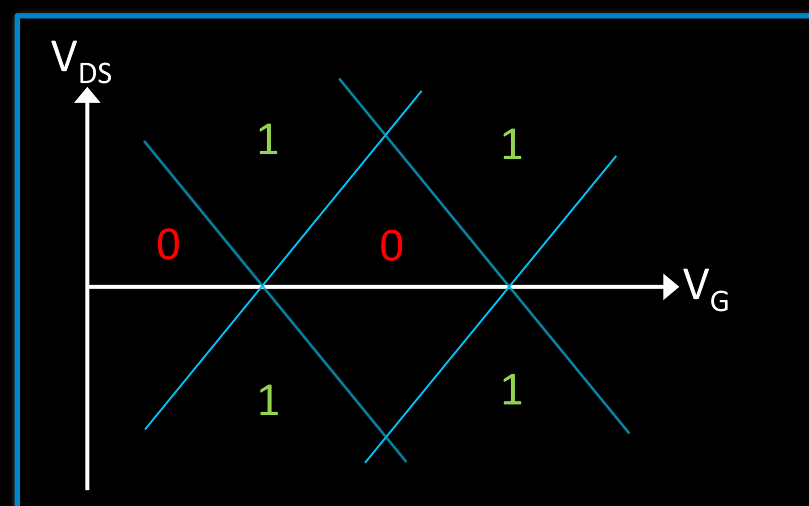




Conductance G vs. V_{DS} and V_G

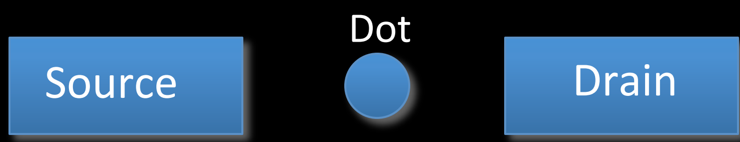
1 = Transistor on (current flow)

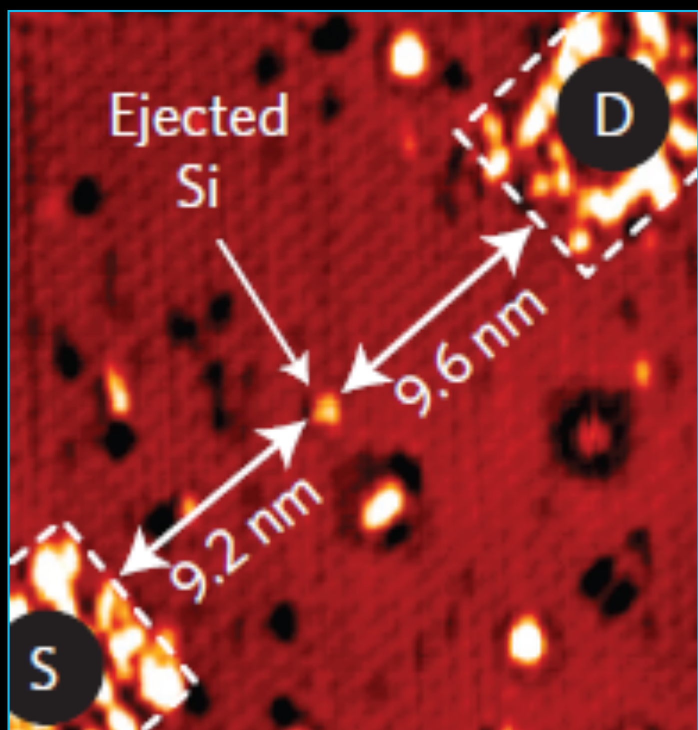
0 = Transistor off (no current flow)

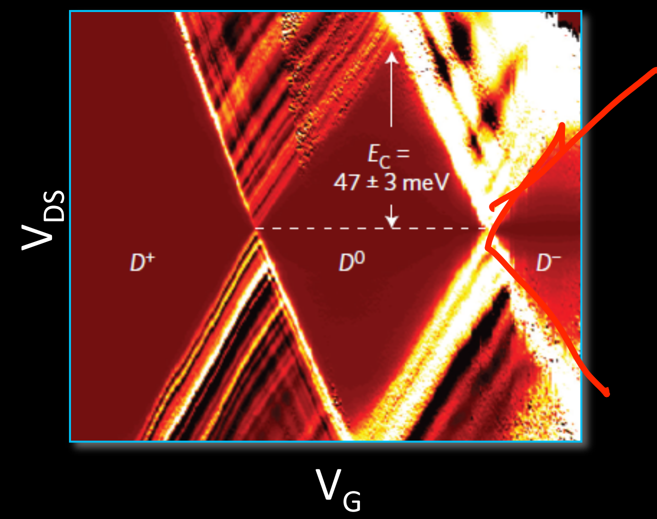


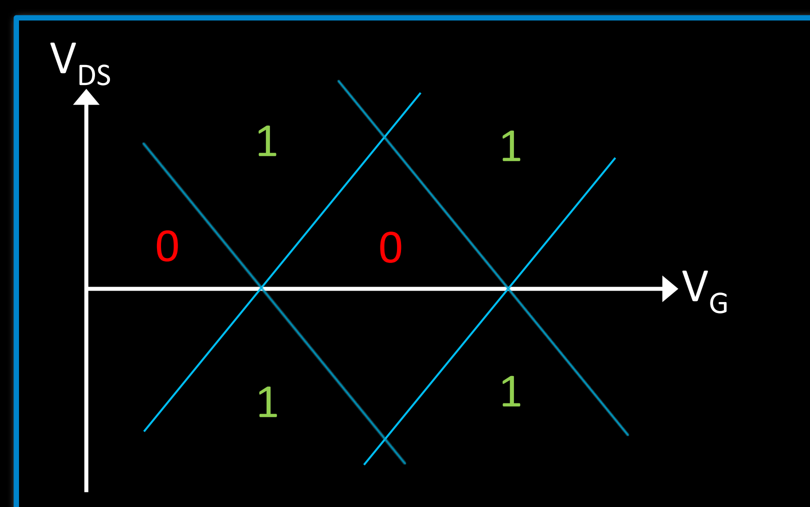
Charge Stability Diagram

Experimental Data









A single-atom transistor,
M. Fuechsle et.al.
Nature Nanotechnology, 2012

The single-atom transistor

Presentation Outline

- Why?
  - Continuum invalid
    => finite atoms/electrons
- What is it?
  - Coulomb diamond
  - How is it built?
  - Results
- How to model this?
  - NEMO
- Where to study this?
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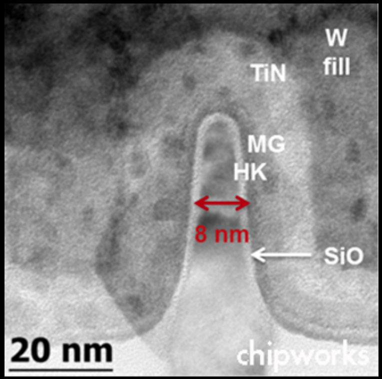
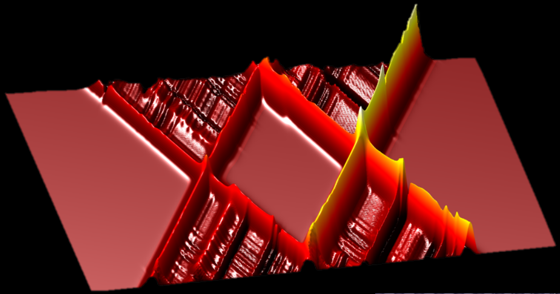
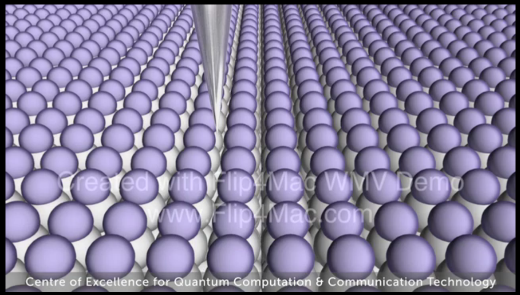
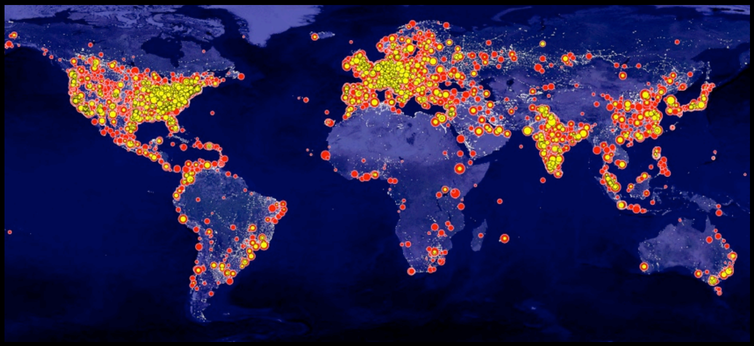








CENTRE FOR
QUANTUM COMPUTATION &
COMMUNICATION TECHNOLOGY

AUSTRALIAN RESEARCH COUNCIL CENTRE OF EXCELLENCE

A designed single electron transistor!
How did we get there?

Experimental Efforts: STM Lithography

Objectives

- Precise donor placement
- Place "many" donors in ultra-scaled region

Scanning Tunneling Microscopy

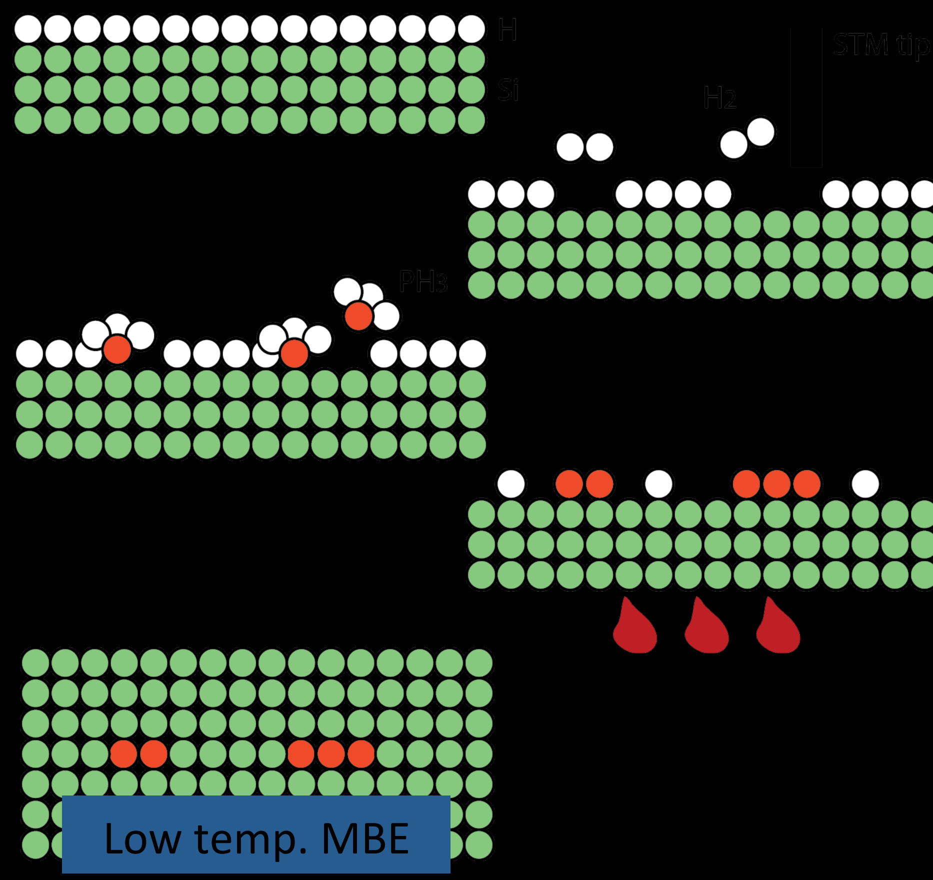
- Device surface imaging
- Control/pattern at atomic scales

Eagler et al, Nature (1990)

- Densely P δ-doped Si (Si:P) device

- Doping control ~ $5x10^{-10}$(m)
- Up to 1/2.9ML (1 P atom per every 2.9 Si atoms)

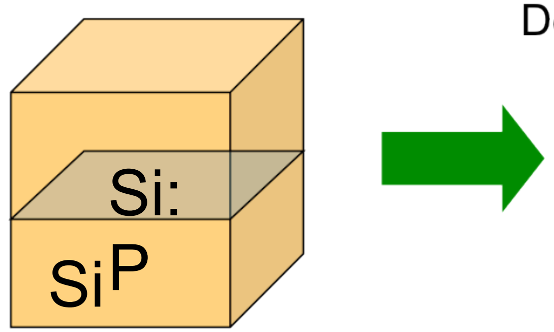
Fabricating single ML thick P doped planes using STM lithography

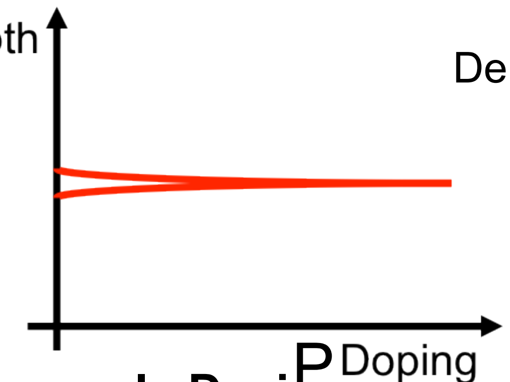


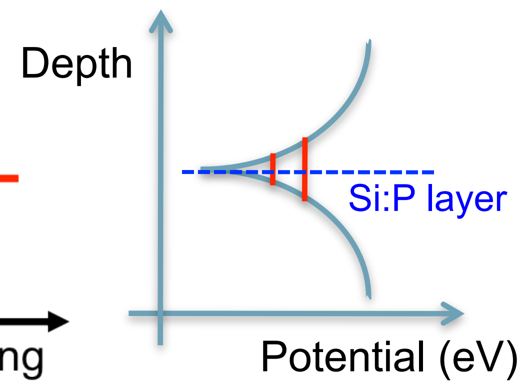
Ruess et al., Nano Lett. (2004)

Picture edited

- **Densely Phosphorus δ-doped Si (Si:P) device**
  - » Thin densely P doped layer in low-doped/intrinsic Si bulk
  - » Electrons strongly confined in P doped layer

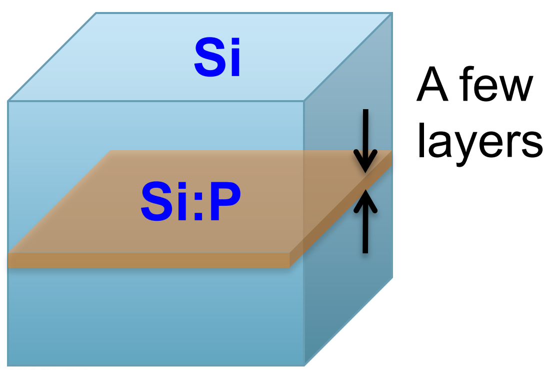




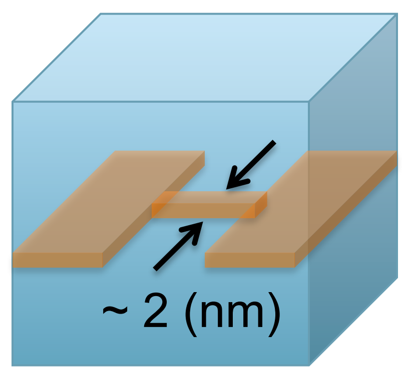


- **Prototype: Novel Structures/ Nanoscale Devices**

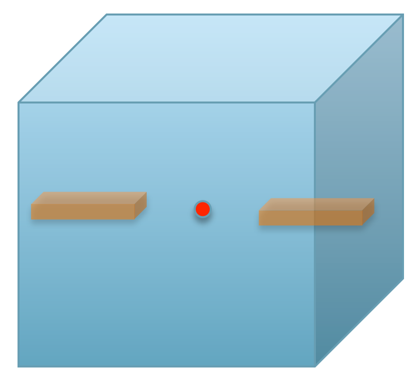
2-D electron reservoirs (Shallow Junctions)



Ultra-narrow NW channel (Interconnector)



Single donor device with NW leads

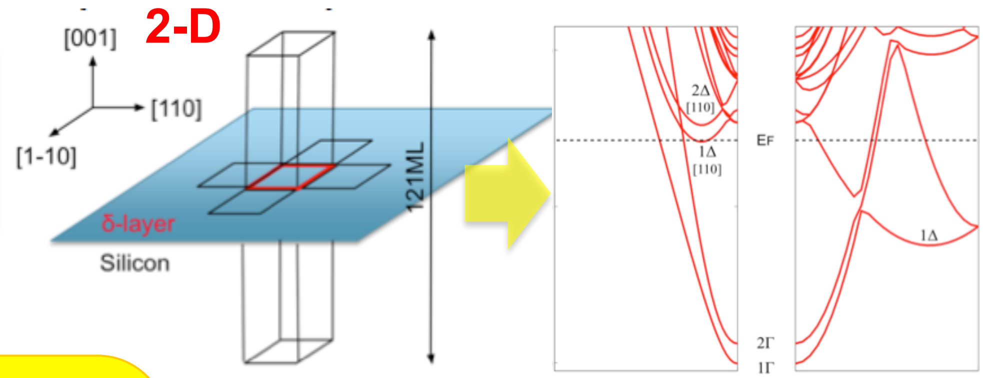


Single Impurity Outline

1) Si:P Doping Plane (2-D)

1A) Semi-metallic property

1B) Sensitivity to doping disorder



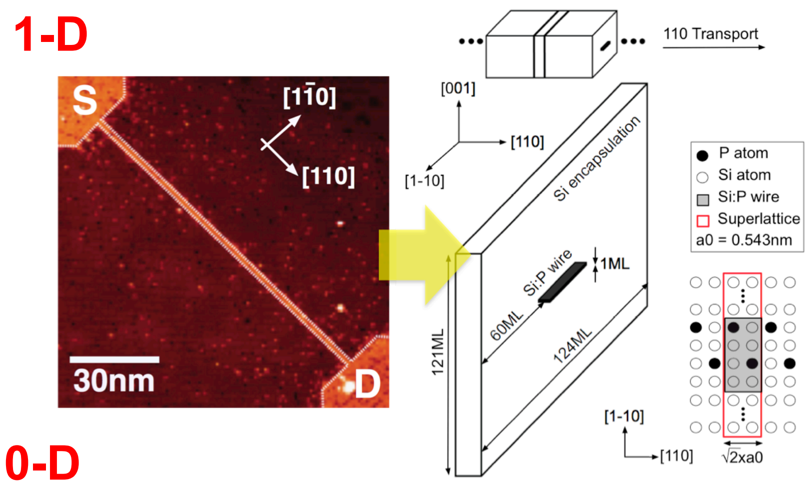
2) Si:P Nanowire (1-D)

2A) Semi-metallic property

2B) Modulation of channel conductance

2C) Resistance-limit of Si Nanowire

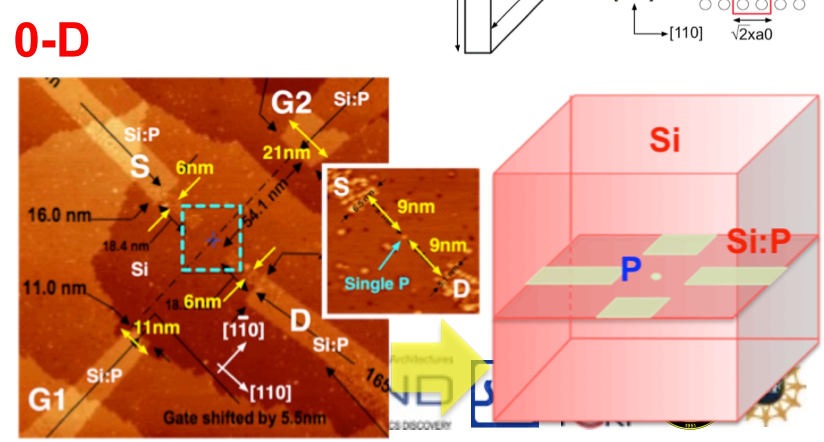
2D) Sensitivity of resistance to doping disorder



3) Single-donor Quantum-dot (0-D)

3A) Channel Modulation

→ Single-electron transport



2-D Doping Plane (1A): Semi-metallic Property

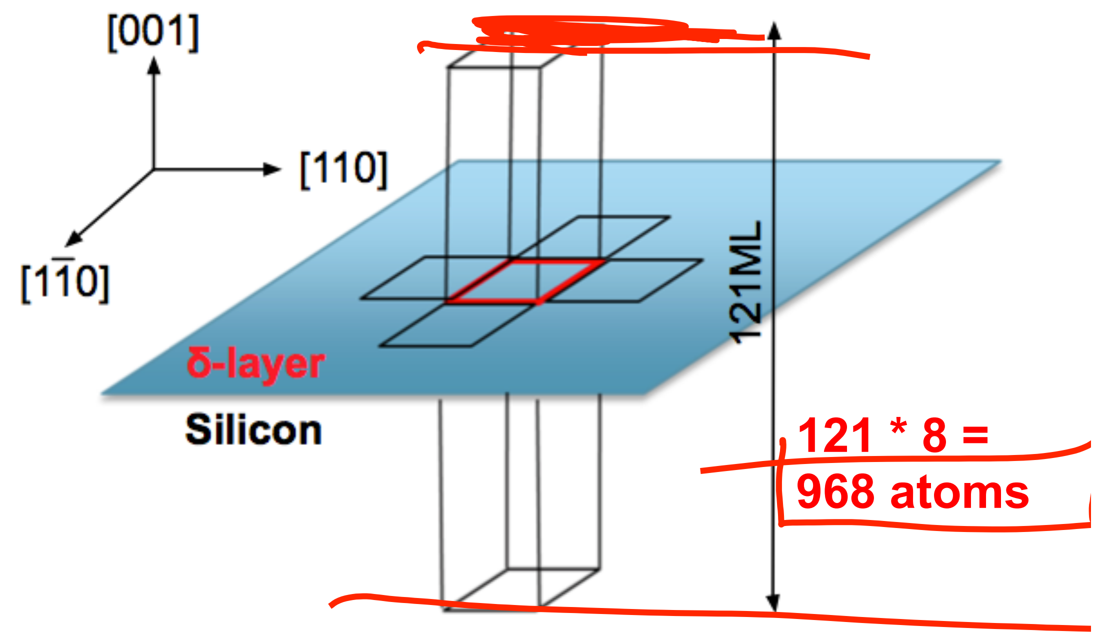
Objective
- Explain metallic property of 1/4ML doped 2-D Si:P layer

Approach
- Supercell, 2-D periodic BC
- Dispersion at charge neutrality

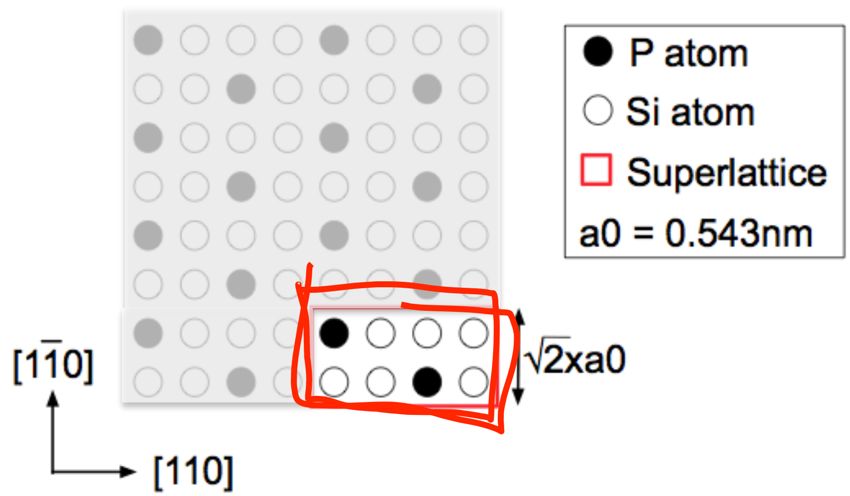
Results
- Donor-bands in Si gap
- Non-zero DOS near EF
- Semimetal → DOS Fluctuation
- Agree with previous studies
- Our approach:
  → Much larger systems!

(1A)
Int'l Workshop for Comp. Elec. (2009)
IEEE NANO (2010)

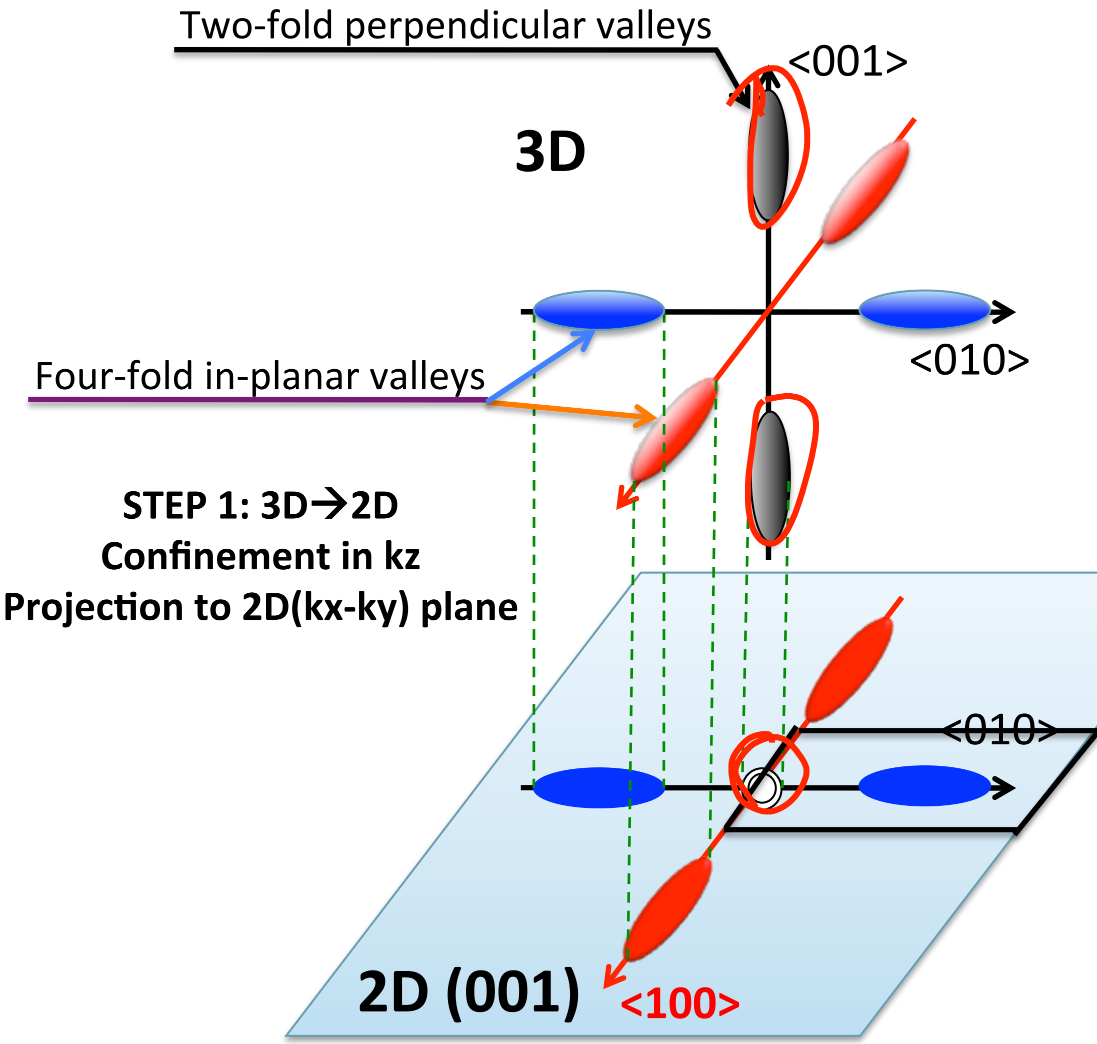
Schematic of Supercell

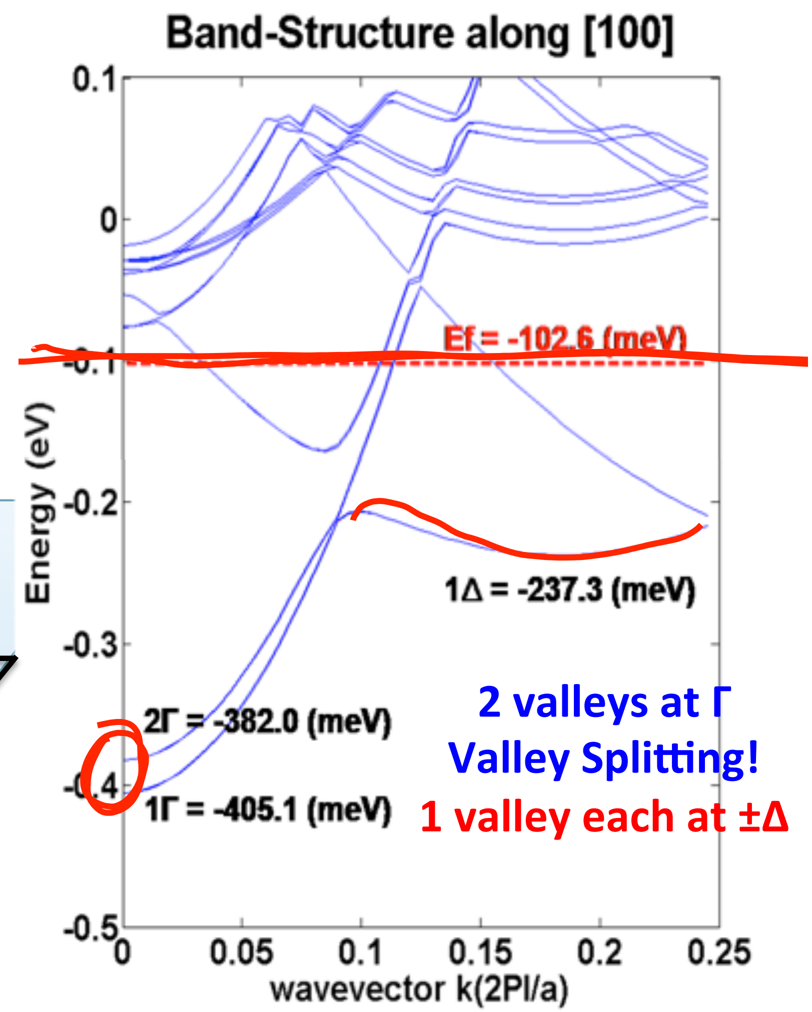


Atomic Profile on Doping Plane



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

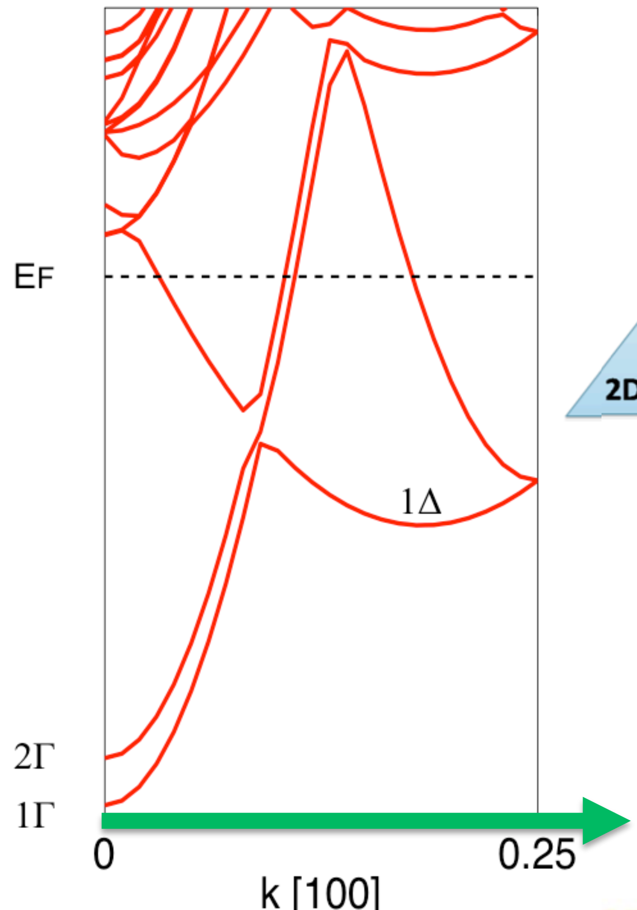


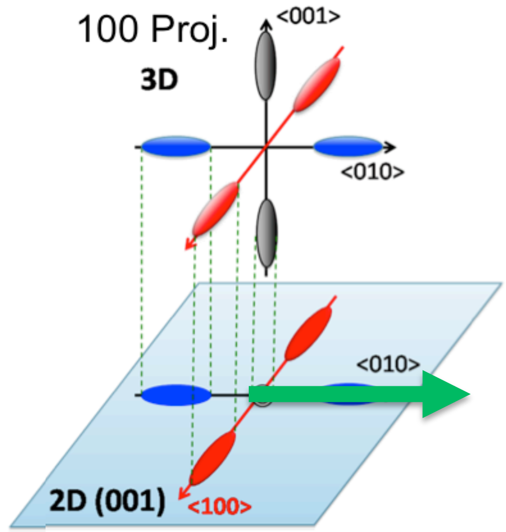


Bandstructure at charge neutrality

- **Donor bands are observed below the Si bulk band gap**
  - » Conduction band minimum of Si bulk → 0(eV)

Bandstructure and Projection of 6 ellipsoids in Si bulk conduction band





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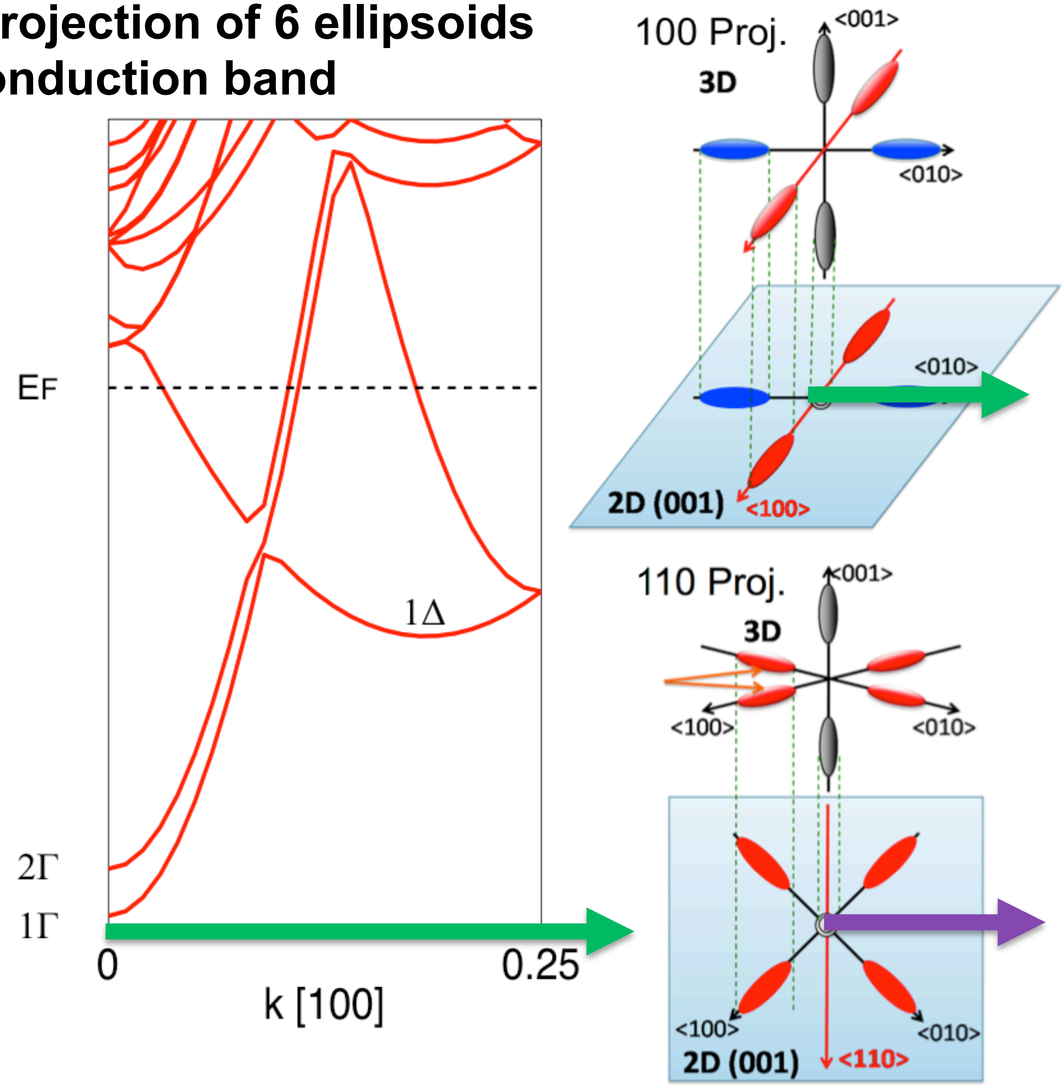

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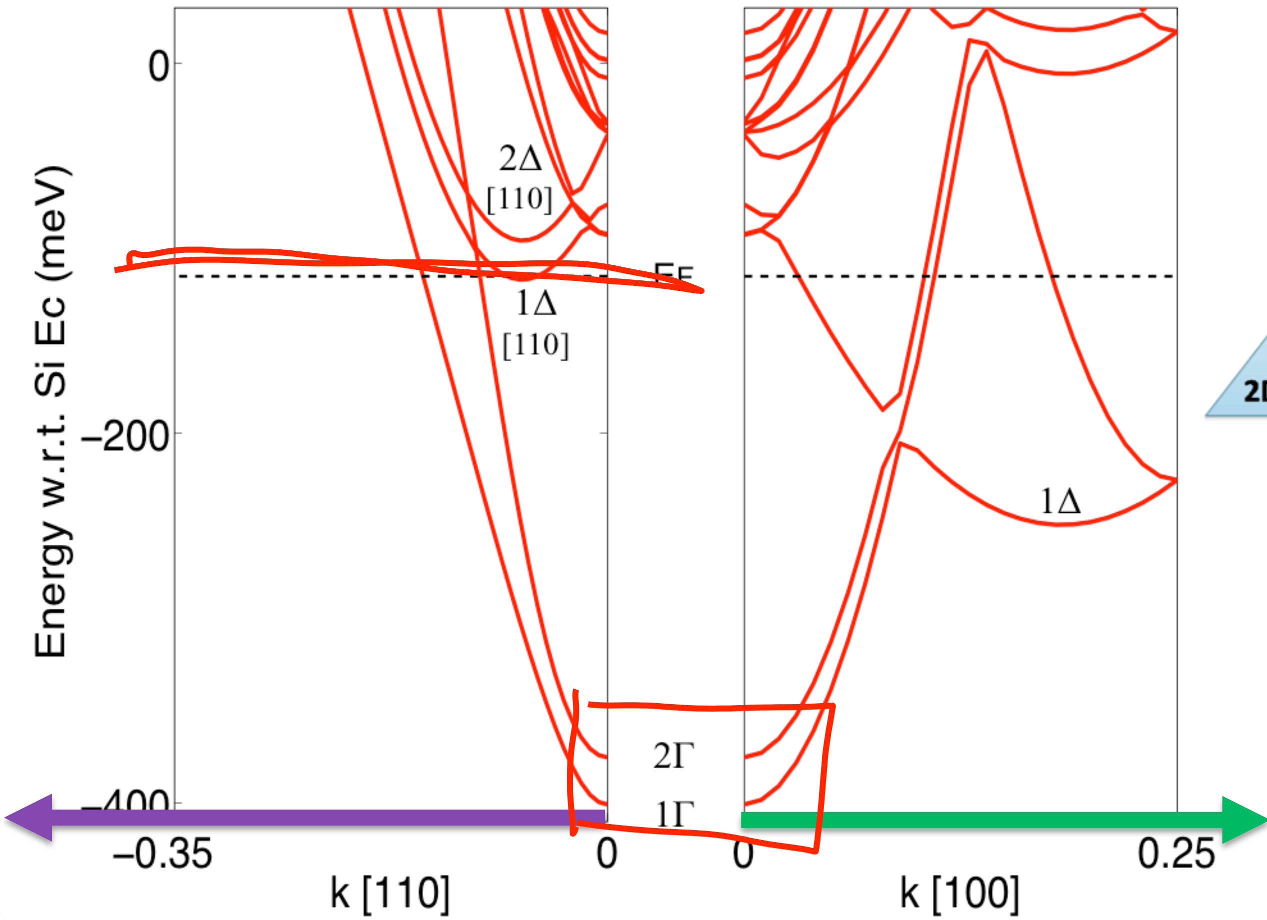
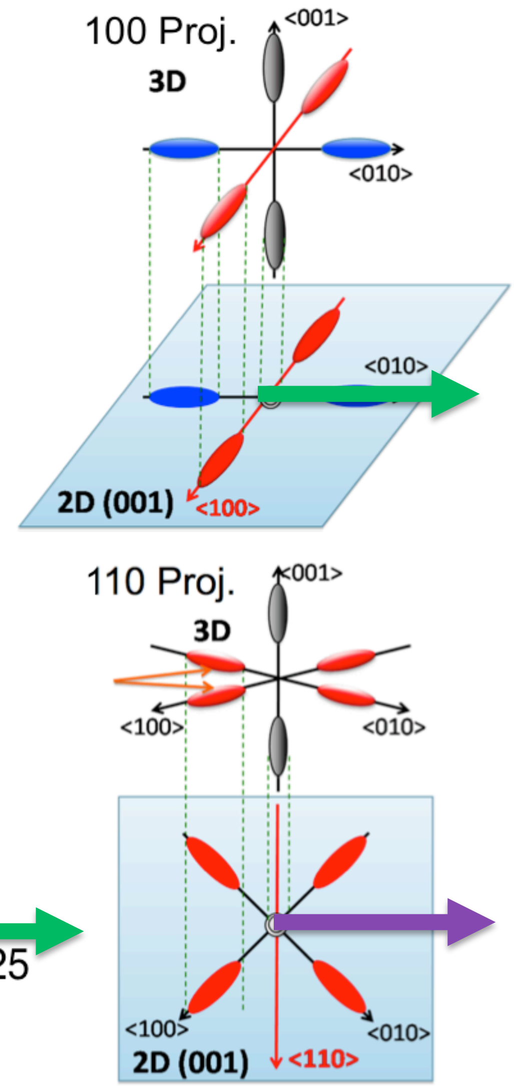
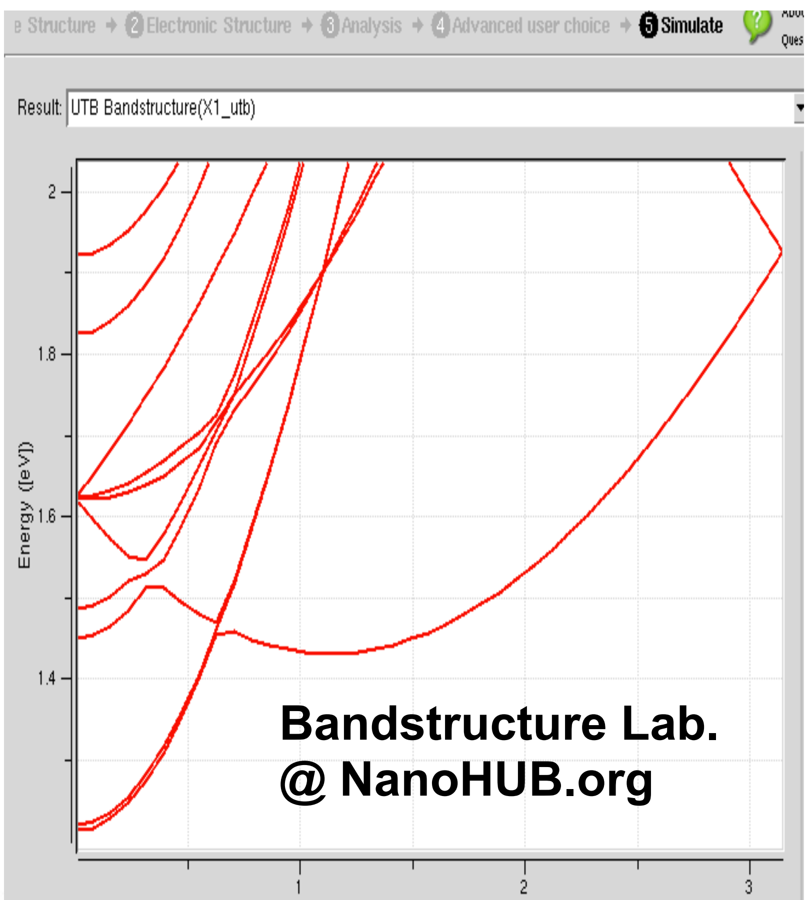
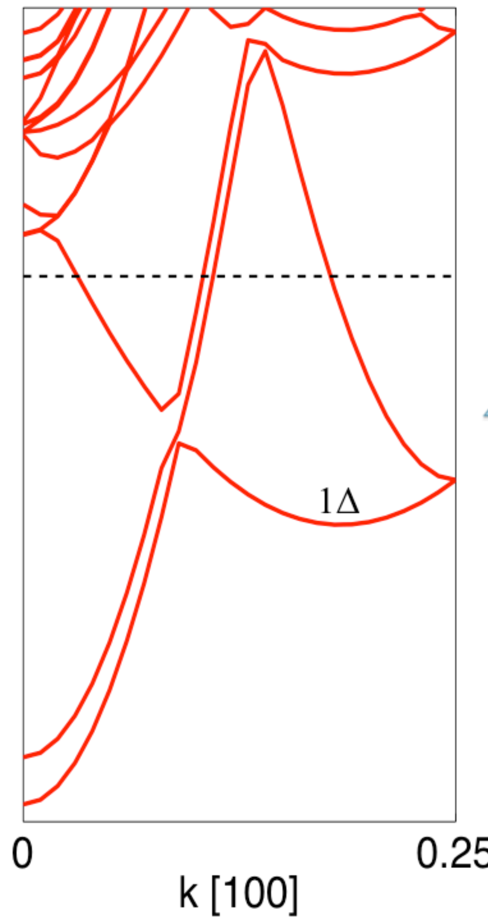


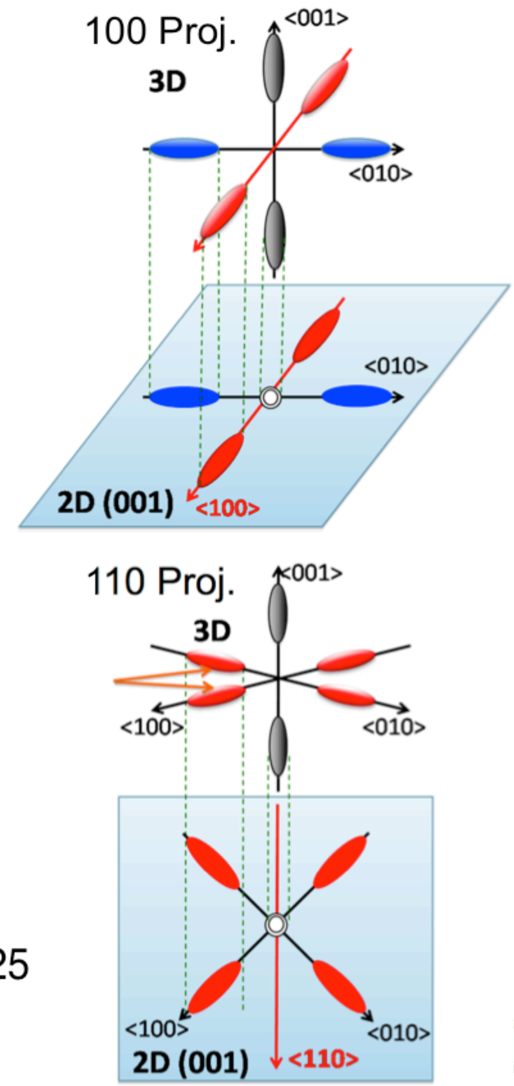


Band-Projection: A comparison to Si UTB



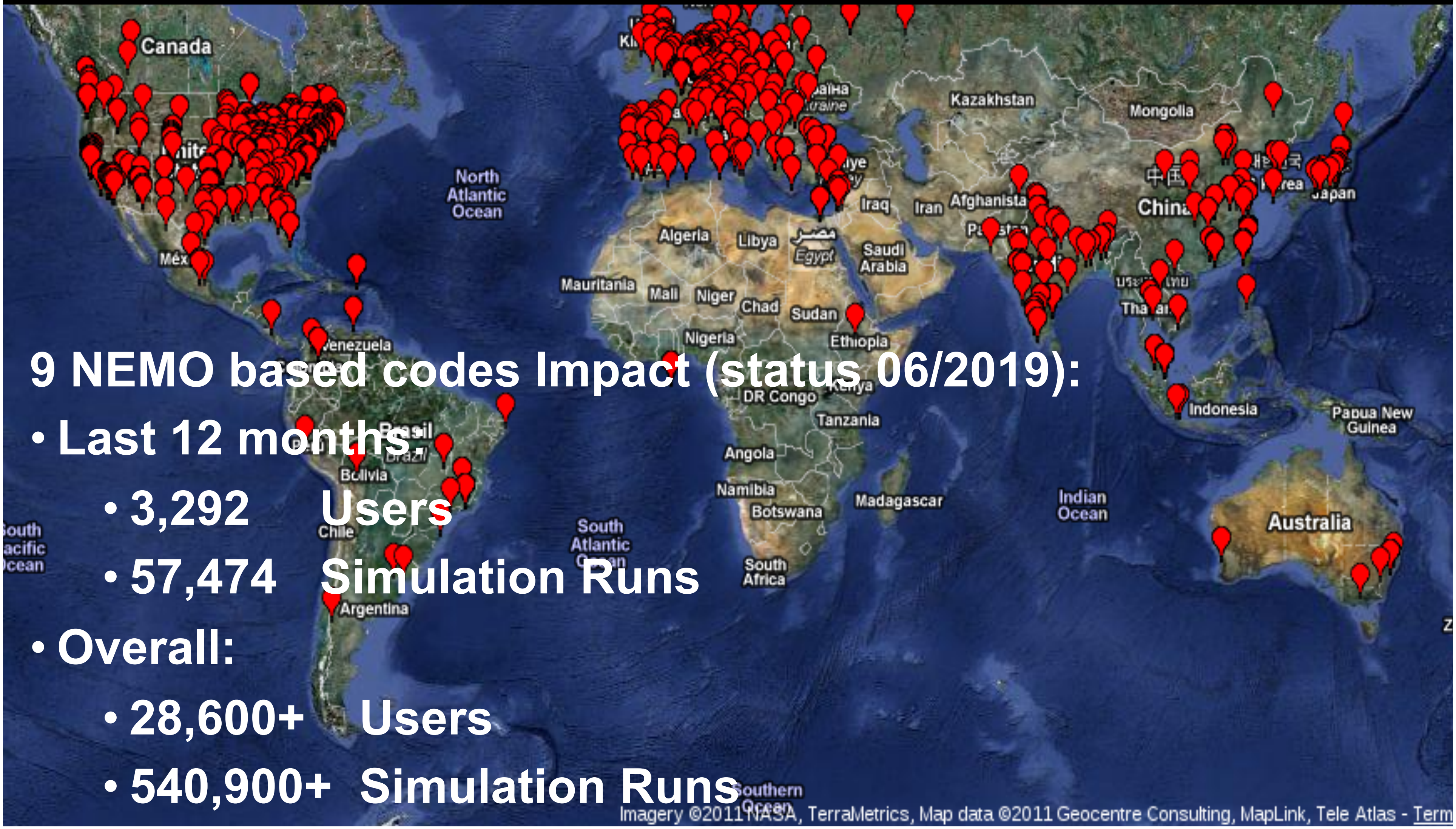
:tion of 6 ellipsoids
:ction band





39 Klimeck tools:
- **>71,000 users**
- **>2.3 million simulations**

Classroom use:
>11,000 students
>64 universities



9 NEMO based codes Impact (status 06/2019):
- **Last 12 months:**
  - **3,292 Users**
  - **57,474 Simulation Runs**
- **Overall:**
  - **28,600+ Users**
  - **540,900+ Simulation Runs**

Single Impurity Outline

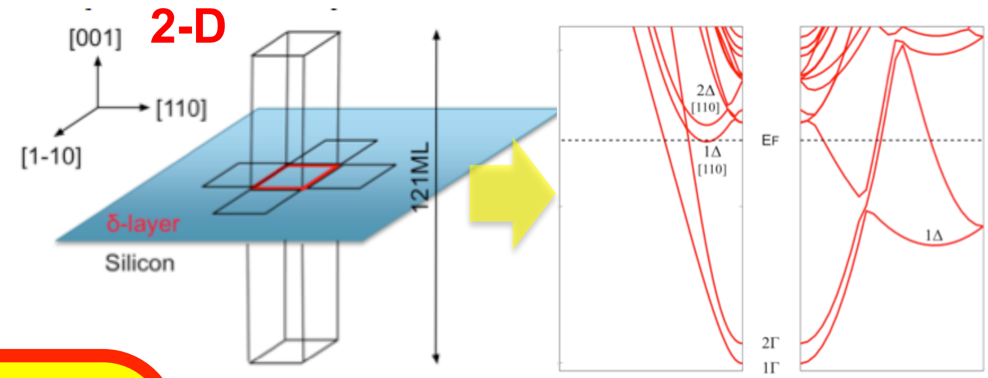
1) Si:P Doping Plane (2-D)

1A) Semi-metallic property

1B) Sensitivity to doping disorder

121 * 8 = 968 atoms

2-D



2) Si:P Nanowire (1-D)

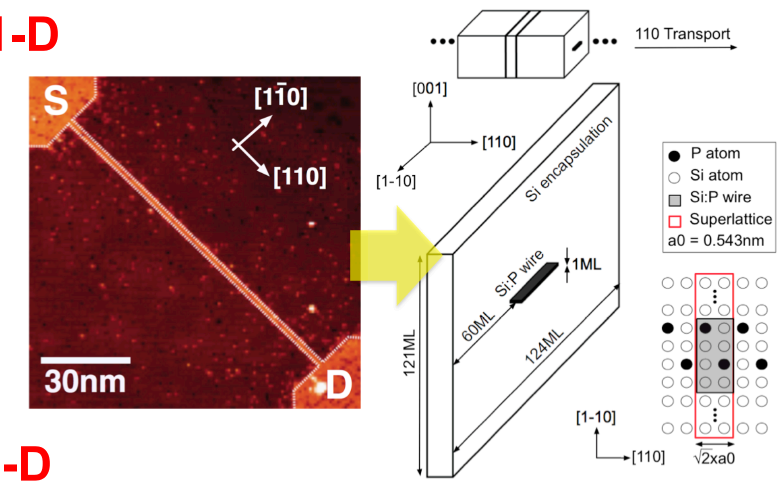
2A) Semi-metallic property

2B) Modulation of channel conductance

2C) Resistance-limit of Si Nanowire

2D) Sensitivity of resistance to doping disorder

1-D

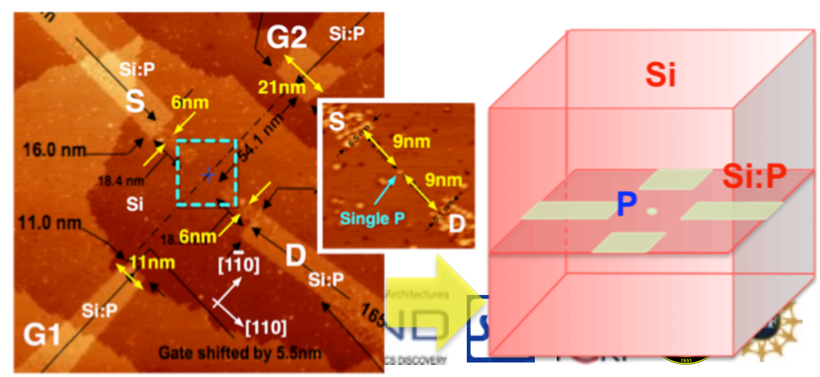


3) Single-donor Quantum-dot (0-D)

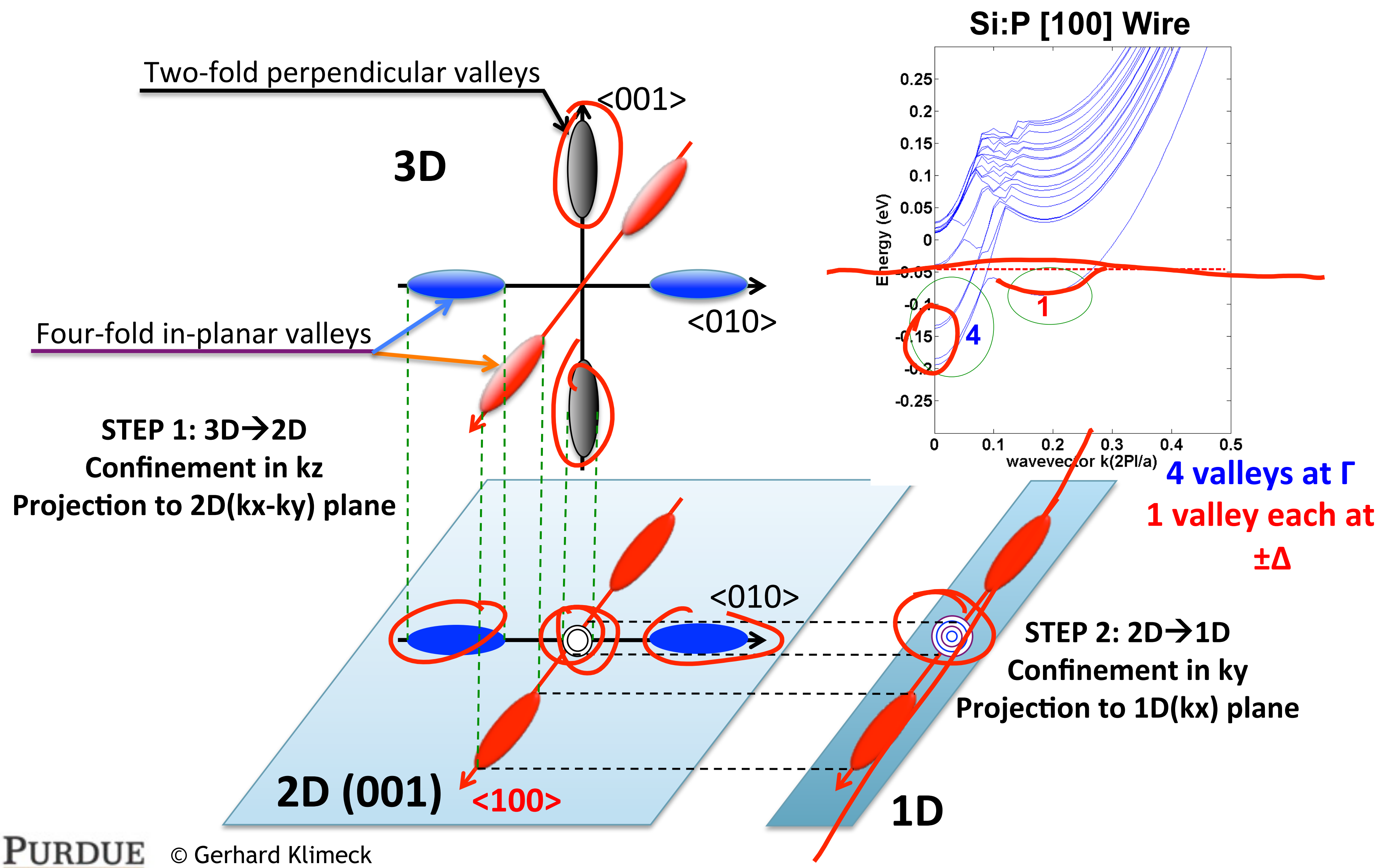
3A) Channel Modulation

→ Single-electron transport

0-D

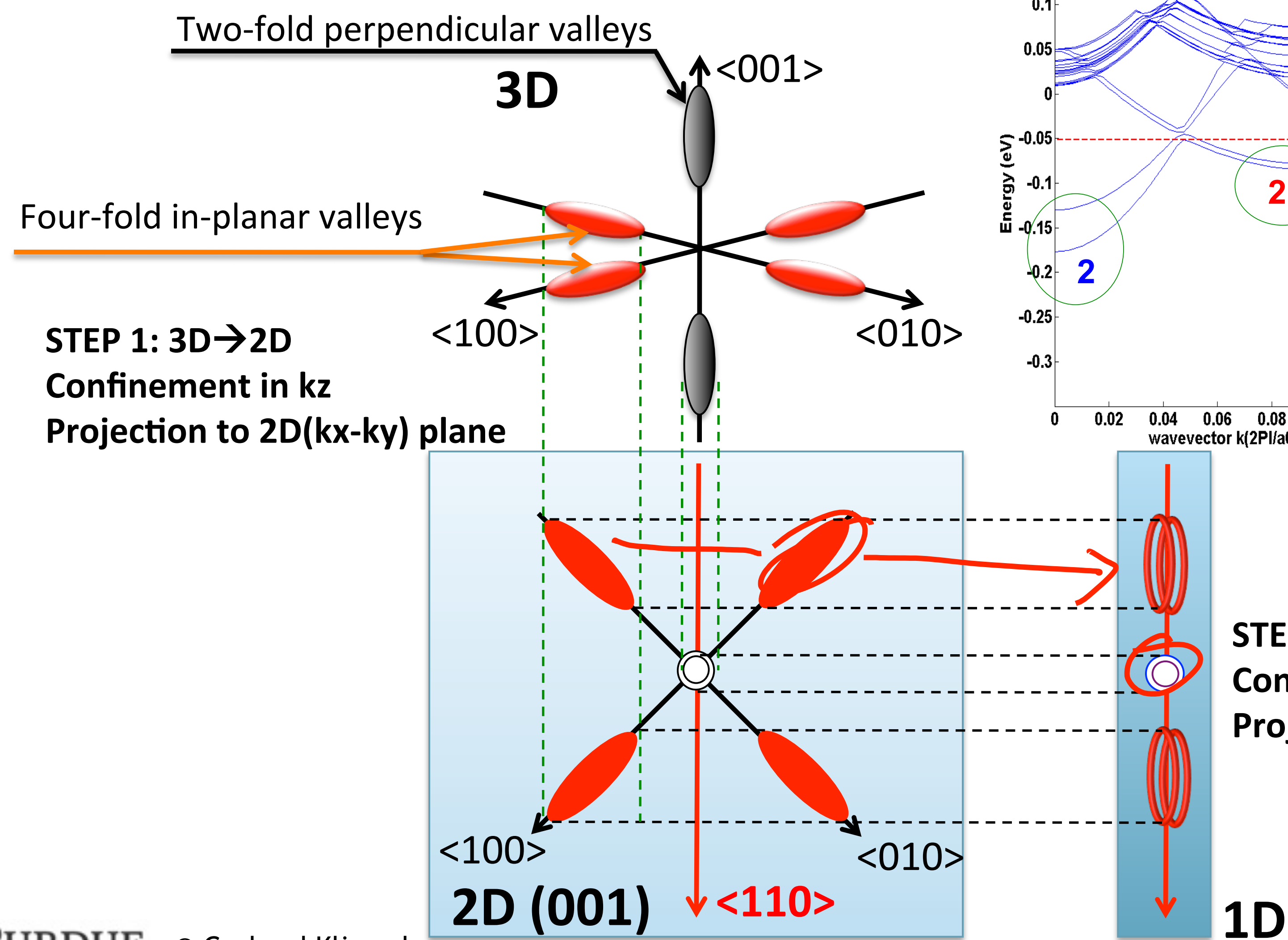


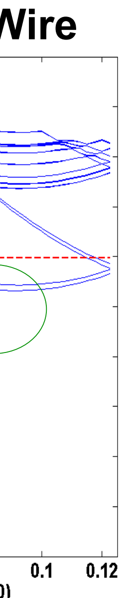
- 3D→2D→1D projection of Si [100] nanowire



Band projection in [110] Si:P wires

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



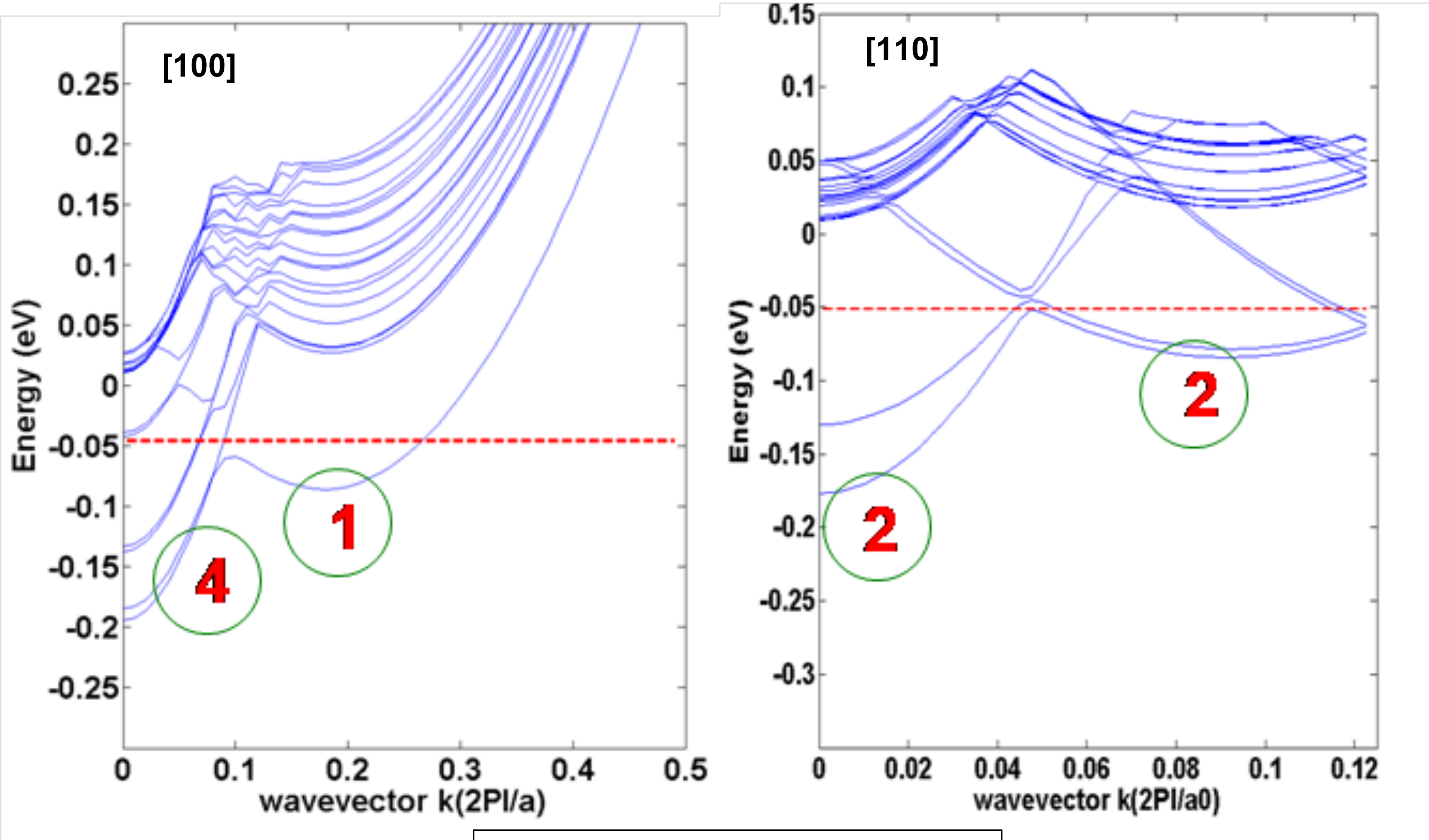


STEP 1: 3D→2D
Confinement in kz
Projection to 2D(kx-ky) plane

2 valleys at Γ
2 valley each at ±Δ

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

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



Wires are metllic with:
G(Ballistic) ~ 6($2e^2/h$)

1-D Nanowire (2A): Semi-metallic Property

Objective
- Experiment: Ohmic conduction
- Explain metallic property of 1/4ML doped Si:P nanowire

Approach
- Supercell, 1-D periodic BC
- Dispersion at charge neutrality

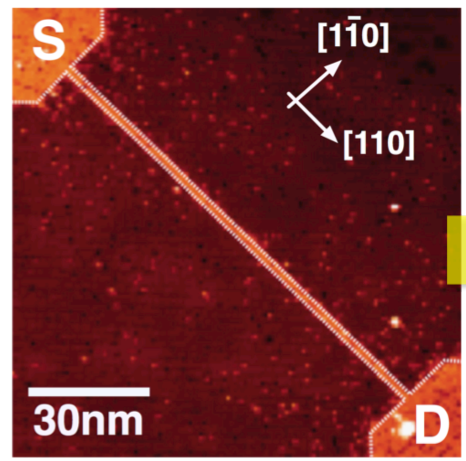
Remark
- Expensive computation.
  → compared to 2-D Si:P plane

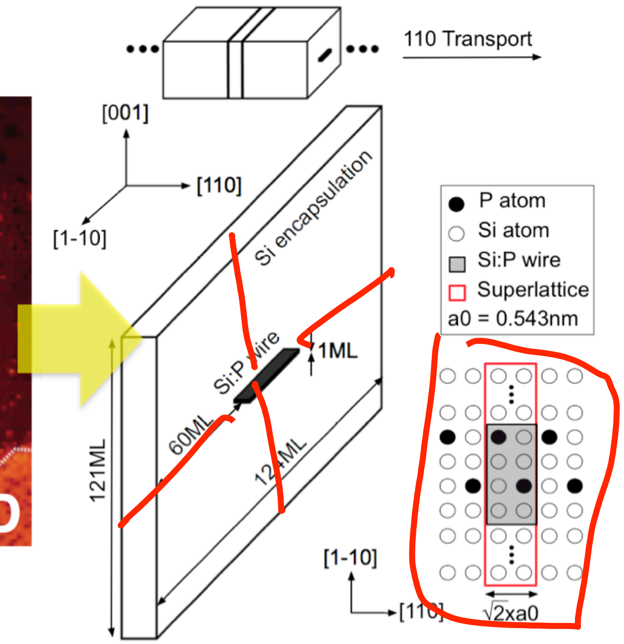
Results
- Donor bands : 6 modes
- Non-zero DOS near EF
- Semimetal → DOS Fluctuations

(2A) IEEE Silicon Nanoelectronics Workshop (2010)

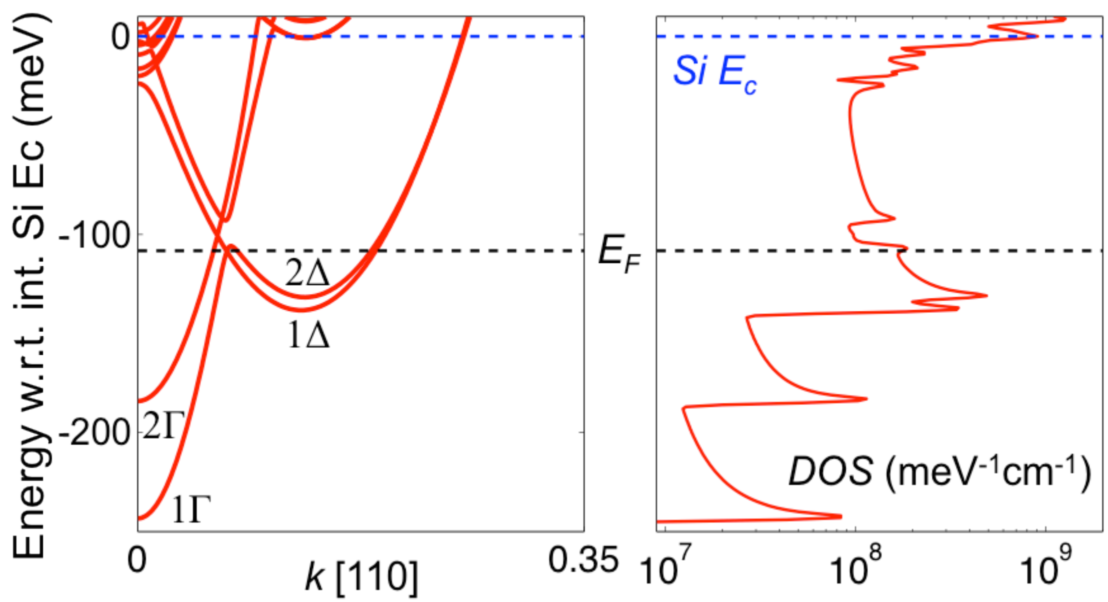
121 * 124 * 2 = 30,008 atoms

Real NW and Supercell





Dispersion and DOS



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1B) Sensitivity to doping disord

121 * 8 = 968 atoms

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2A) Semi-metallic property

2B) Modulation of channel conductance

2C) Resistance-limit of Si Nanowire

2D) Sensitivity of resistance to doping disorder

121 * 124 * 2 = 30,008 atoms

3) Single-donor Quantum-dot (0-D)

3A) Channel Modulation

→ Single-electron transport

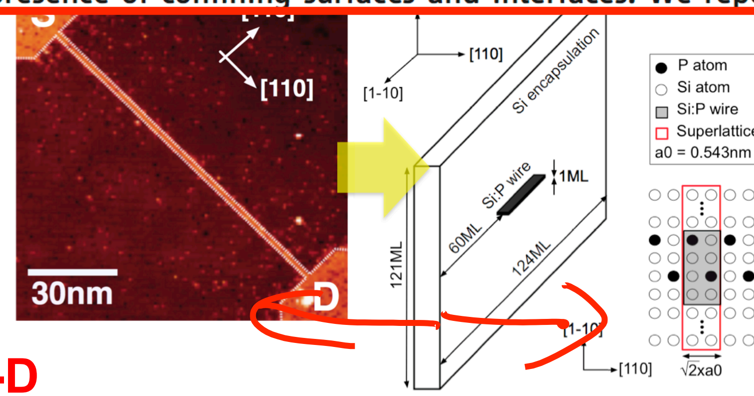
40 x 40 x 10 nm^3 ~ 1million atoms

Ohm's Law Survives to the Atomic Scale

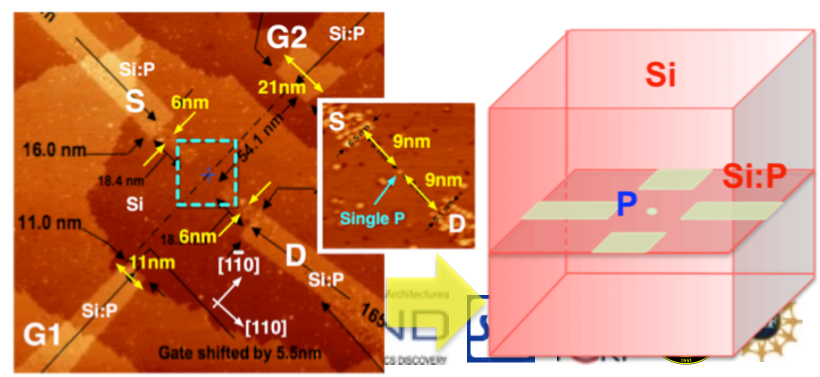
B. Weber,[1] S. Mahapatra,[1] H. Ryu,[2]* S. Lee,[2]
W. C. T. Lee,[1] G. Klimeck,[2] L. C. L. Hollenber

As silicon electronics approaches the atomic sc
in size to the active device components. Maint
challenging because of the presence of confining surfaces and interfaces. We repor

Science AAAS

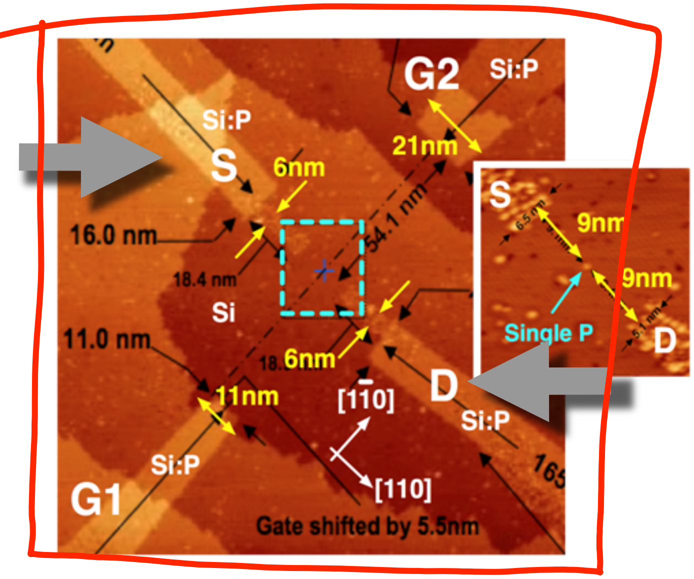


0-D

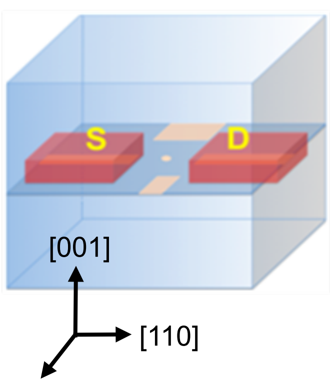


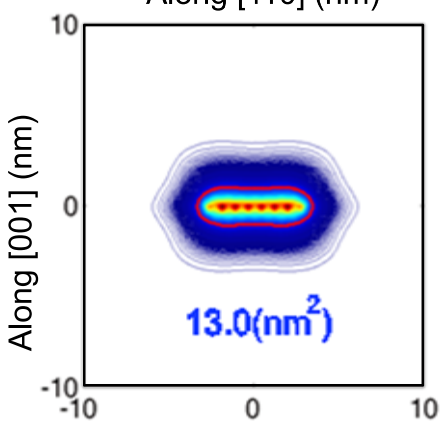
Modeling of Si/P contacts

- Leads show *semi-metallic* behavior (non-zero DOS near E_F)
- Electrons strongly confined to leads (leads densely doped)

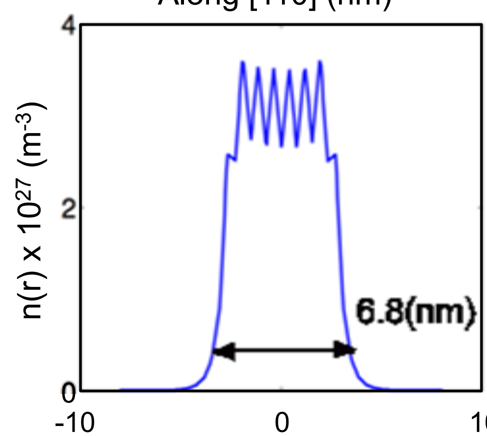


Source/Drain

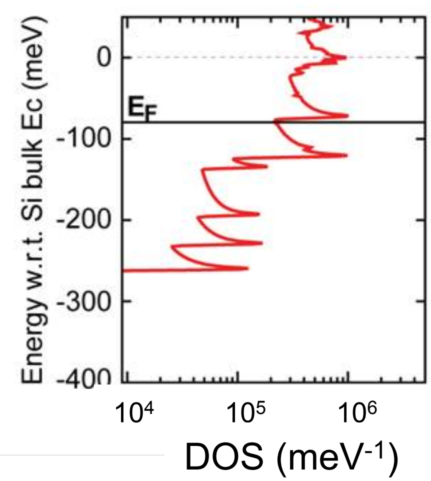




Spatial electron distribution

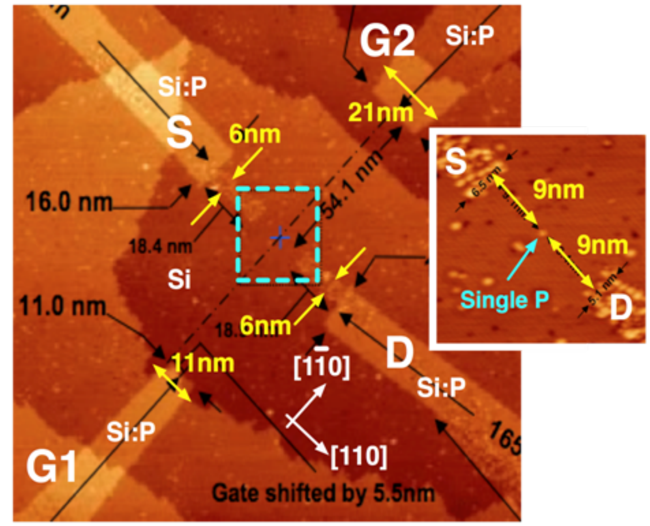


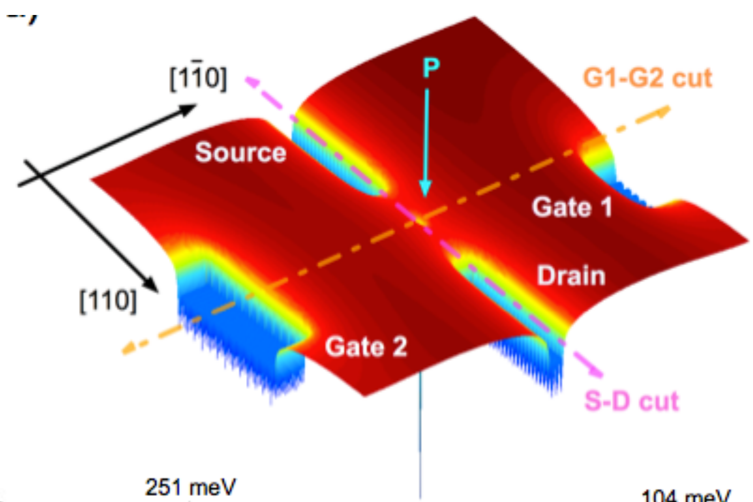
Electron density



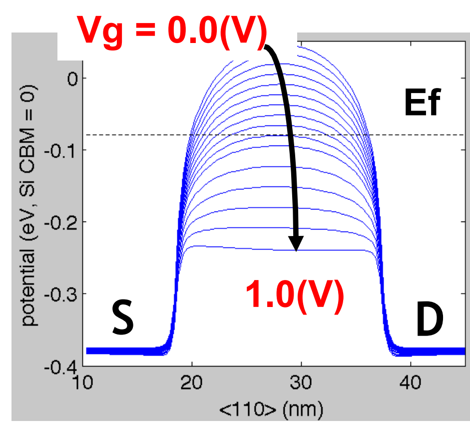
Potential profile

- Thomas-Fermi calculation for potential landscape *without* ionized donor
  Klimeck et al, APL (1995)
  40 x 40 x 10 nm^3 ~ 1million atoms
- Donor potential
  - ✓Empty state: Analytical Coulomb potential
    R.Rahman et al. PRL 2007,
    Lansbergen, Nature Physics, 4, 656 (2008)
  - ✓Filled state: "Screened" potential by an electron from self-consistent simulation

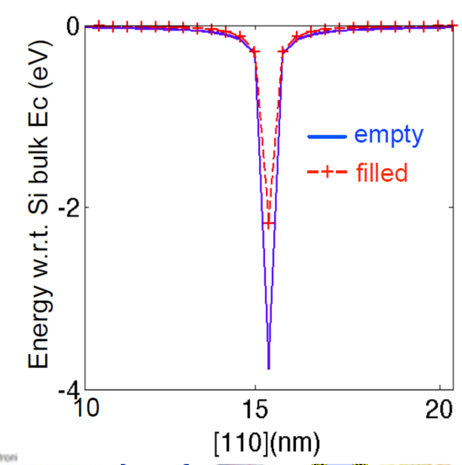


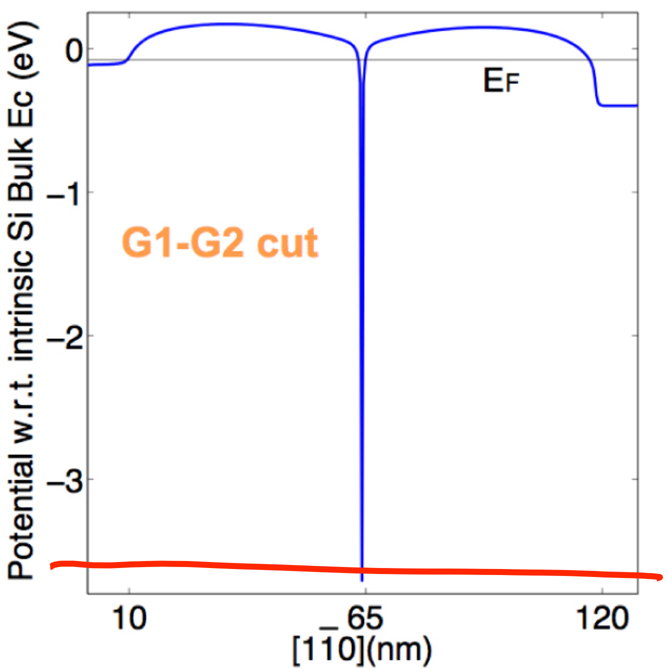


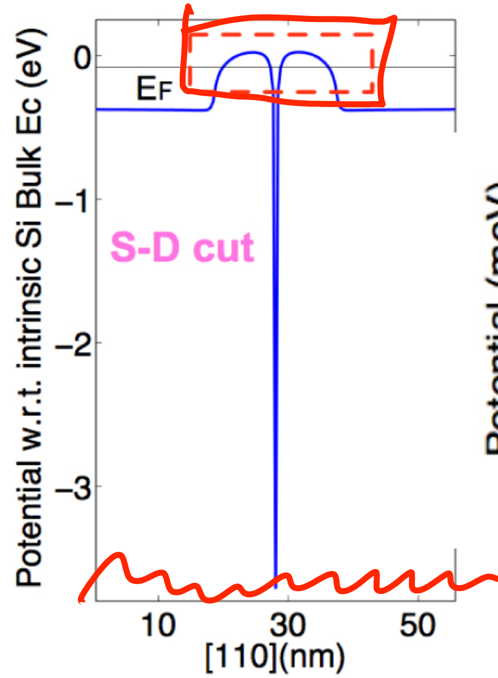
Potential profile

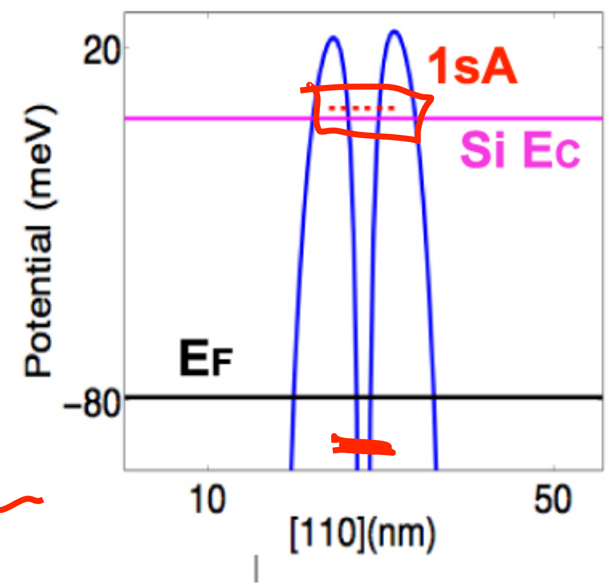


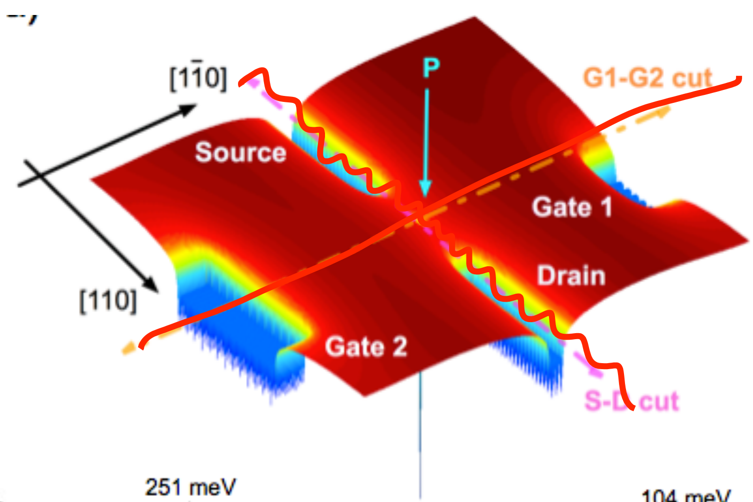
Donor potential









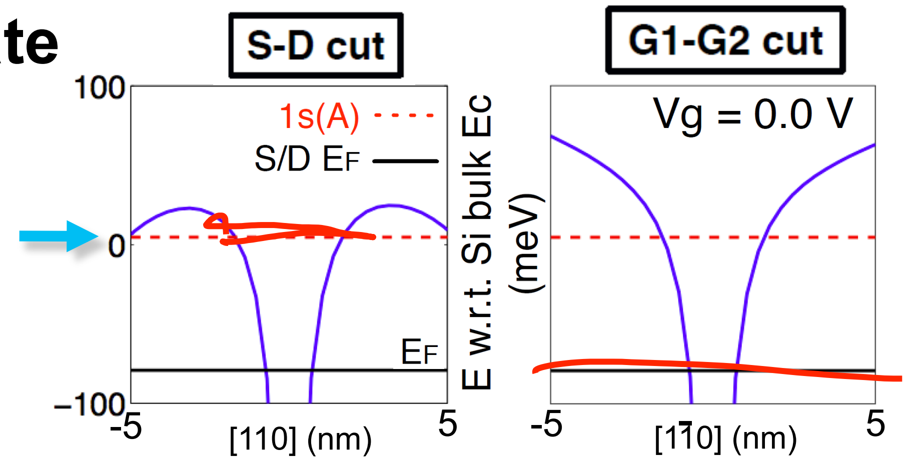


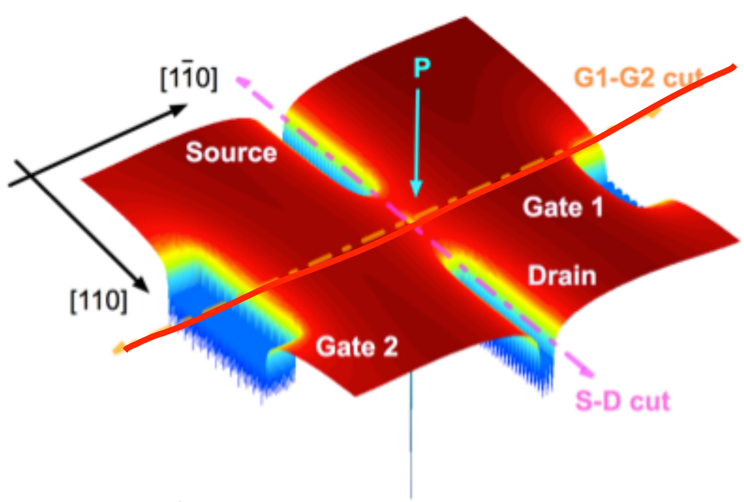
Channel State Electrostatics (Equilibrium)

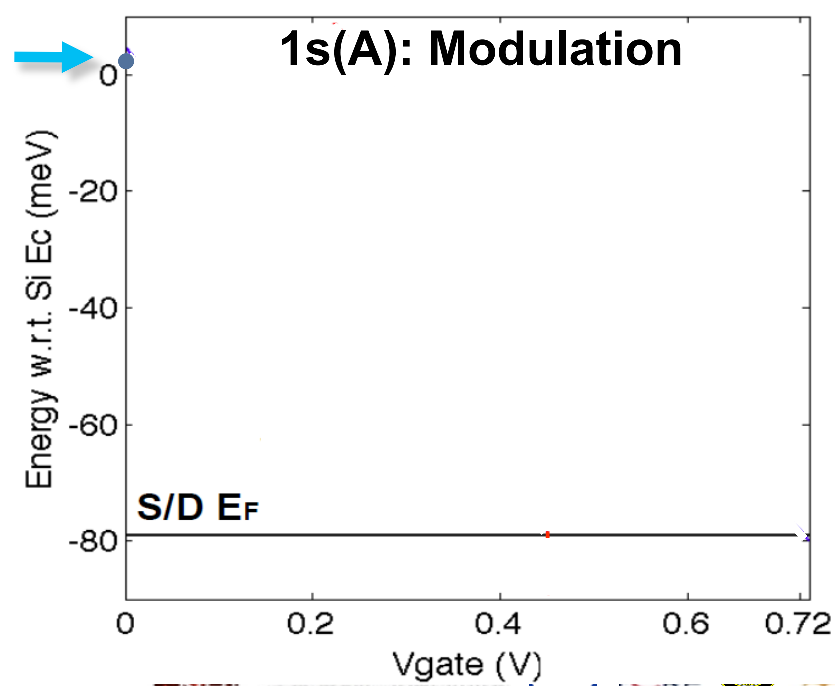
- **Channel empty at equilibrium**
- 1s(A) ground state ~ 84meV above Ef
- S-D barrier heights ~ 104 meV
- G1-G2 barrier heights ~ 251 meV

Gate Modulation of Channel state

- Donor potential along S-D and G1-G2
- Vds = 0, sweep Vg
- If ground state 1s(A) = Ef
  → donor confinement potential changes
  → donor from D^+ to D^0 regime







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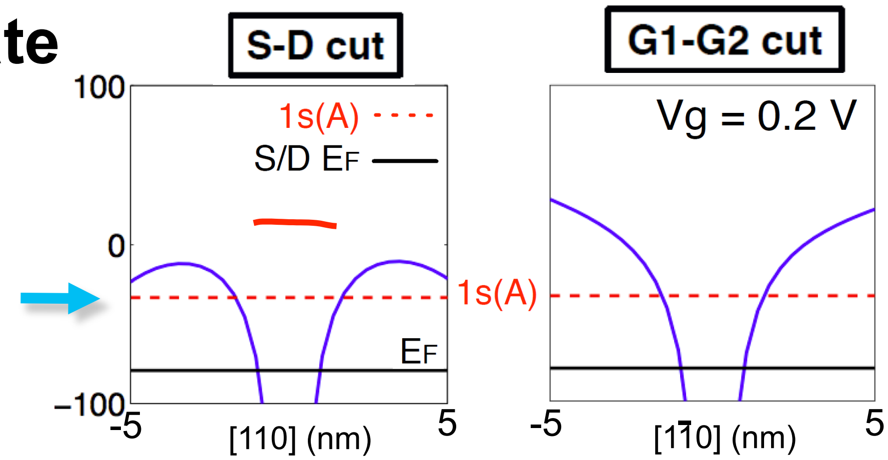

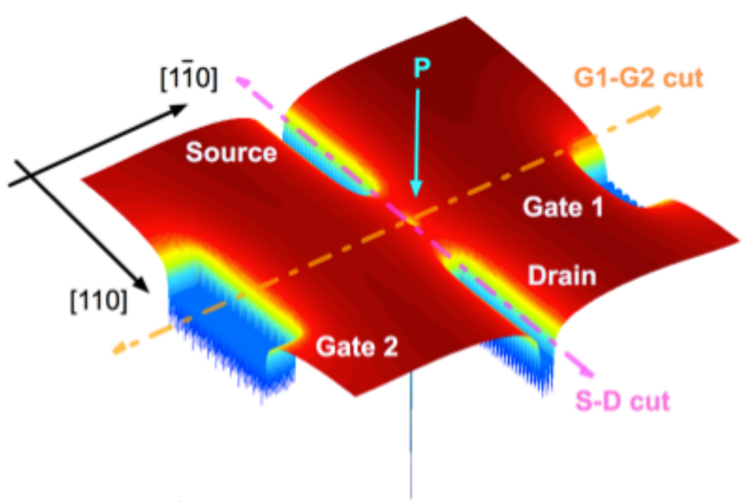

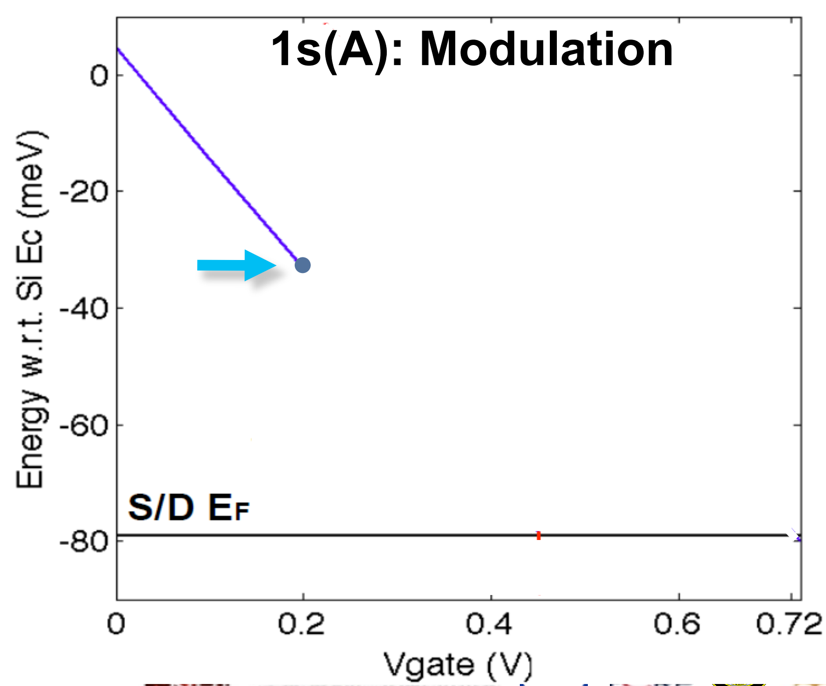

Results: Gate Modulation

Gate Modulation of Channel state

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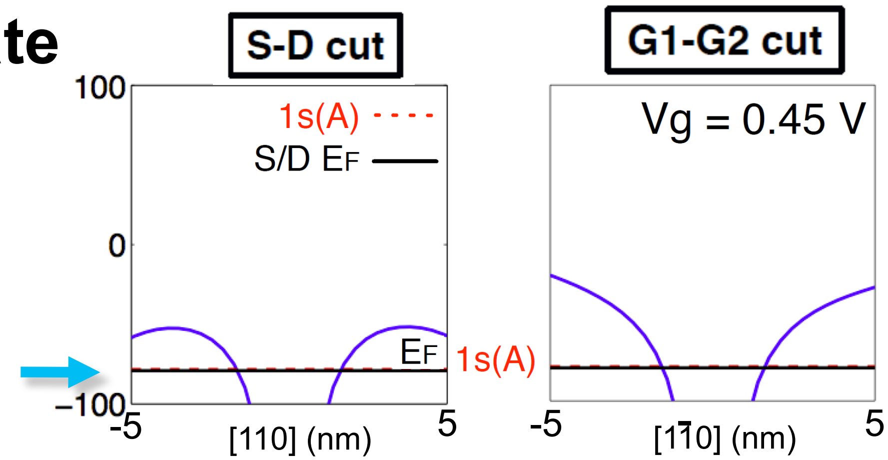

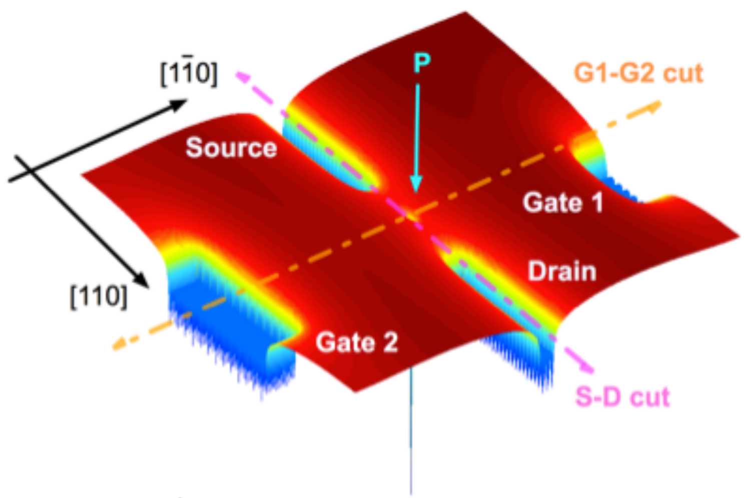

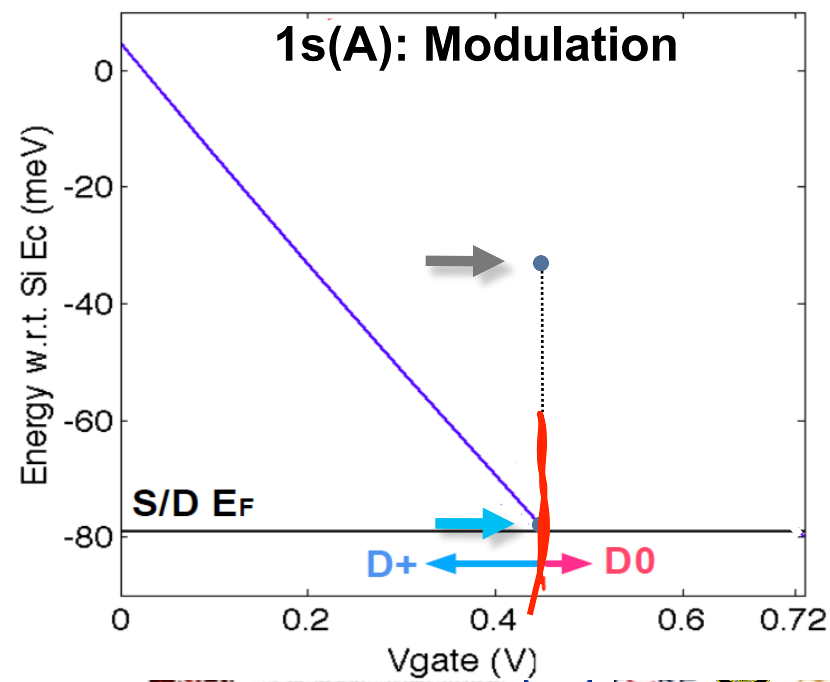

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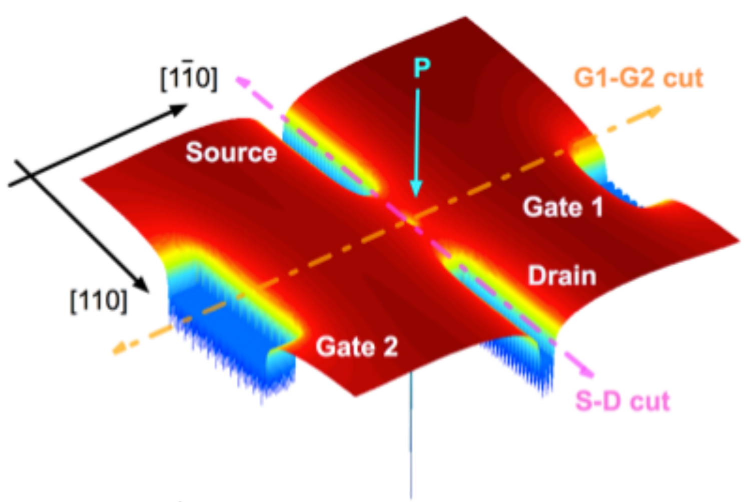

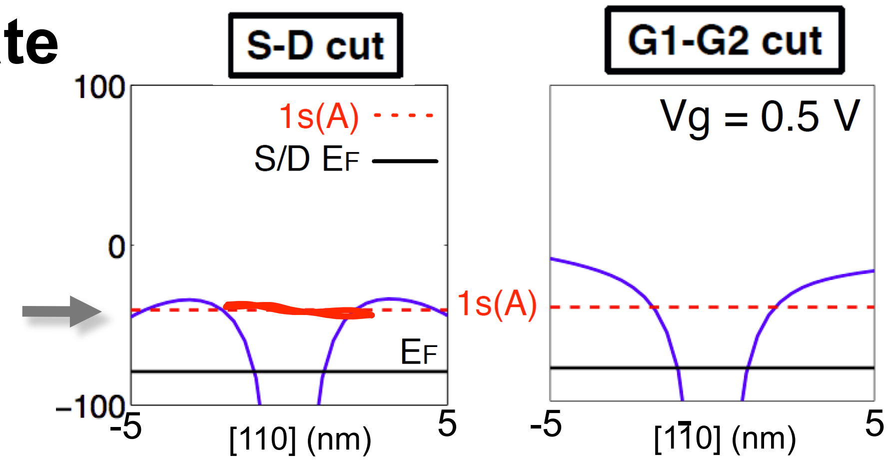

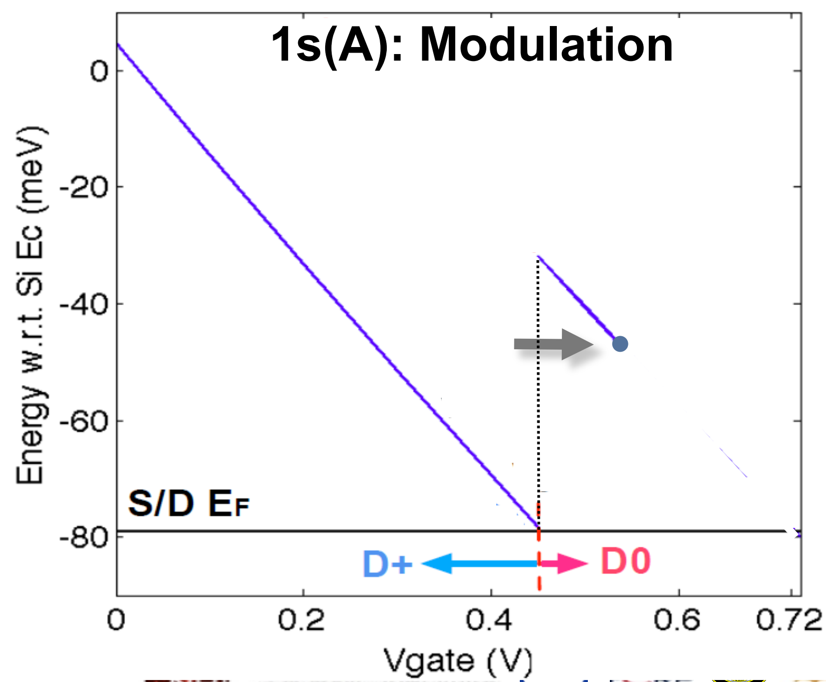

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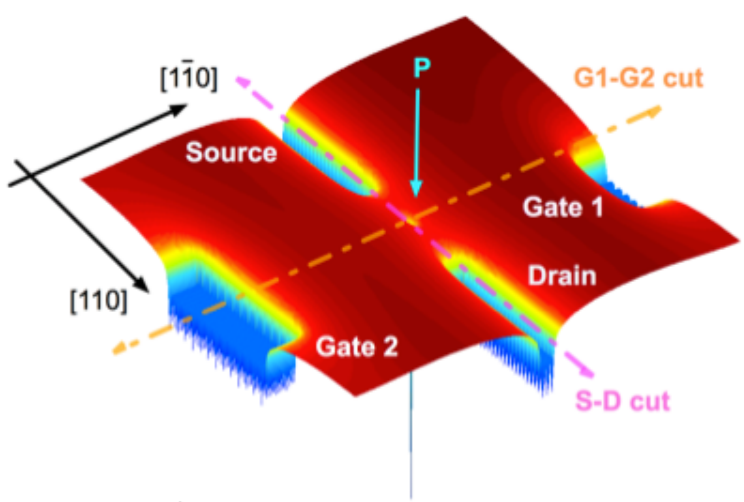

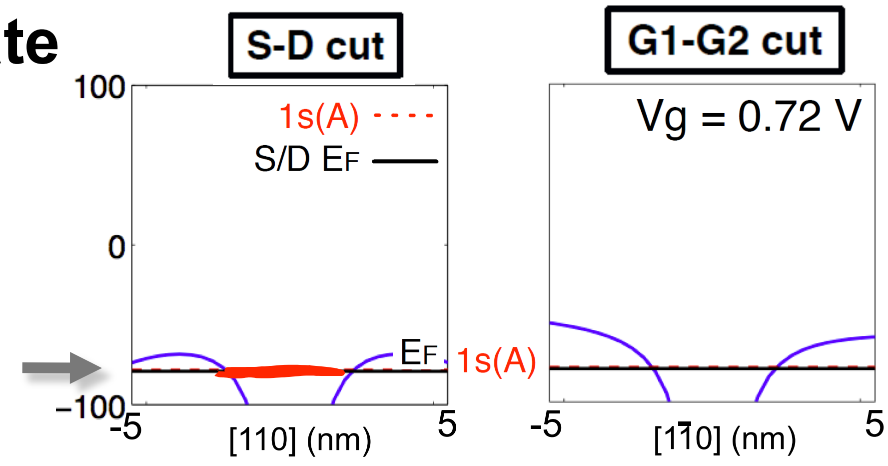

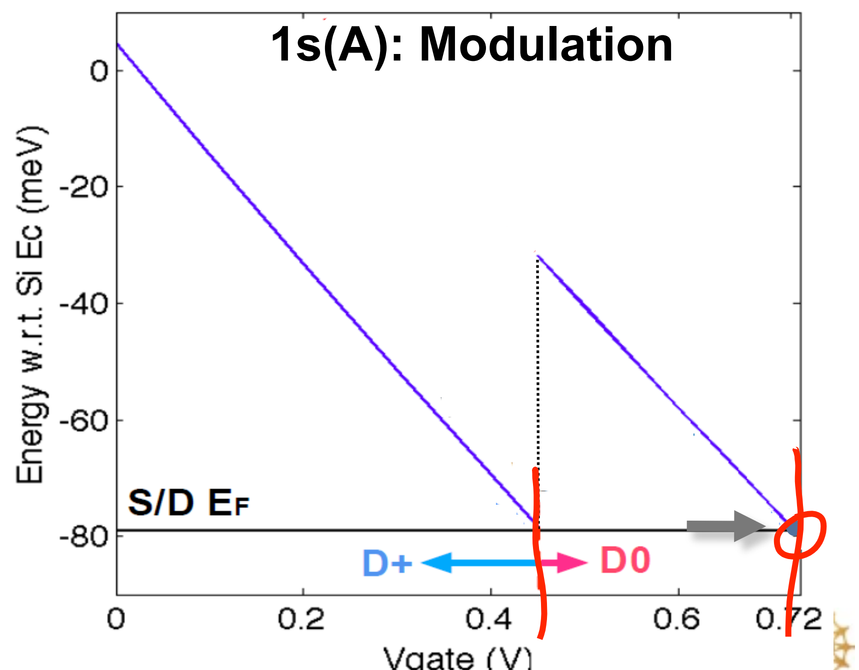

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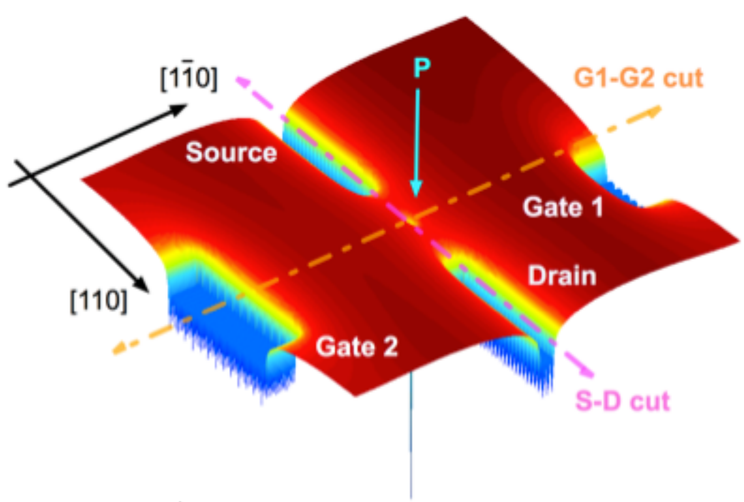
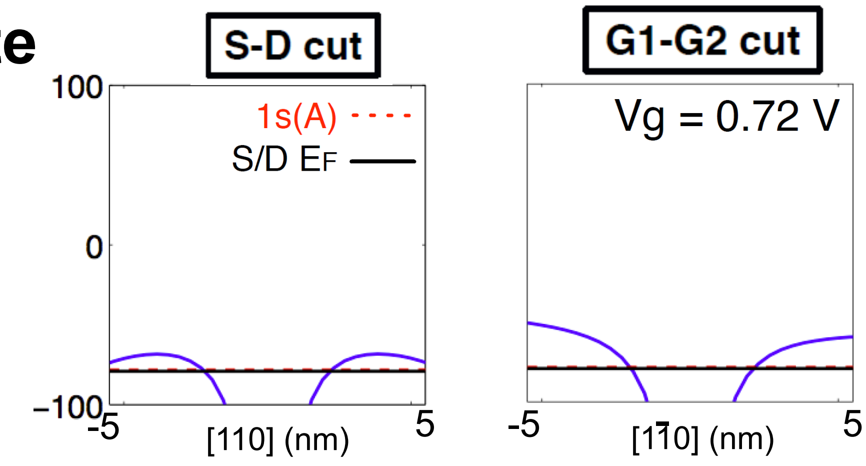
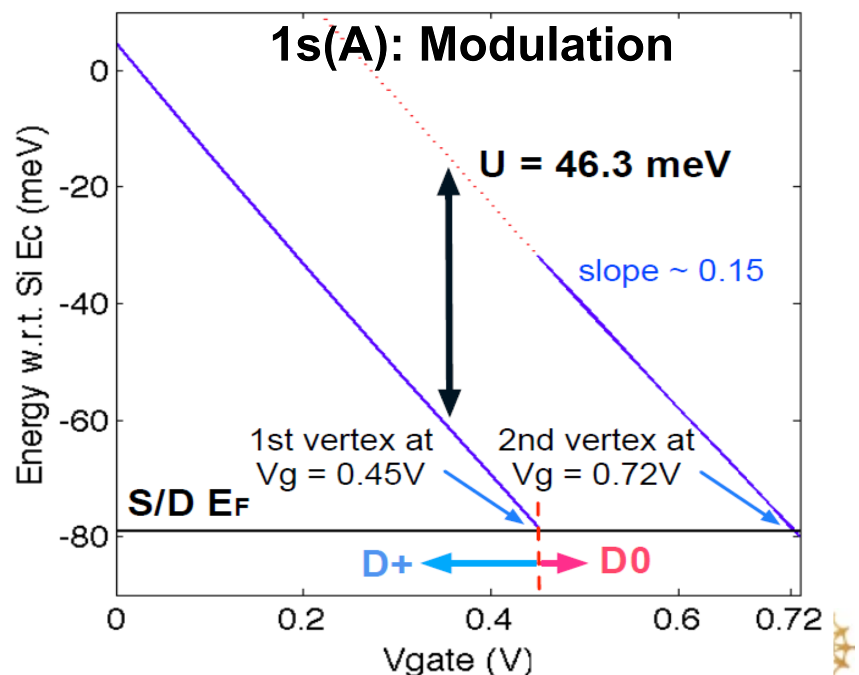
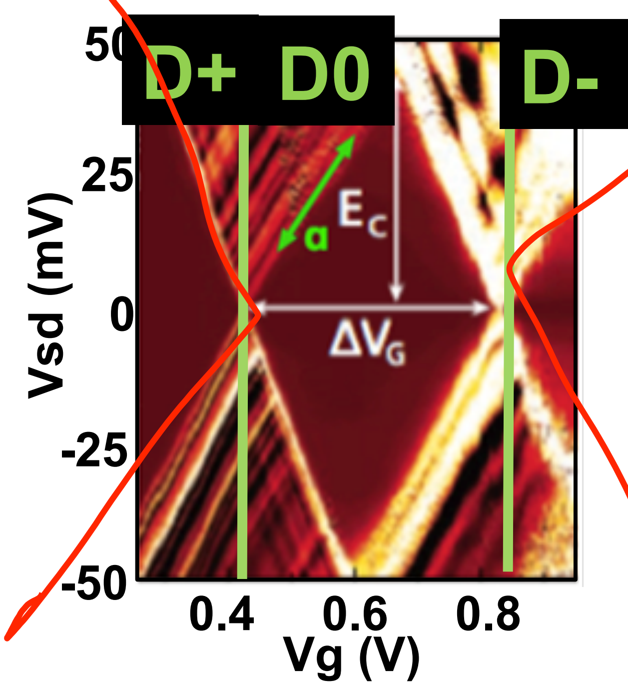


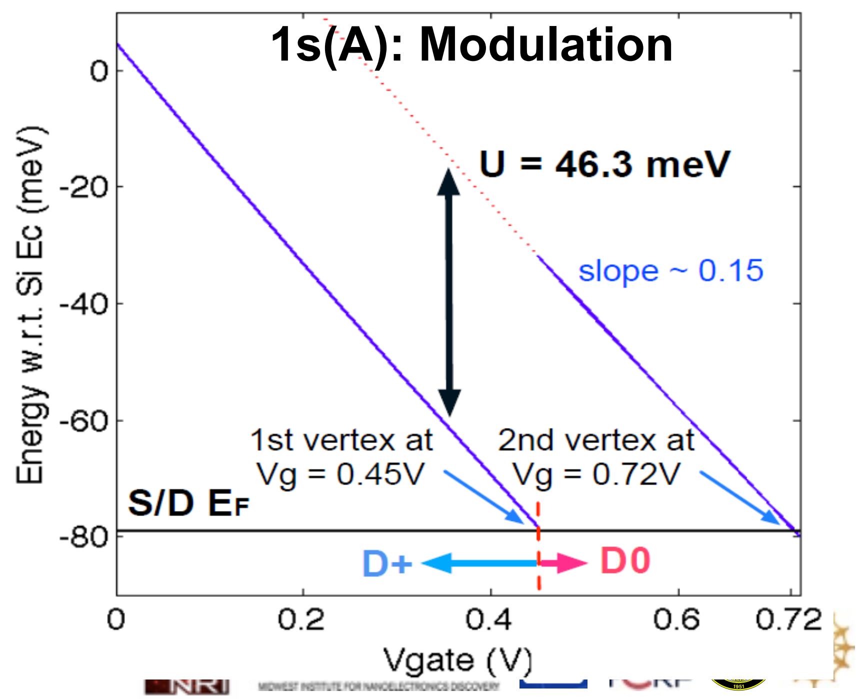




Gate Modulation of Channel state (theory vs. experiment)

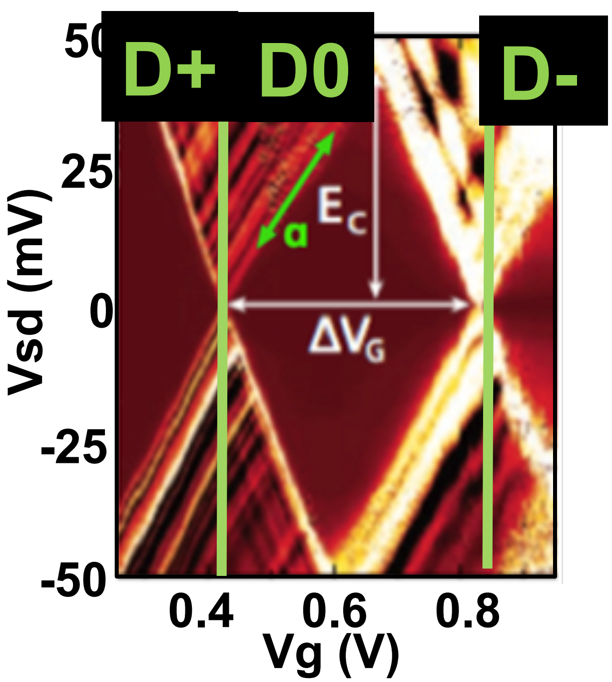
- Close match of transitions points (D+ to D0 at **0.45V**, D0 to D- at **0.72V**)
  Comparison: Experiment (~**0.4V** and ~**0.8V**)
- Close match of charging energy: U= **46.3meV**
  Comparison: Experiment Charging energy Ec= **~47+2meV**
- Gate lever-arm: Theory U/ΔVg = **0.11**,
  Comparison: Experiment Ec/ ΔVg = **0.15**

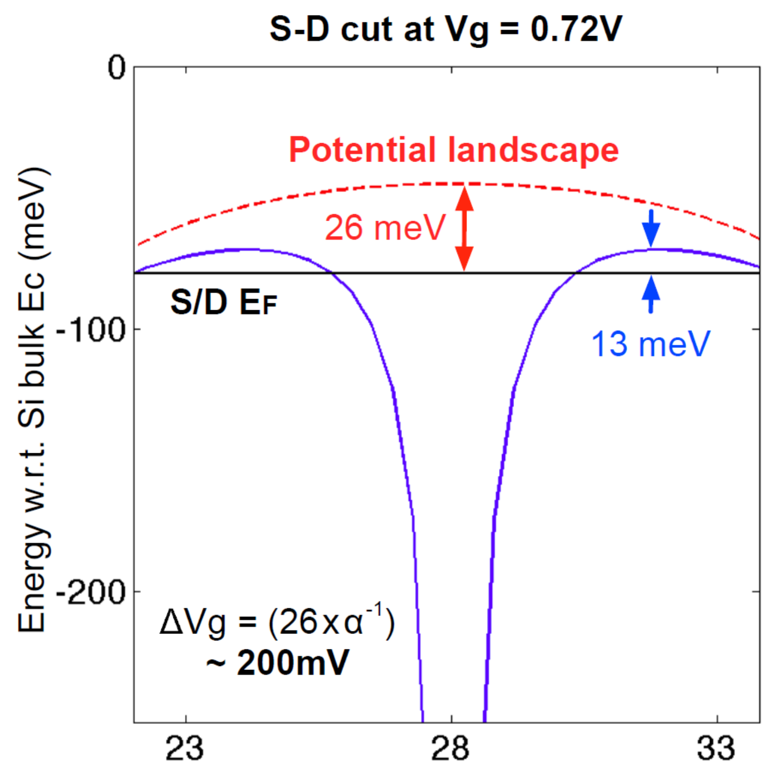




Gate Modulation of Channel state (theory vs. experiment)

- Results explain extension of Coulomb Diamond into D- (two-electron) regime
- Weak channel barrier at second transition point (~ 13 meV)
- Channel electrons no longer confined for Vg greater ~ 1V





(Ongoing) Calculation of Coulomb Diamond

Objective:

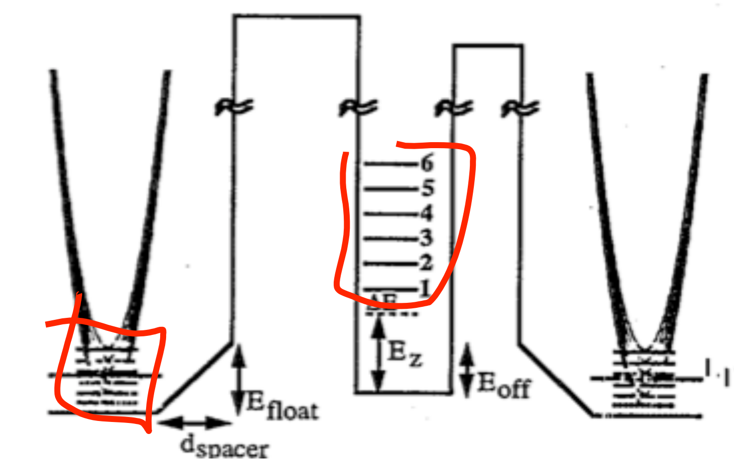
- Construct a coulomb diamond of the single donor QD device.

Problems:

- Understand the “full” coulomb diamond measured at T=4K considering:
  - ✓ DOS of Si:P wire leads.
  - ✓ Excited single donor states.
  - ✓ Inelastic scattering for the transport.

Approach:

- Rate-equation formalism coupled with tight-binding Schrödinger-Poisson solver.



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Elastic and inelastic scattering in quantum dots in the Coulomb-blockade regime

Gerhard Klimeck,* Roger Lake,† and Supriyo Datta
Purdue University, School of Electrical Engineering, West Lafayette, Indiana 47907-1285

Garnett W. Bryant
U.S. Army Research Laboratory, Microphotonic Devices Branch, Adelphi, Maryland 20783-1197
(Received 28 March 1994)

Starting from a rate-equation model proposed by Beenakker, we calculate current-voltage char-

(Ongoing) Calculation of Coulomb Diamond

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- Construct a coulomb diamond of the single donor QD device.

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Approach:

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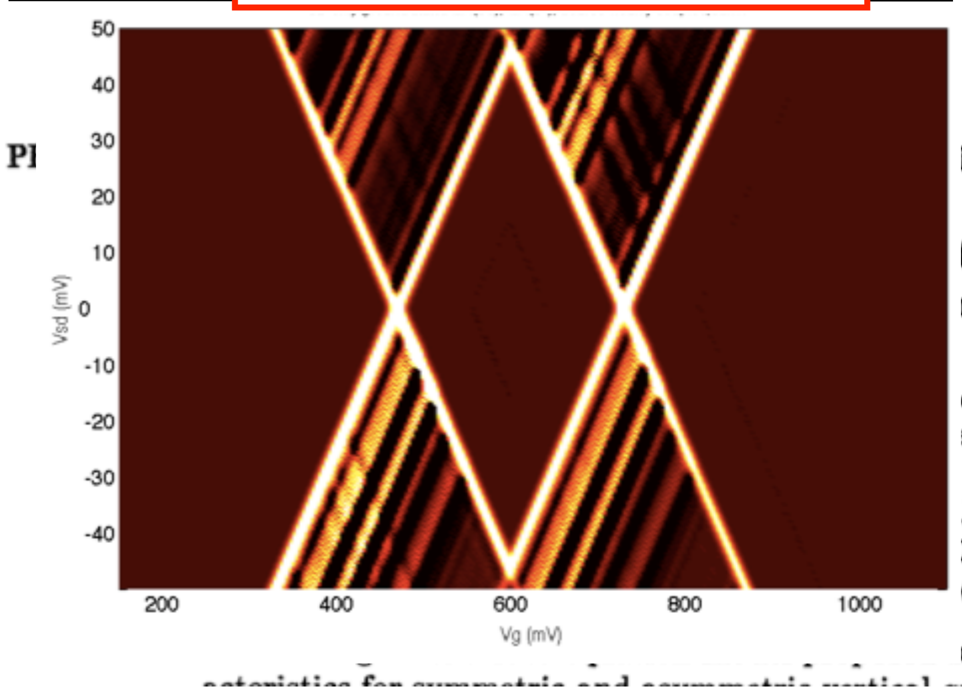
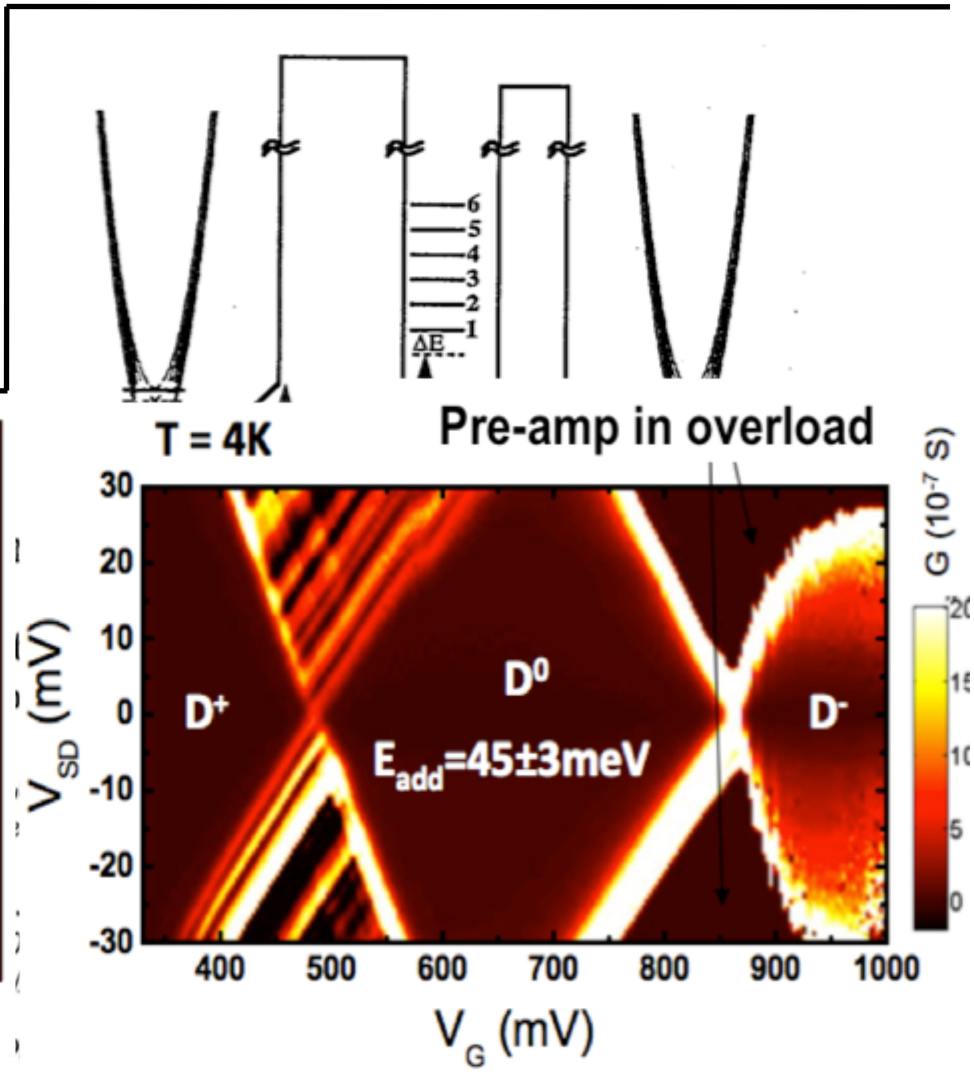
Result we have so far





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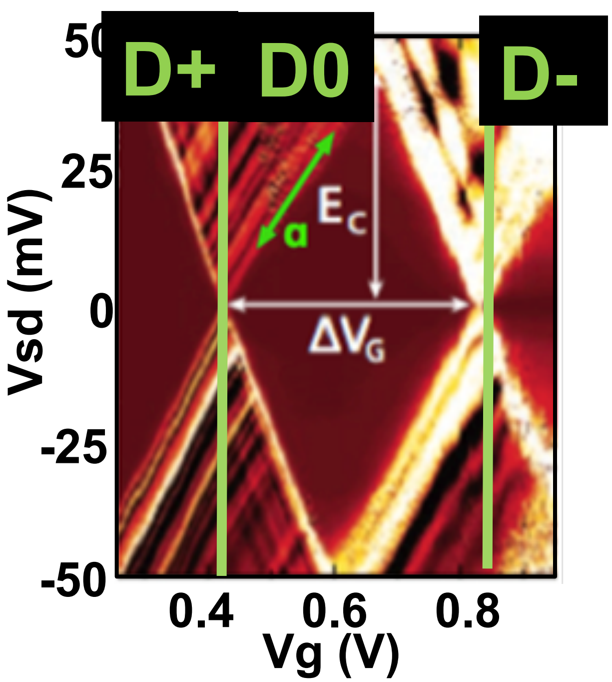
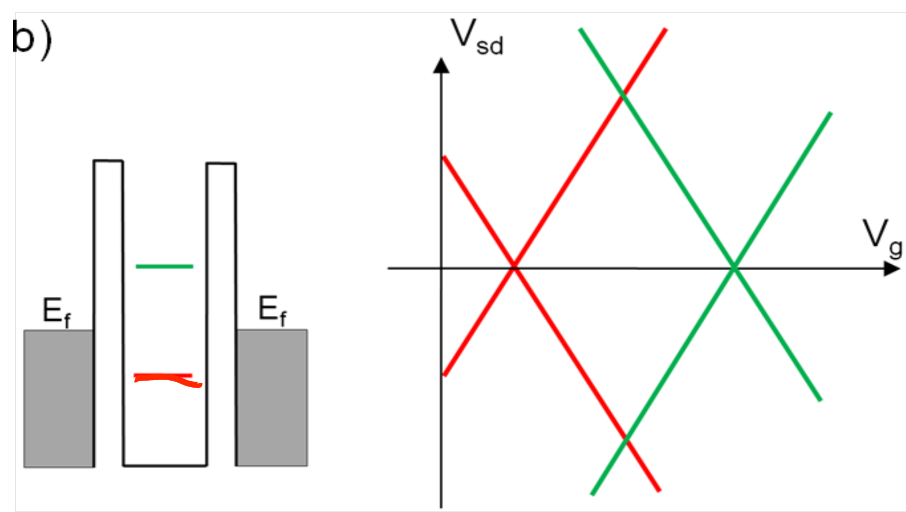
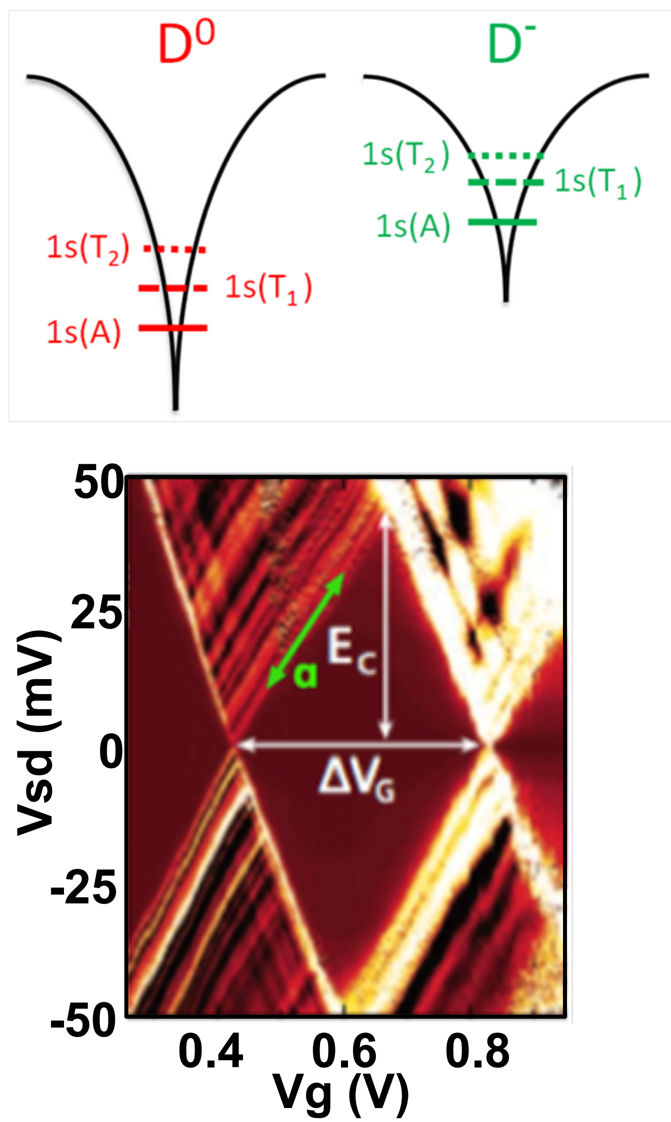
- Weak channel barrier at second transition point (~ 13 meV)
- Channel electrons no longer confined for Vg greater ~ 1V



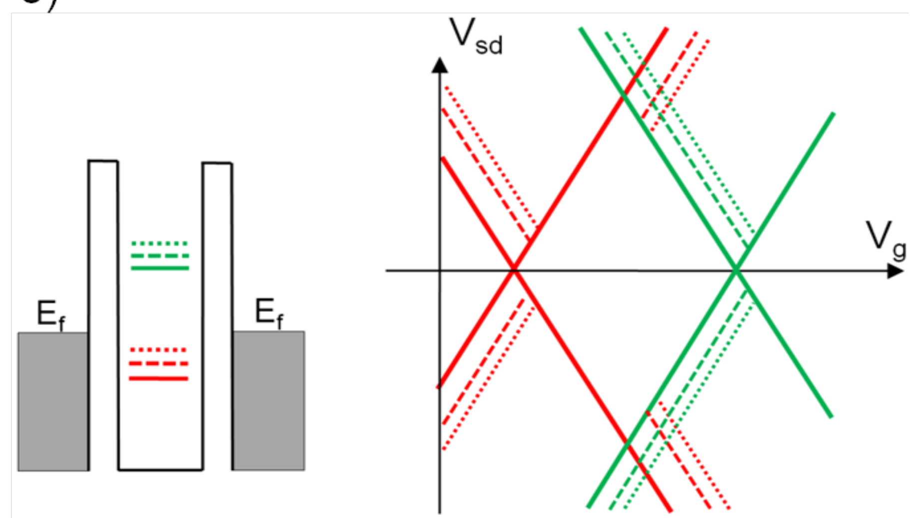


Impurity Excited States

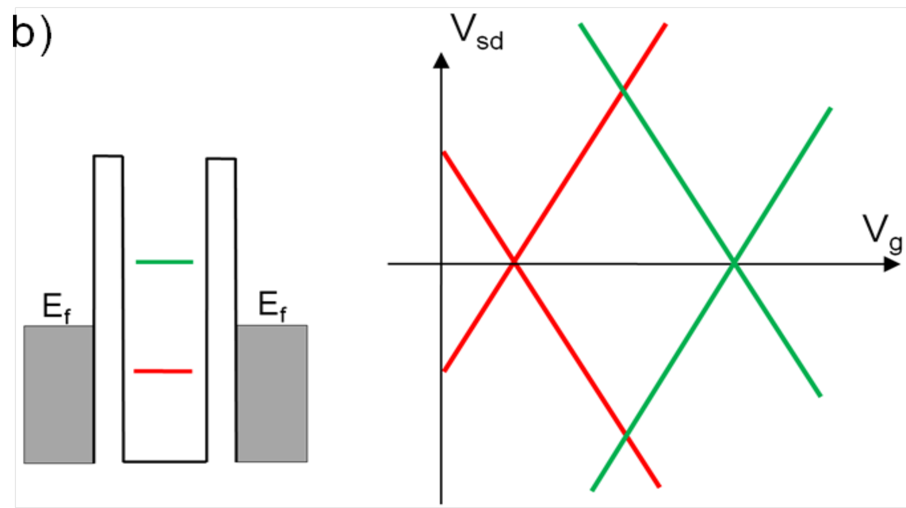
a)



c)

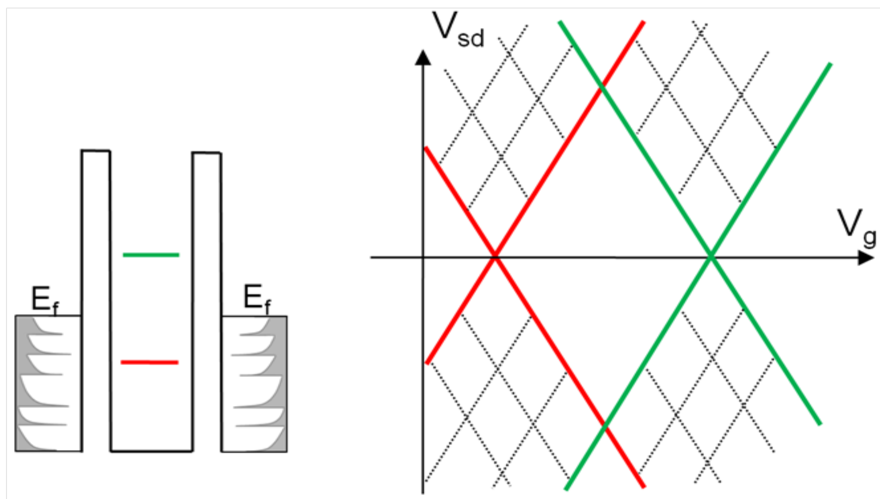


b)

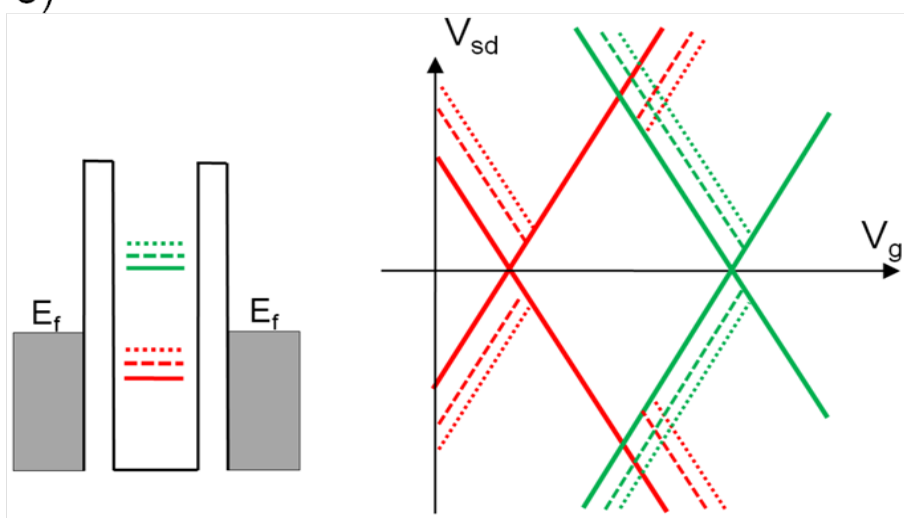


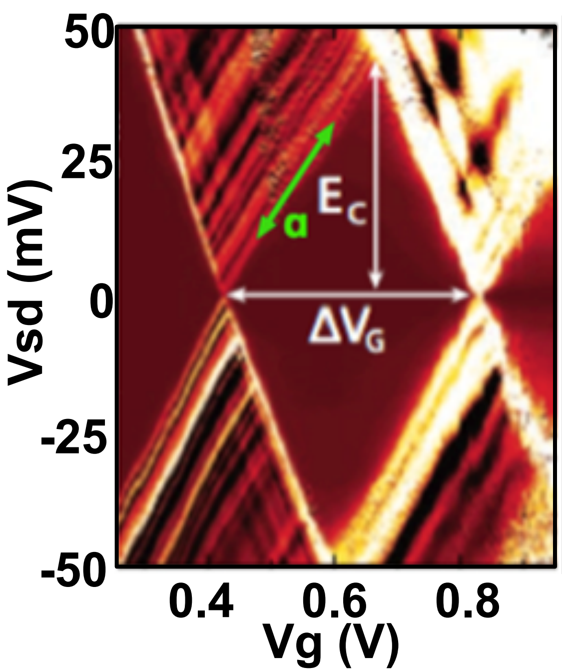
Quantum Transport Theory With Coulomb Blockade, Excited States, Lead DOS

d)

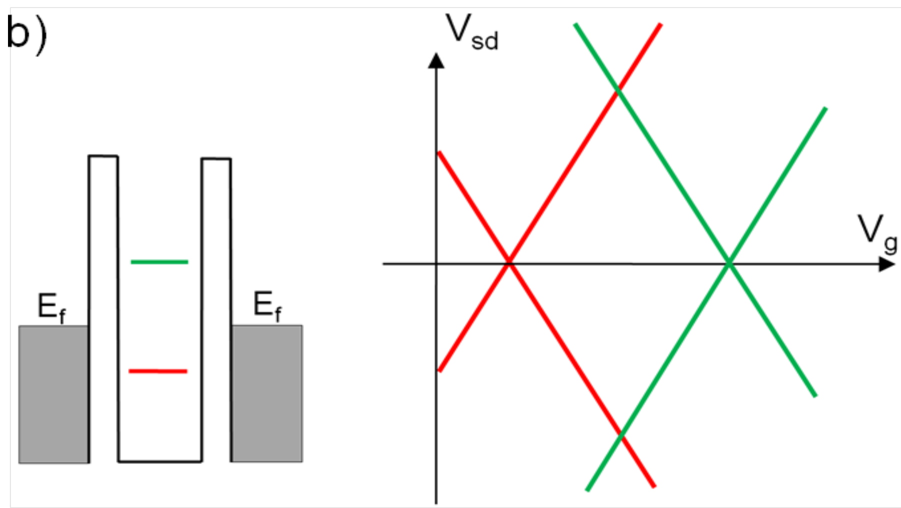


c)

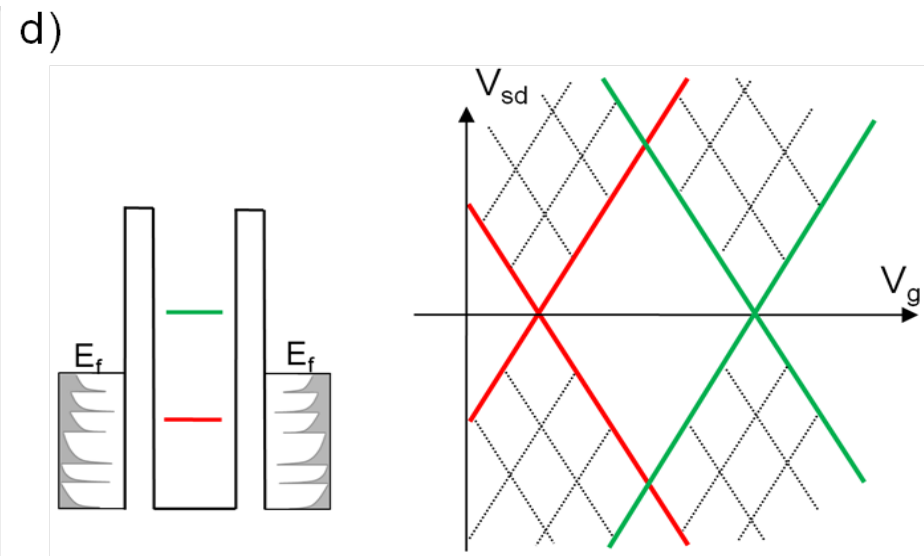


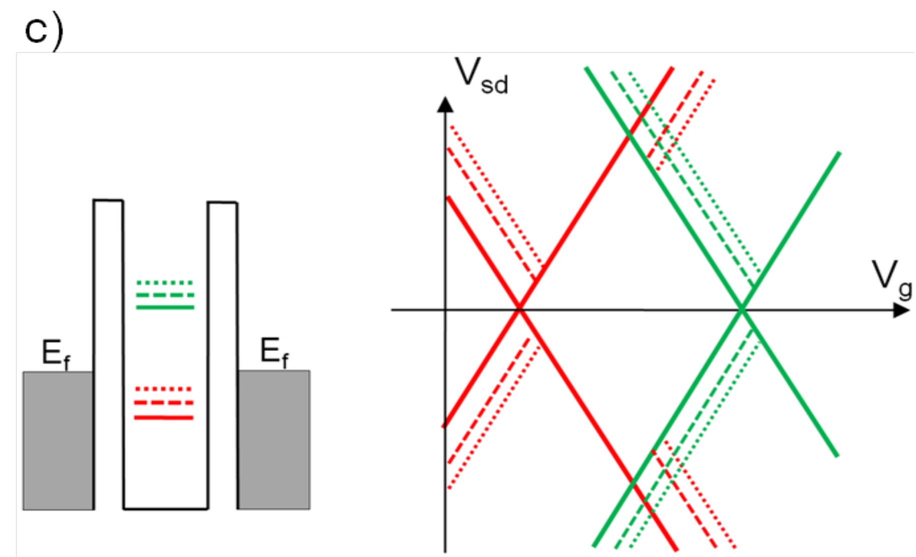


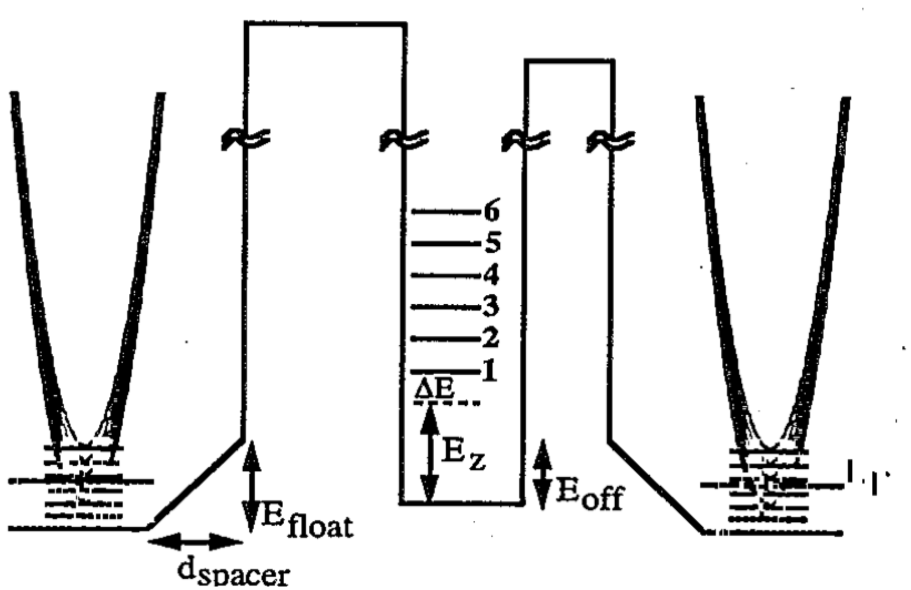
b)

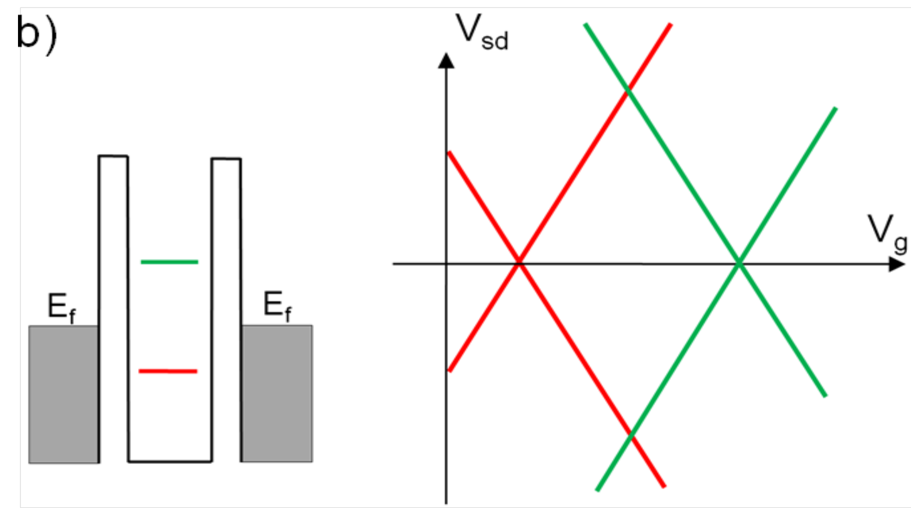


Quantum Transport Theory With Coulomb Blockade, Excited States, Lead DOS









1) Si:P Doping Plane (2-D)

1A) Semi-metallic property

1B) Sensitivity to doping disord

2) Si:P Nanowire (1-D)

2A) Semi-metallic property

2B) Modulation of channel conductance

2C) Resistance-limit of Si Nanowire

2D) Sensitivity of resistance to doping disorder

3) Single-donor Quantum-dot (0-D)

3A) Channel Modulation

→ Single-electron trans

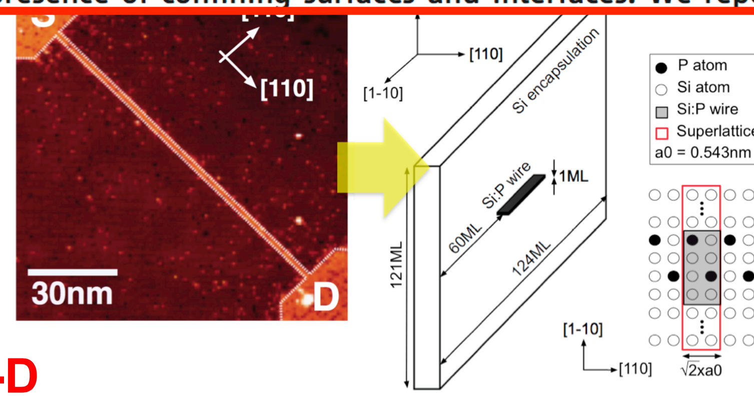
Will briefly explain a t

Ohm's Law Survives to the Atomic Scale

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

As silicon electronics approaches the atomic sc
in size to the active device components. Maint
challenging because of the presence of confining surfaces and interfaces. We repor

Science AAAS

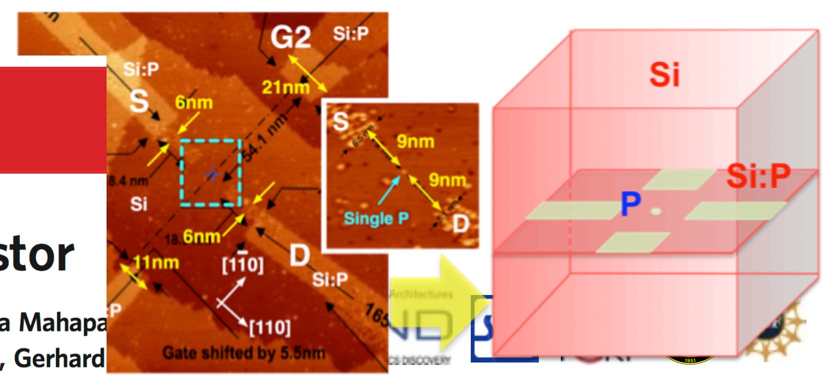


0-D

nature nanotechnology

A single-atom transistor

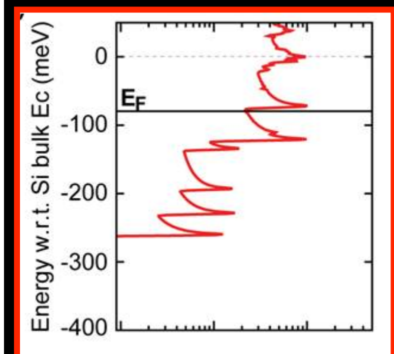
Martin Fuechsle[1], Jill A. Miwa[1], Suddhasatta Mahapa
Oliver Warschkow[1], Lloyd C. L. Hollenberg[3], Gerhard

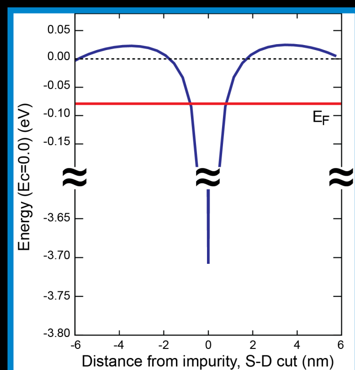


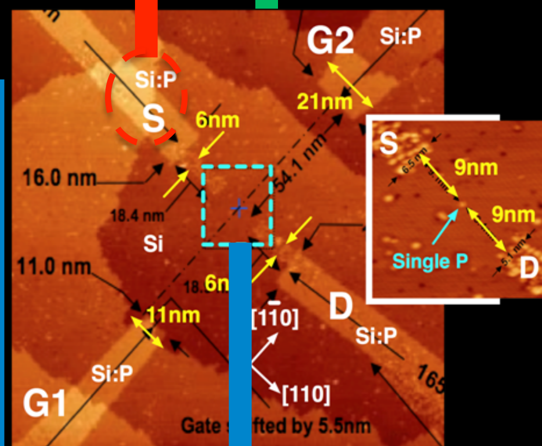
A multi-scale modeling procedure

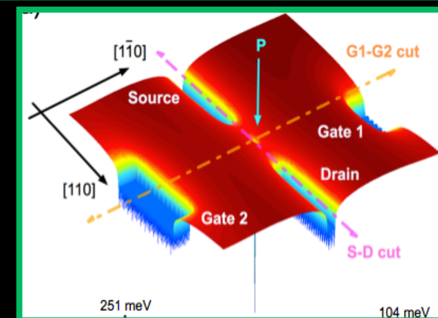
1. Contact modeling
- Atomistic modeling on the leads
- Charge-potential self-consistency
- *Semi-metallic*, DOS profile

2. Potential profile
- Semi-classical potential profile
- Superpose w. donor potential

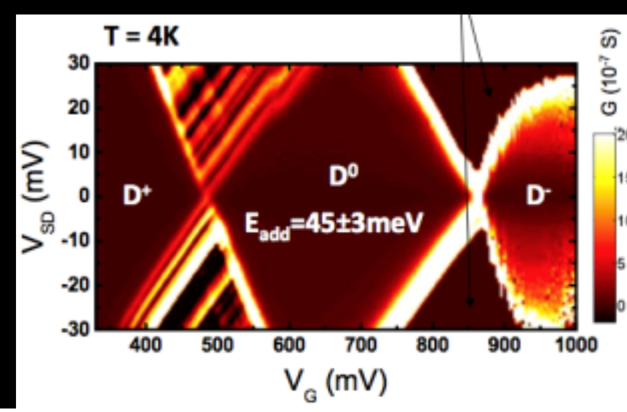








3. Charge filling
- Potential profile → Hamiltonian
- Compute eigenstates w.r.t E_F at every V_G
- Transition, charging energy and gate modulation



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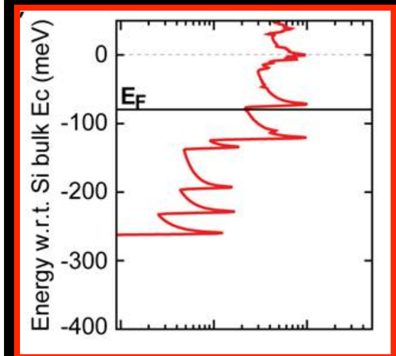

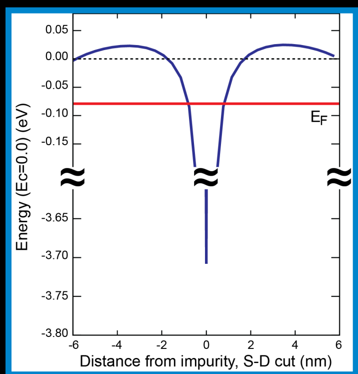

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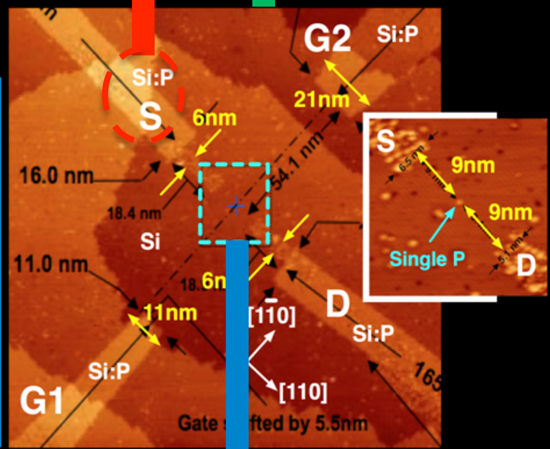
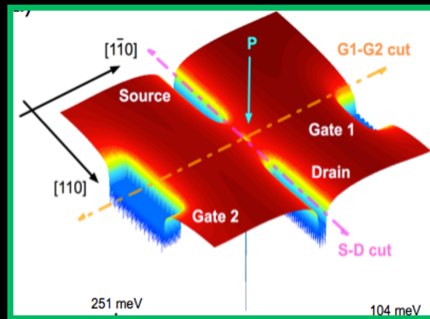
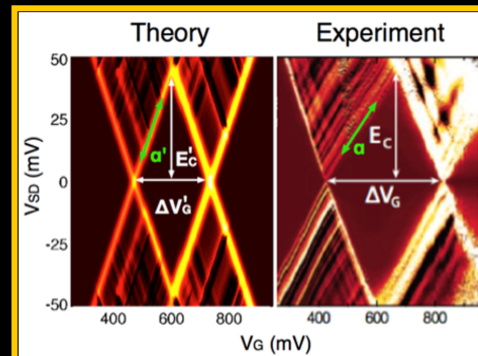






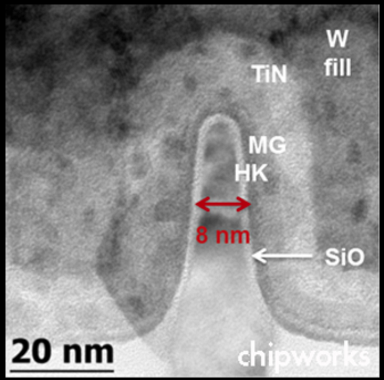
3. Charge filling
- Potential profile → Hamiltonian
- Compute eigenstates w.r.t E_F at every V_G
- Transition, charging energy and gate modulation

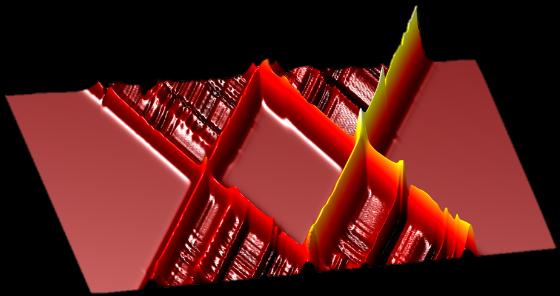
4. Coulomb diamond
- DOS profile of S/D and Charge filling information
- Rate equation formalism

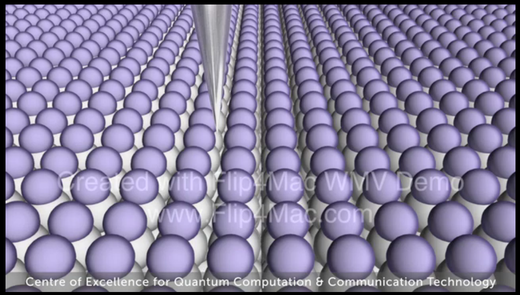
The single-atom transistor

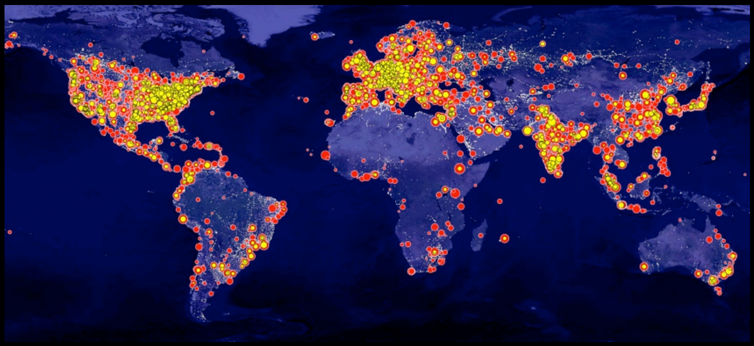
Presentation Outline

- Why?
  – Continuum invalid
    => finite atoms/electrons
- What is it?
  – Coulomb diamond
  – How is it built?
  – Results
- How to model this?
  – NEMO
- Where to study this?
  – nanoHUB.org

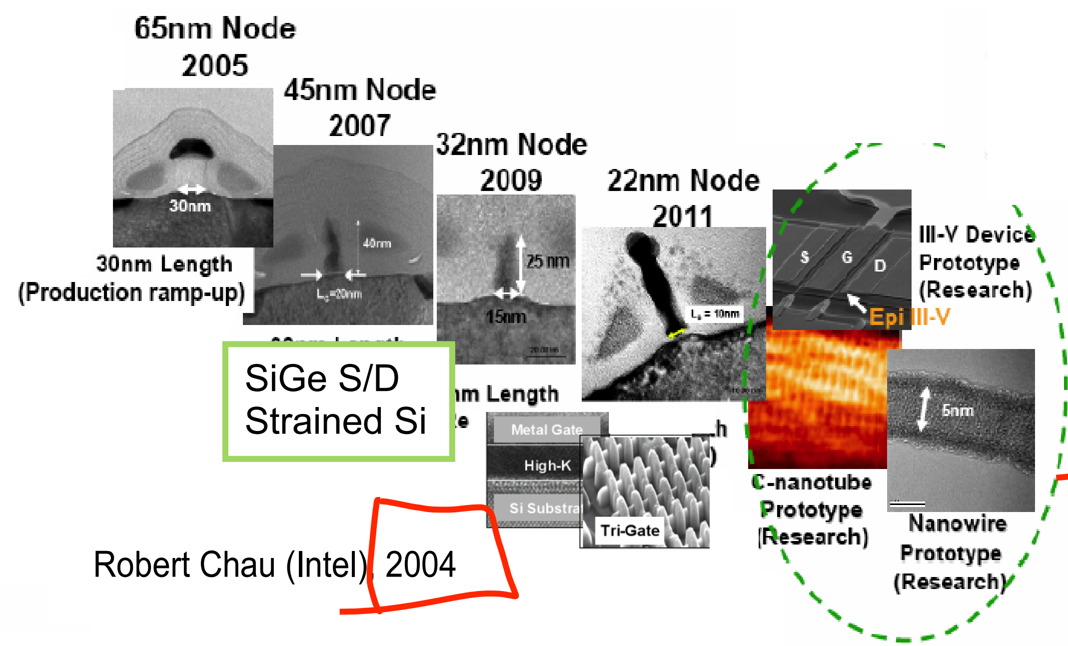








Industrial Device Trends and Challenges



Questions / Challenges

- Strain ?
- Quantization?
- Crystal orientation?
- Atoms are countable; does granularity matter? Disorder?
- New material or new device?

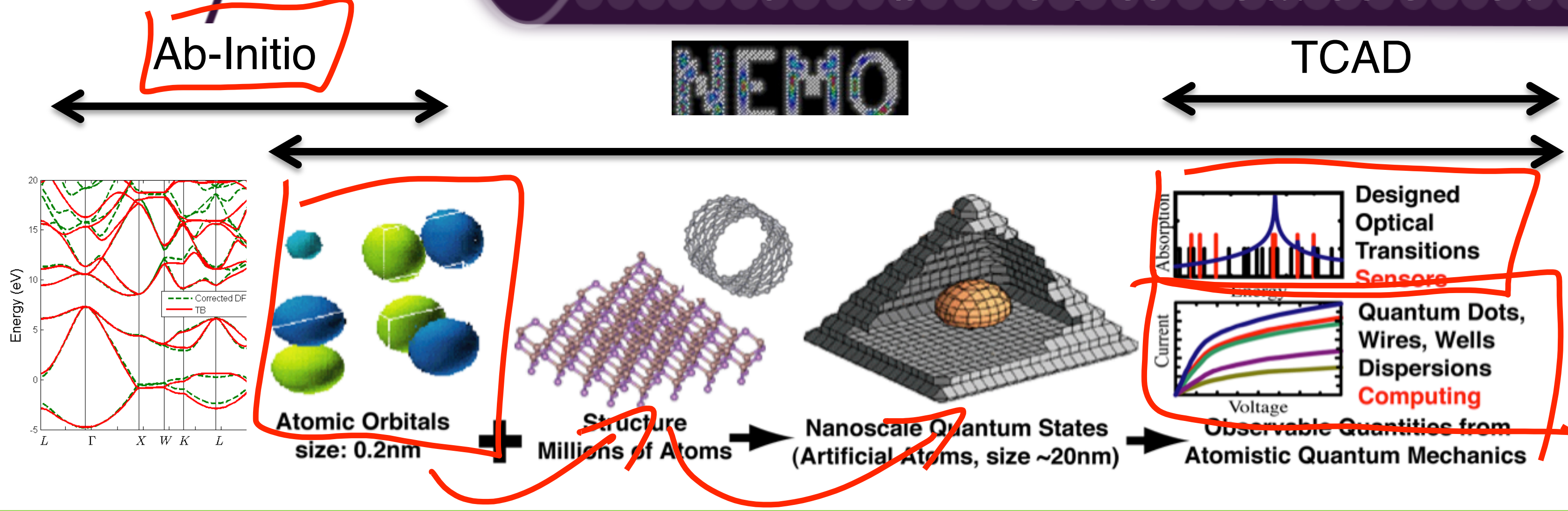
Assertions of importance

- High bias / non-equilibrium
- Quantum mechanics
- Atomistic representation
  - » Band coupling, non-parabolicity, valley splitting
  - » Local (dis)order, strain and orientation

Observations:

- 3D spatial variations on nm scale
- Potential variations on nm scale
- New channel materials (Ge, III-V)

NEMO5 - Bridging the Scales
From Ab-Initio to Realistic Devices



Goal:
- Device performance with realistic extent, heterostructures, fields, etc. for new / unknown materials

Problems:
- Need ab-initio to explore new material properties
- Ab-initio cannot model non-equilibrium.
- TCAD does not contain any real material physics

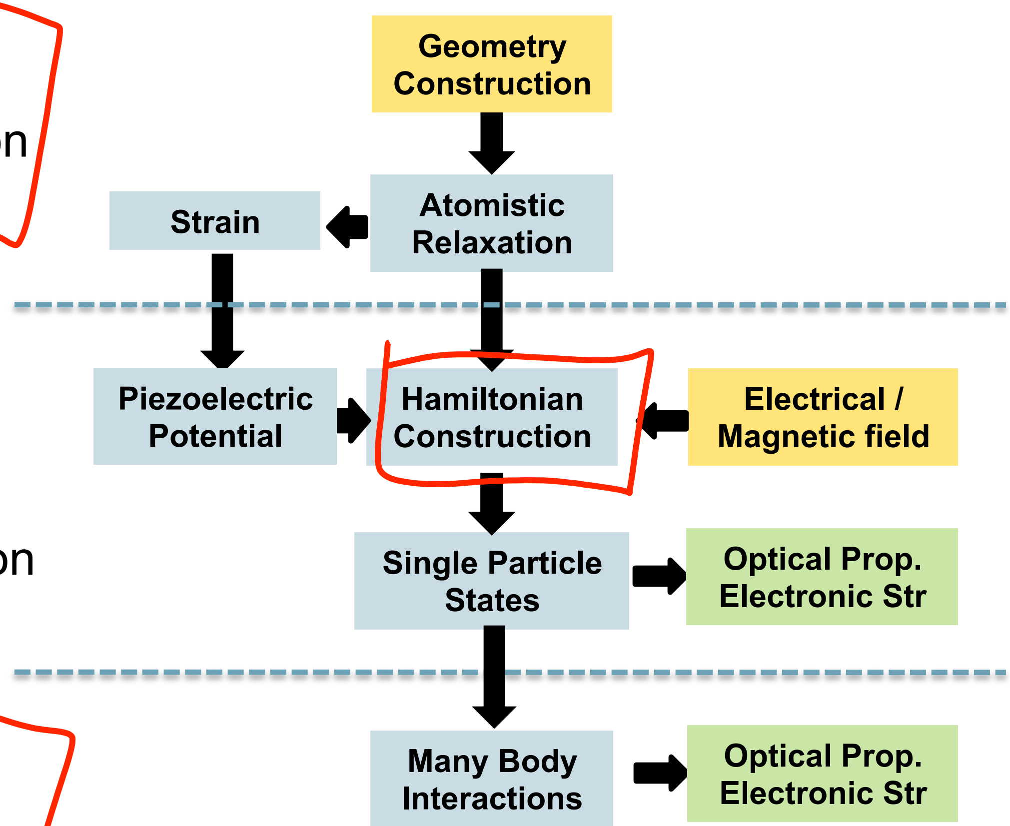
Approach:
- Ab-initio:
  - Bulk constituents
  - Small ideal superlattices
- Map ab-initio to tight binding (binaries and superlattices)
- Current flow in ideal structures
- Study devices perturbed by:
  - Large applied biases
  - Disorder
  - Phonons

NEMO - Multi-Scale Modeling

Atom Positions ~10-50 million atoms

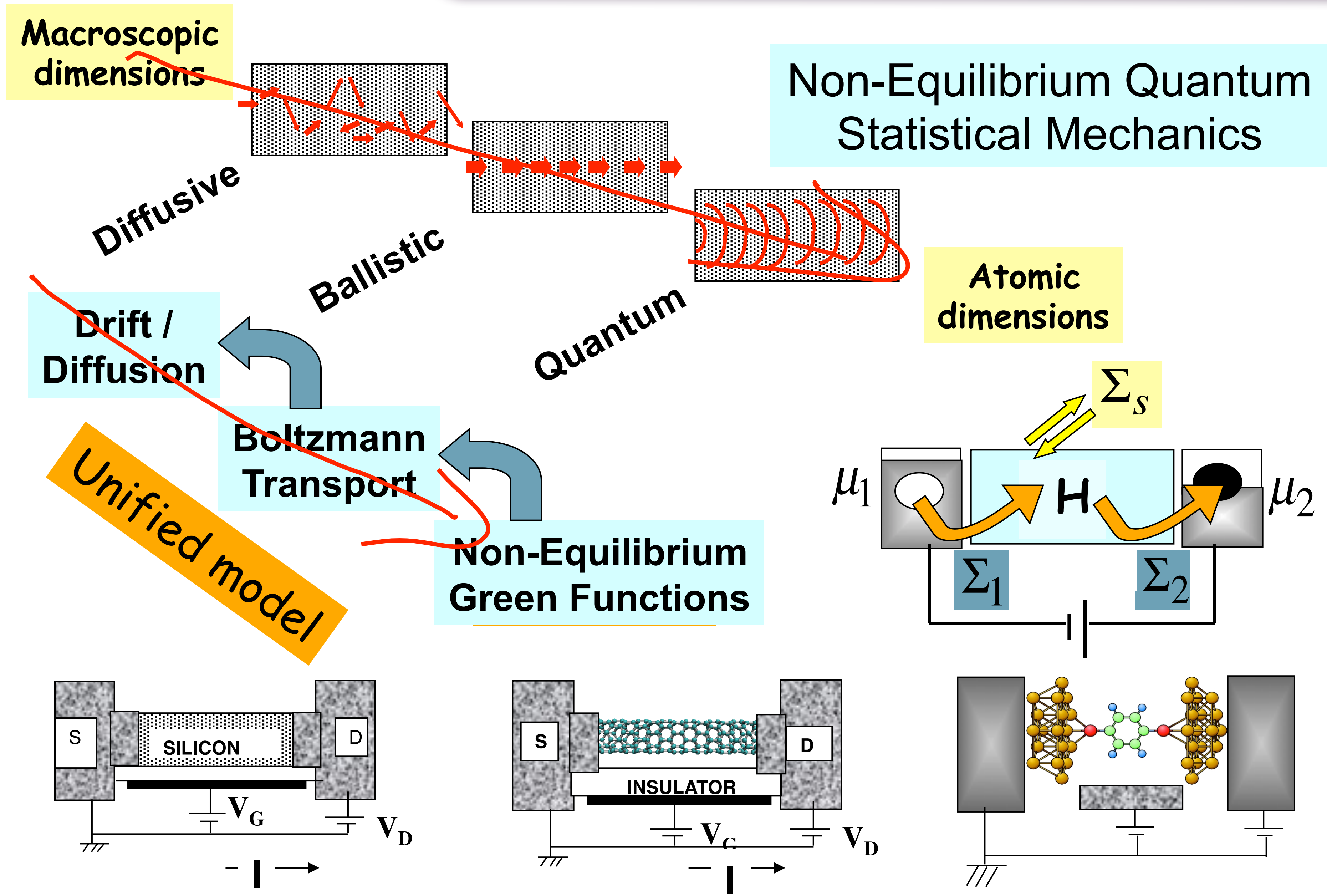
Valence Electrons ~0.5-10 million

e-e interactions Few States

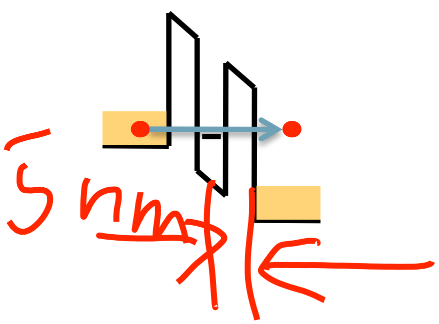


- Valence Force Field (VFF) Method
- Piezoelectric eff. Pol. charge density
- Empirical tight binding $sp^3d^5s^*$ + spin orbit
- SCP: Poisson + LDA
- Slater Determinants

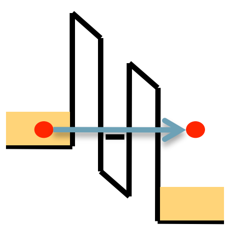
Quantum Transport far from Equilibrium

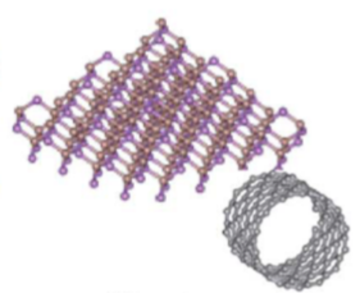


	NEMO-1D
Transport	Yes
Dim.	1D
Atoms	~1,000
Crystal	[100] Cubic, ZB
Strain	-
Multi-physics	-
Parallel Comp.	3 levels 23,000 cores

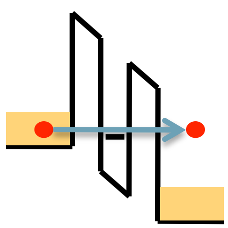


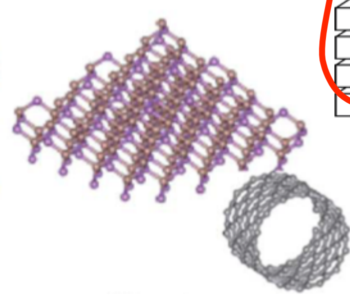
	NEMO-1D	NEMO-3D
Transport	Yes	-
Dim.	1D	any
Atoms	~1,000	50 Million
Crystal	[100] Cubic, ZB	[100] Cubic, ZB
Strain	-	VFF
Multi-physics	-	
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores

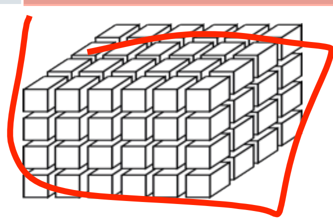




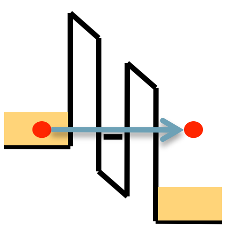
	NEMO-1D	NEMO-3D	NEMO3Dpeta
Transport	Yes	-	-
Dim.	1D	any	any
Atoms	~1,000	50 Million	100 Million
Crystal	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic,ZB, WU
Strain	-	VFF	VFF
Multi-physics	-		
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores

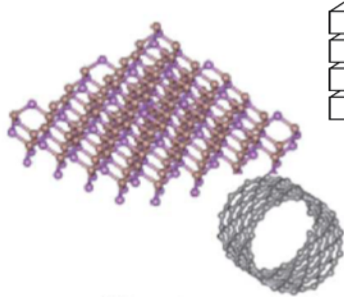


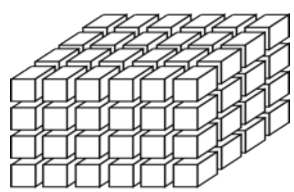


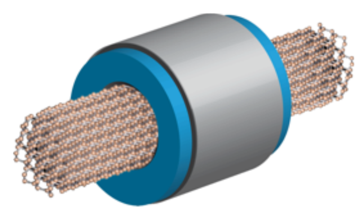


	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN
Transport	Yes	-	-	Yes
Dim.	1D	any	any	any
Atoms	~1,000	50 Million	100 Million	~140,000
Crystal	[100] Cubic, ZB	[100] Cubic, ZB	[100], Cubic,ZB, WU	Any Any
Strain	-	VFF	VFF	-
Multi-physics	-			
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co









	NEMO-1D	NEMO-3D	NEMO3Dpeta	OMEN	NEMO5
Transport	Yes	-	-	Yes	Yes
Dim.	1D	a...	any	any	any
Atoms	~1,000	...n	100 Million	~1_0,000	1... Million
Crystal	[1... ...ZB		[100], ...ubic,ZB, W...		An... Any
Strain	-	V...	VFF		...VFF
Multi-physics	-				Spin, Classical
Parallel Comp.	3 levels 23,000 cores	1 level 80 cores	3 levels 30,000 cores	4 levels 220,000 co	4 levels 100,000 cores

First predictive NEGF tool

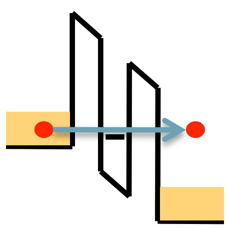
First 10 million atom elctronic structure

First peta-scale Engineering

Silvaco

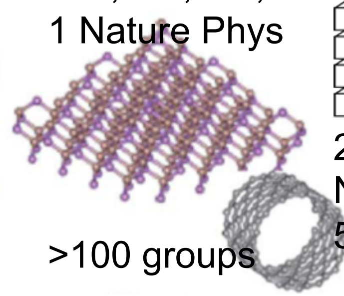
All codes:
>100,000 lines

>300 papers

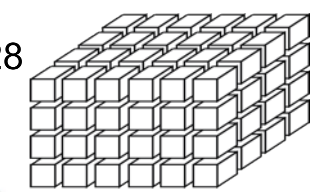


4 top pubs cites:
545,157,128,82
Patents:2

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

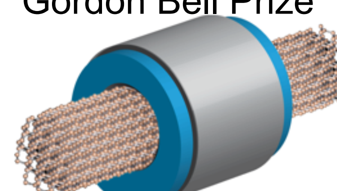


>100 groups



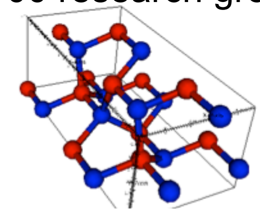
2 pubs in Science & Nature Nano 2012:
50 & 30 cites

Gordon Bell Prize



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

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

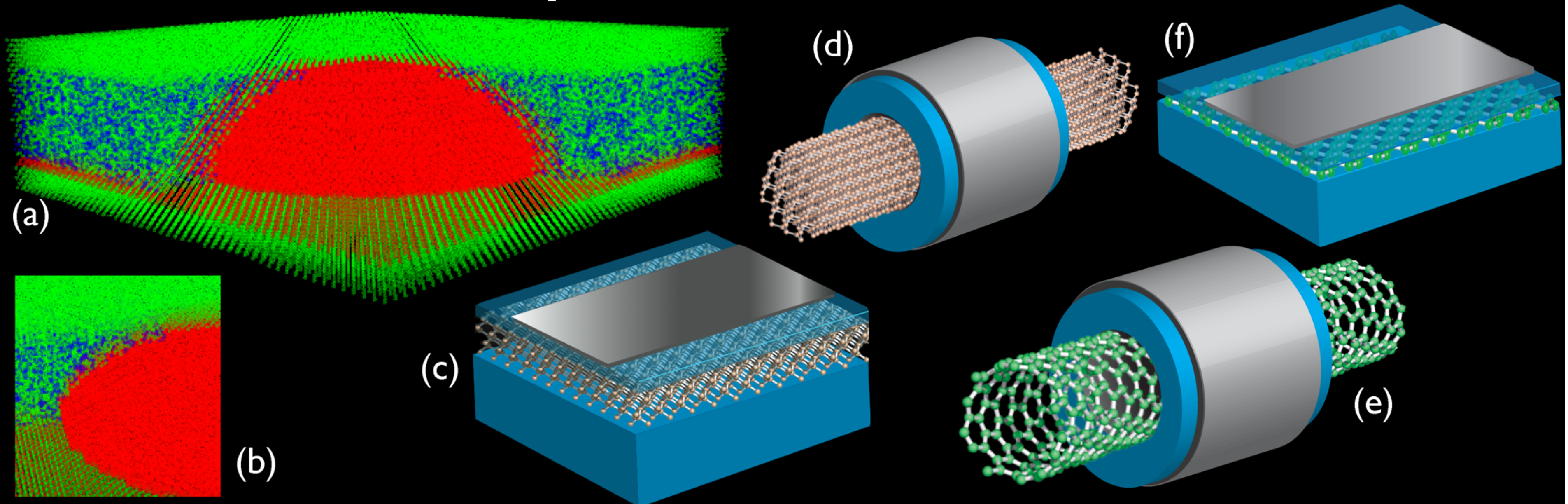


Core Code / Theory Development

- 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-'13)
  - » 5 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,

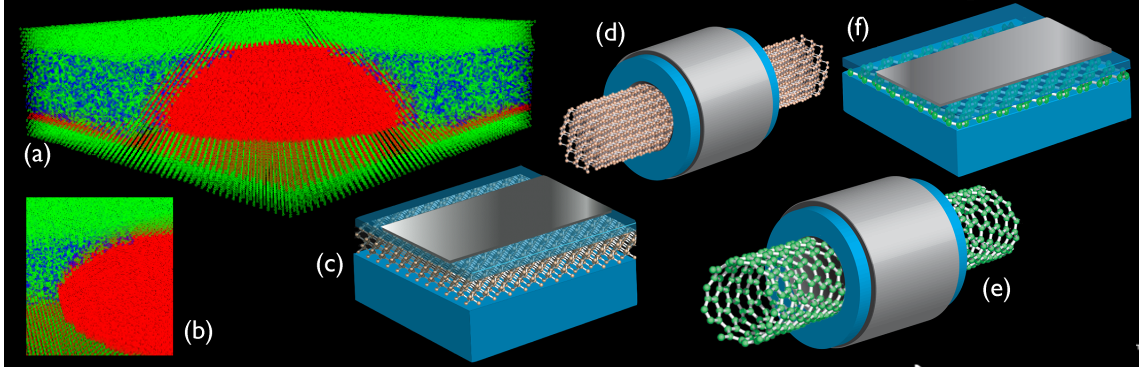
Compute Intensive: NEMO/OMEN



26 years development

- Texas Instruments
- NASA JPL
- Purdue

Compute Intensive: NEMO/OMEN



26 years development

- Texas Instruments
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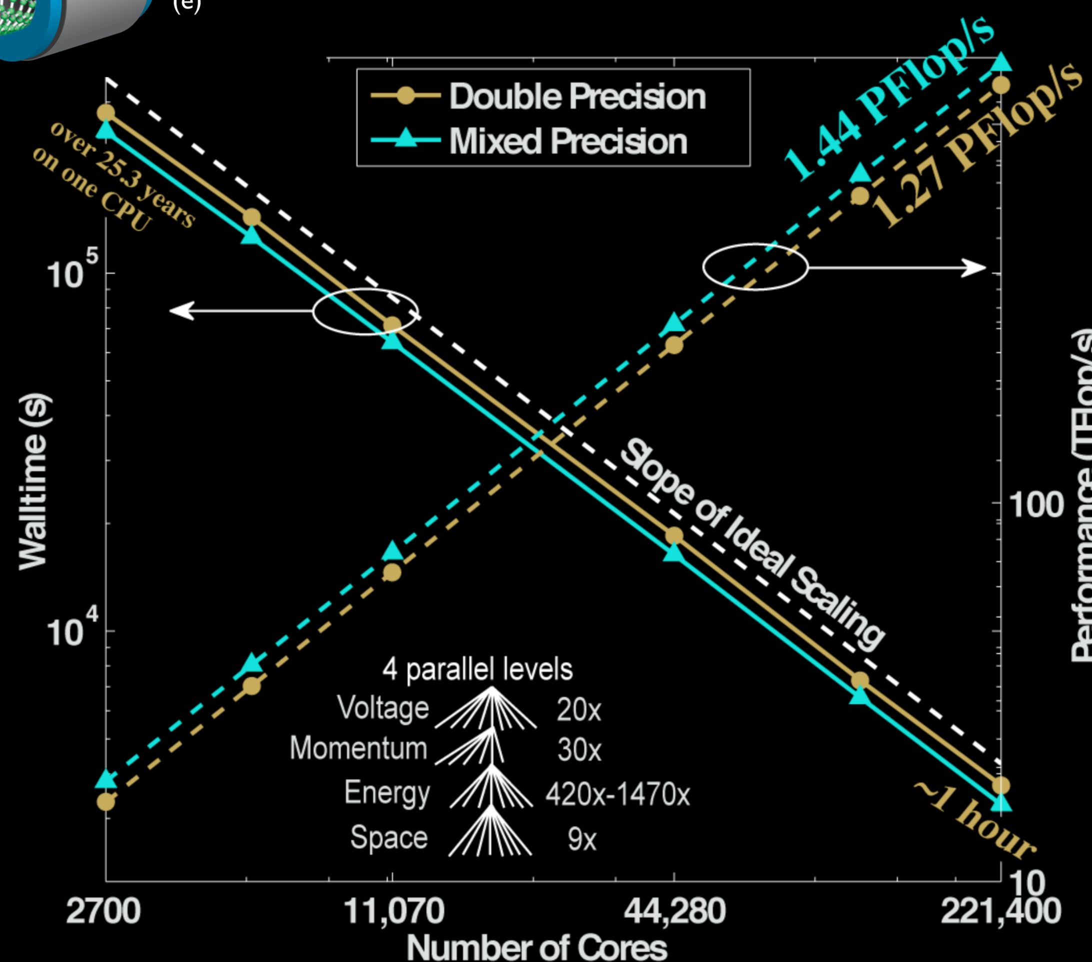
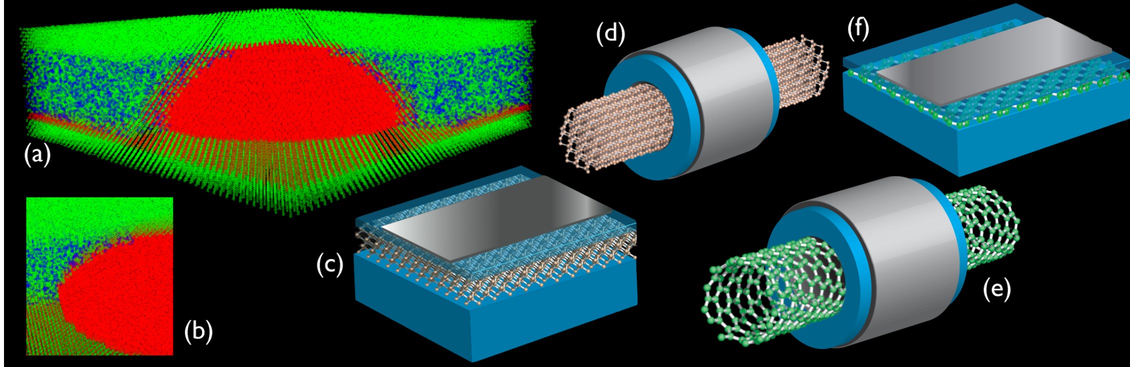
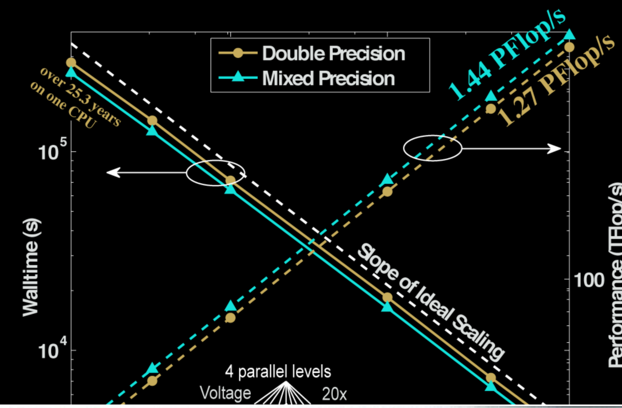
- Peta-scale Engineering



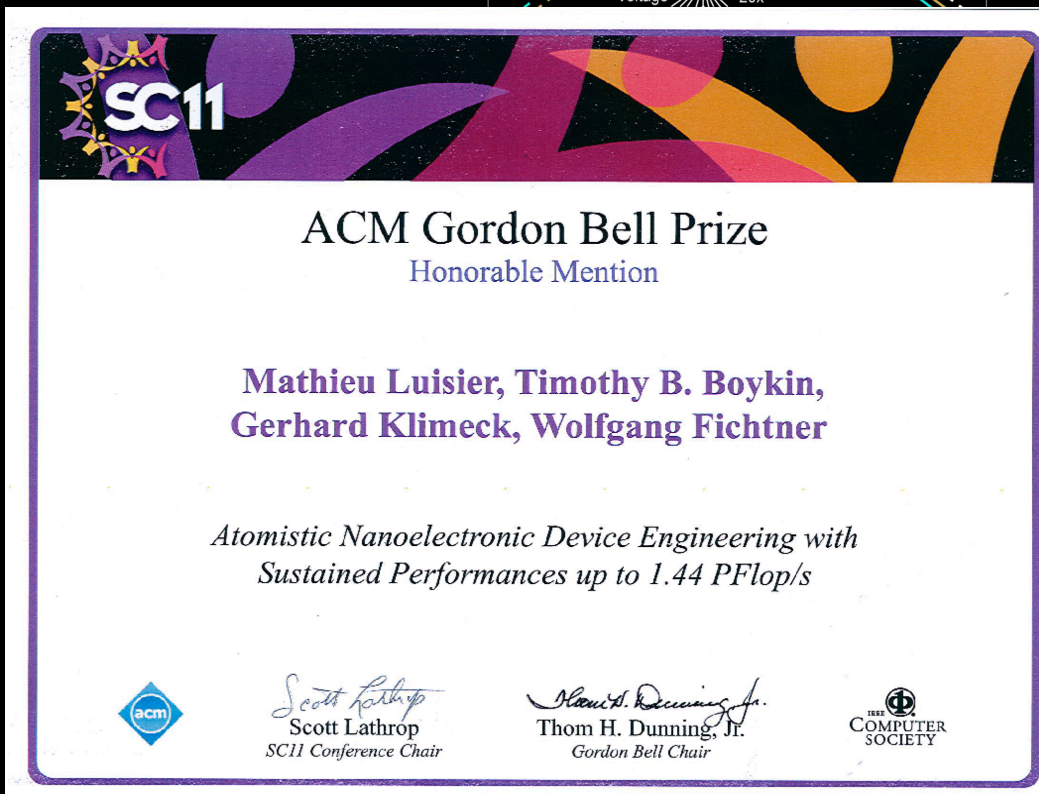
Compute Intensive: NEMO/OMEN





26 years development

- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering
- Gordon Bell



SC11

ACM Gordon Bell Prize

Honorable Mention

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

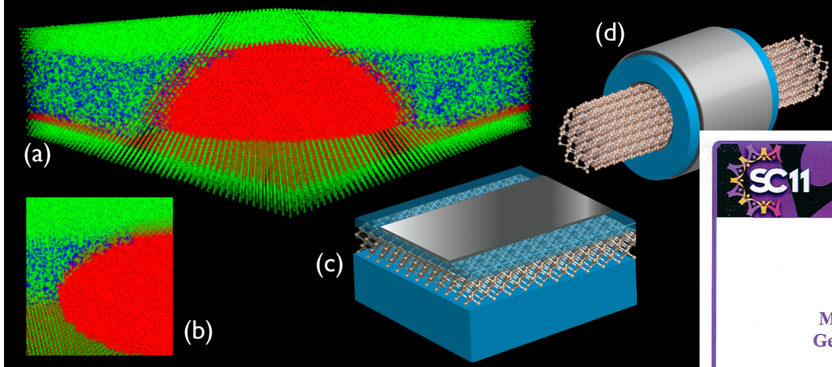
Atomistic Nanoelectronic Device Engineering with Sustained Performances up to 1.44 PFlop/s

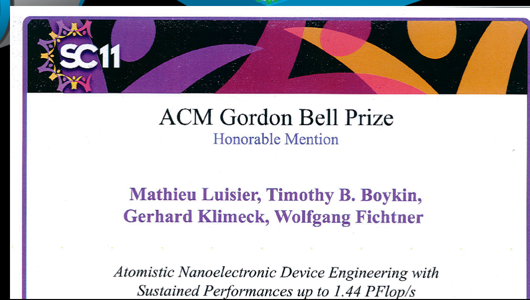
Scott Lathrop
SC11 Conference Chair

Thom H. Dunning, Jr.
Gordon Bell Chair

IEEE Computer Society

Compute Intensive: NEMO/OMEN

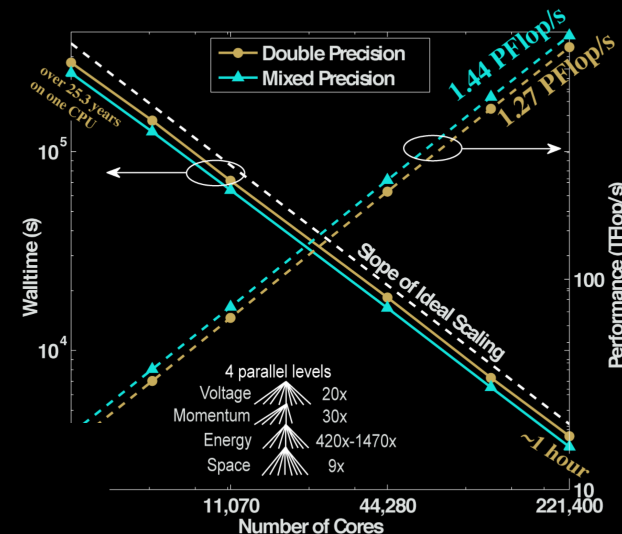


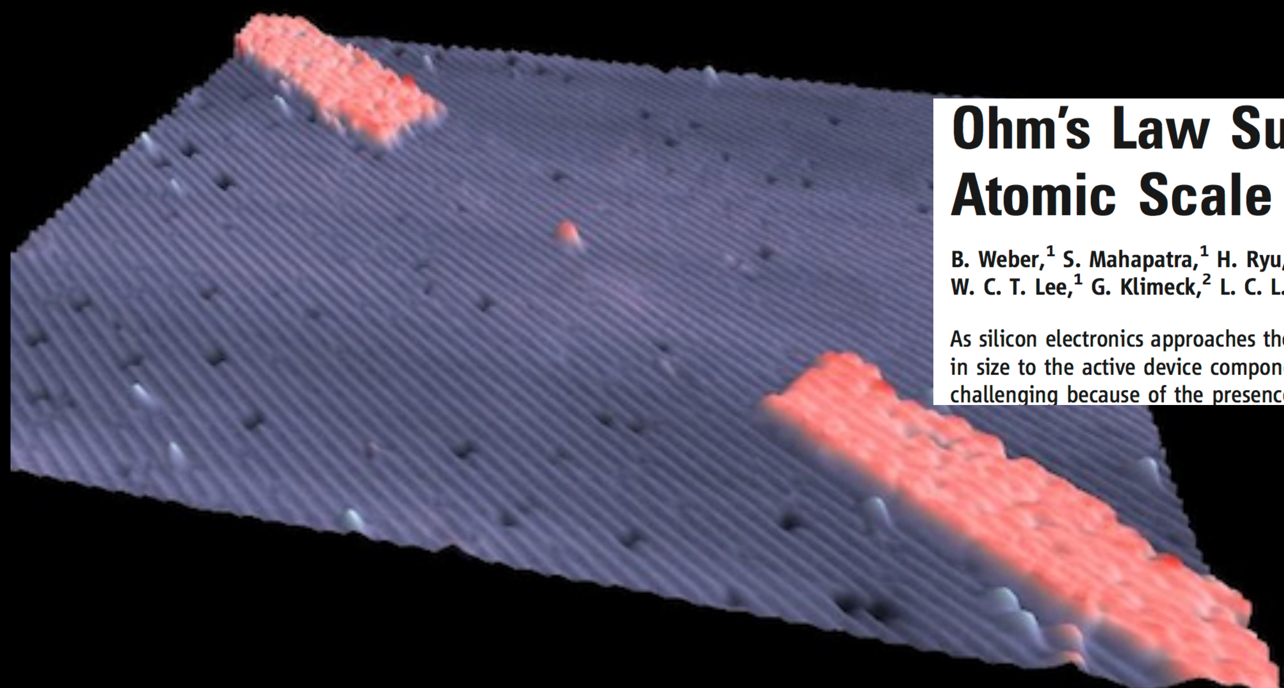


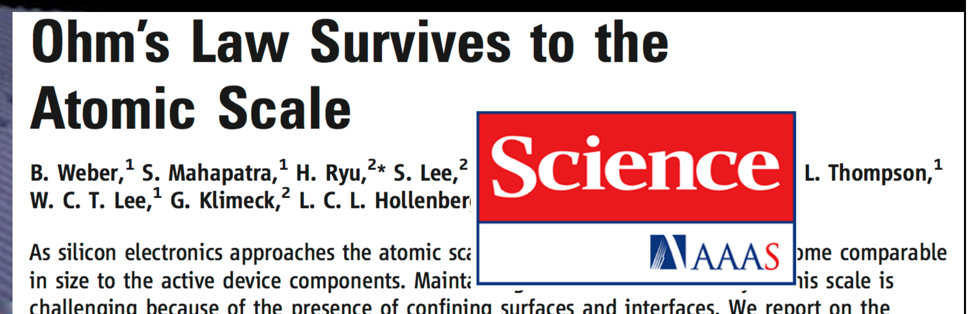
ACM Gordon Bell Prize
Honorable Mention

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

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

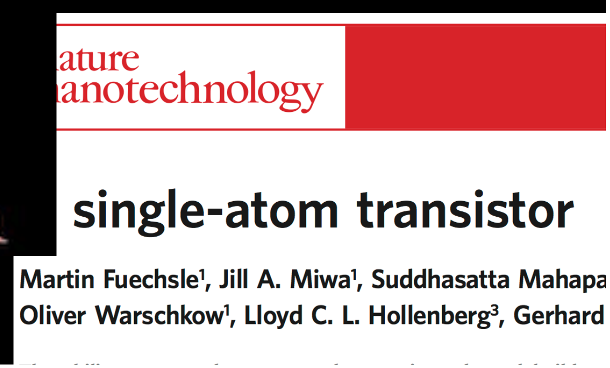





Ohm's Law Survives to the Atomic Scale

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

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

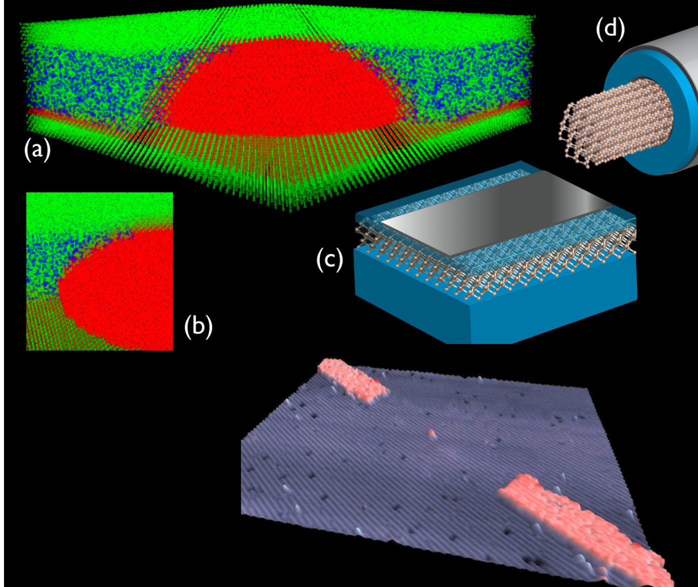


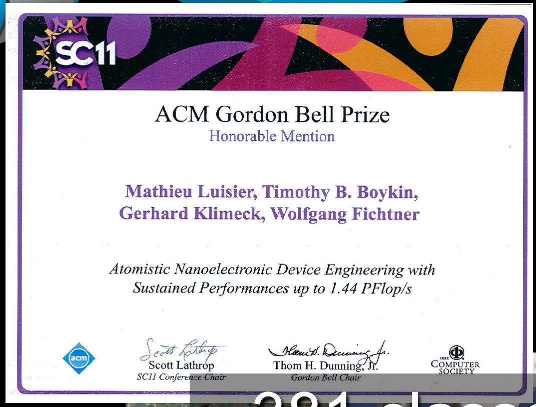
single-atom transistor

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

- Science, Nature Nano

Compute Intensive: NEMO/OMEN

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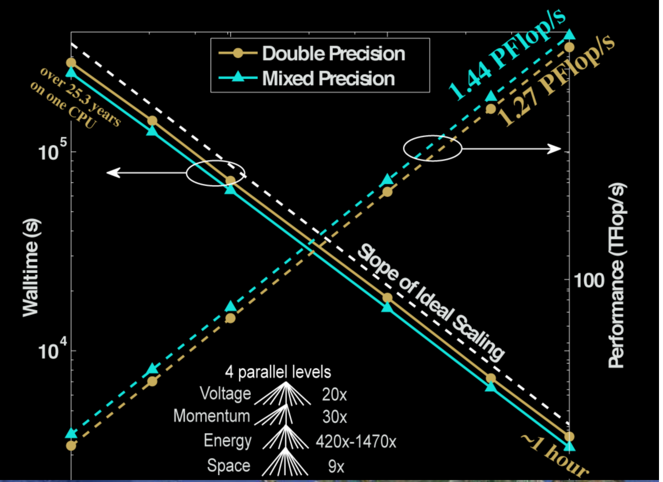
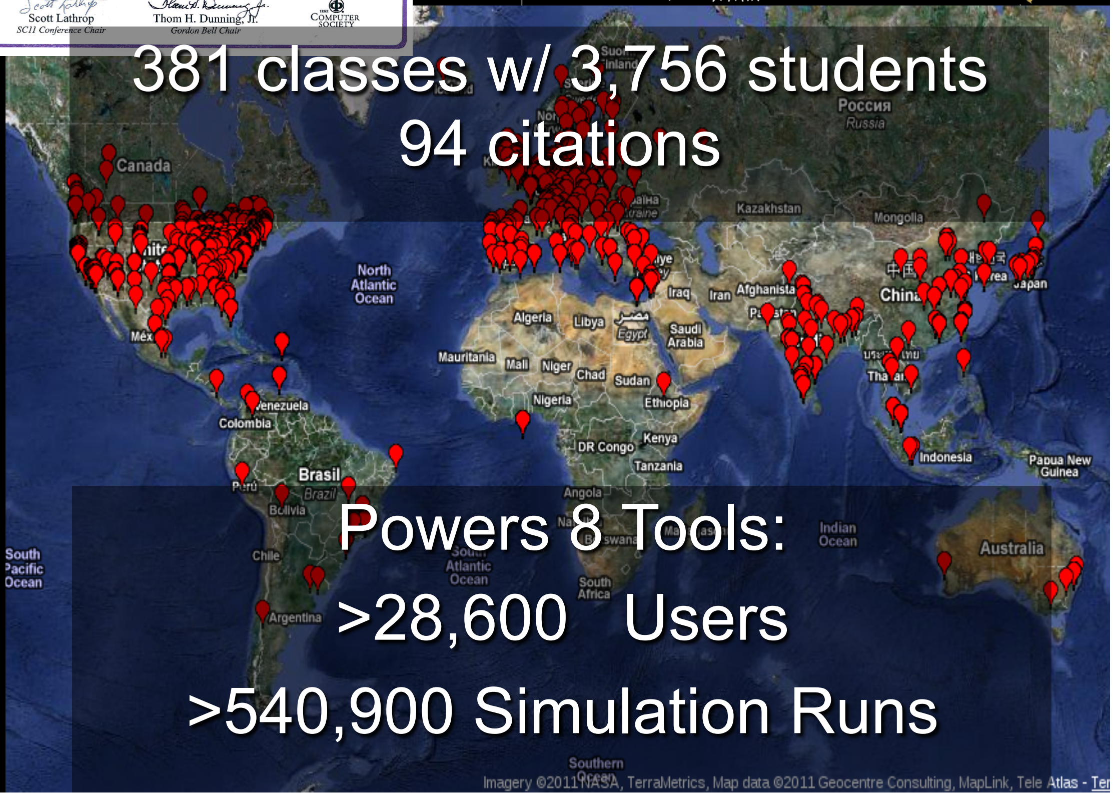


26 years development
- Texas Instruments
- NASA JPL
- Purdue
- Peta-scale Engineering
- Gordon Bell
- Science, Nature Nano



nanoHUB.org – always “on”
New paradigms in global scientific knowledge transfer, publishing, and assessment

Who?

> 2 million users annually

> 1,800 contributors

- 172 countries

- Faculty
- Students
- Industry practitioners

nanoHUB

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nanoHUB

nanoHUB in a nutshell: translating traditional research to new paradigms in publishing, computing, research, & education

What ?
- 600+ nano-Apps in the cloud
- \> 5,000 lectures and tutorials
- \> 100 courses => MOOC

Cyberinfrastructure
24/7 operation with 99.4% uptime

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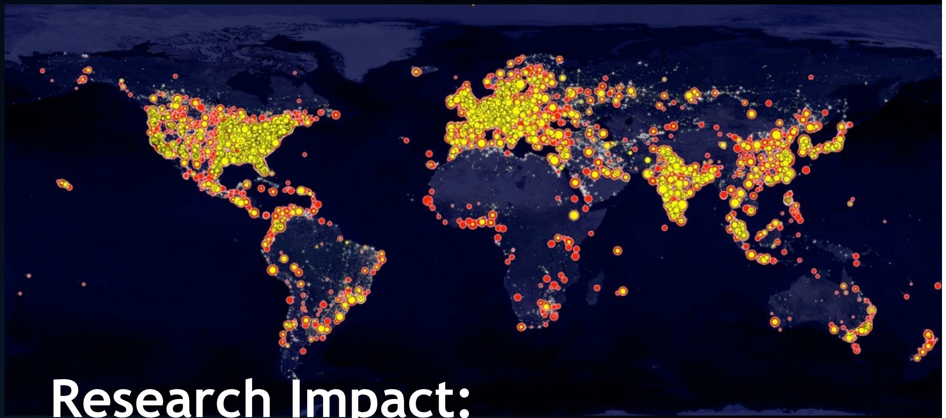

Research Impact:
- nanoHUB tools now listed in

WEB OF SCIENCE Google Scholar

- \> 2,480 papers cite nanoHUB
- \> 54,300 secondary citations
- h-index of 105

Educational Impact
- \>54,800 students use tools in classrooms, >5,345 classes, >185 institutions
- Rapid curriculum change <6 months adoption rate

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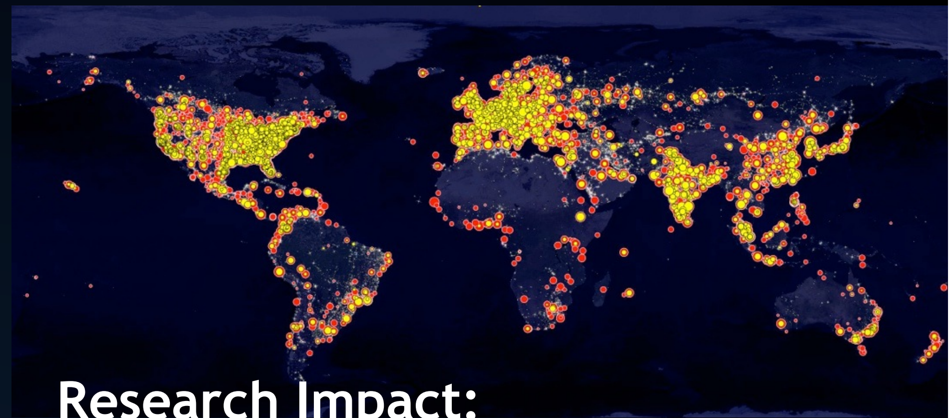
Fundamental changes in approach or underlying assumptions

=> Existence Proofs



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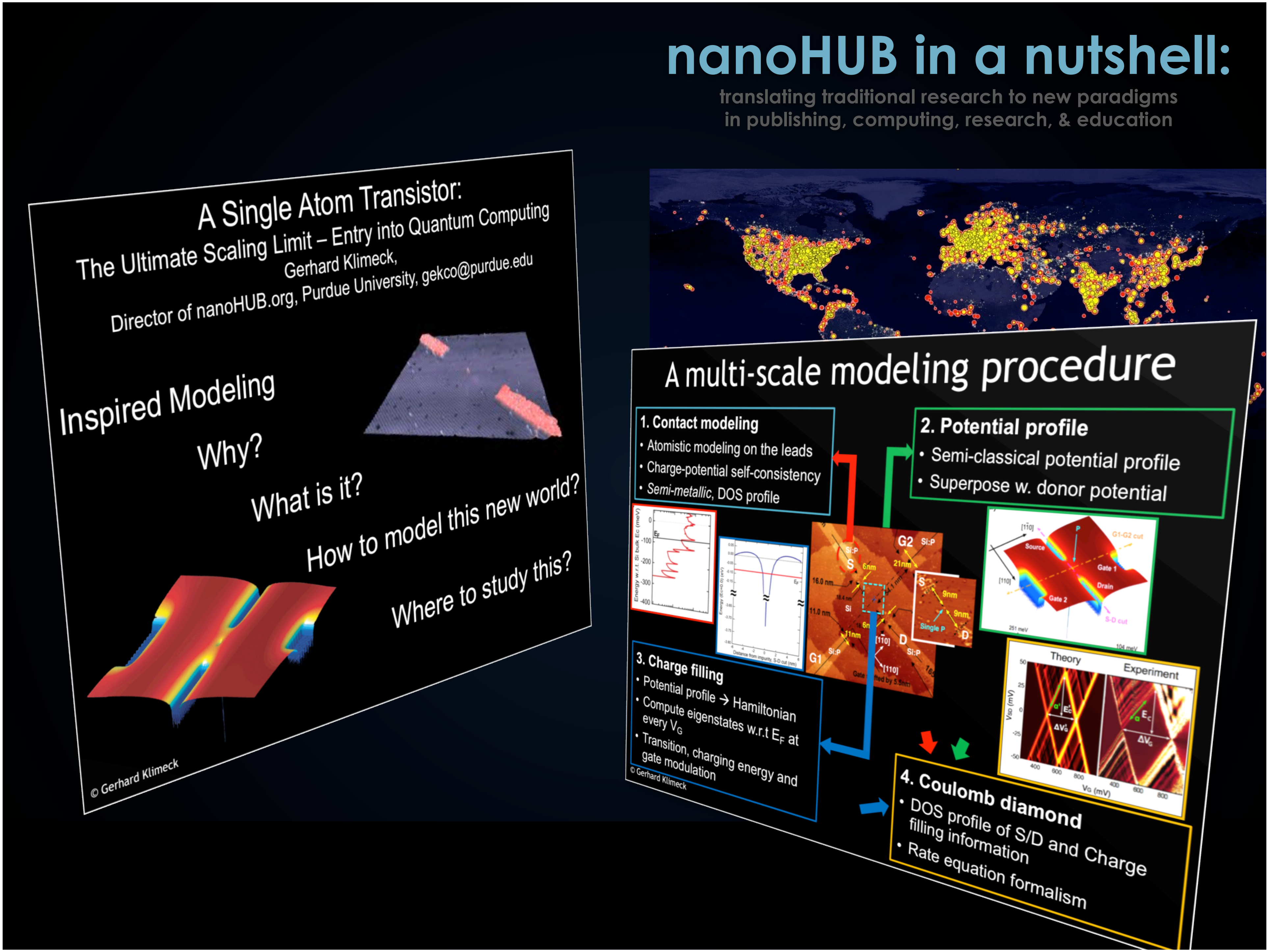
nanoHUB in a nutshell:
translating traditional research to new paradigms
in publishing, computing, research, & education
A Single Atom Transistor:
The Ultimate Scaling Limit – Entry into Quantum Computing
Gerhard Klimeck,
Director of nanoHUB.org, Purdue University, gekco@purdue.edu
Inspired Modeling
Why?
What is it?
How to model this new world?
Where to study this?
© Gerhard Klimeck
A multi-scale modeling procedure
1. Contact modeling
• Atomistic modeling on the leads
• Charge-potential self-consistency
• Semi-metallic, DOS profile
2. Potential profile
• Semi-classical potential profile
• Superpose w. donor potential
3. Charge filling
• Potential profile → Hamiltonian
• Compute eigenstates w.r.t E_F at every V_G
• Transition, charging energy and gate modulation
4. Coulomb diamond
• DOS profile of S/D and Charge filling information
• Rate equation formalism
Theory
Experiment
© Gerhard Klimeck

A Single Atom Transistor:

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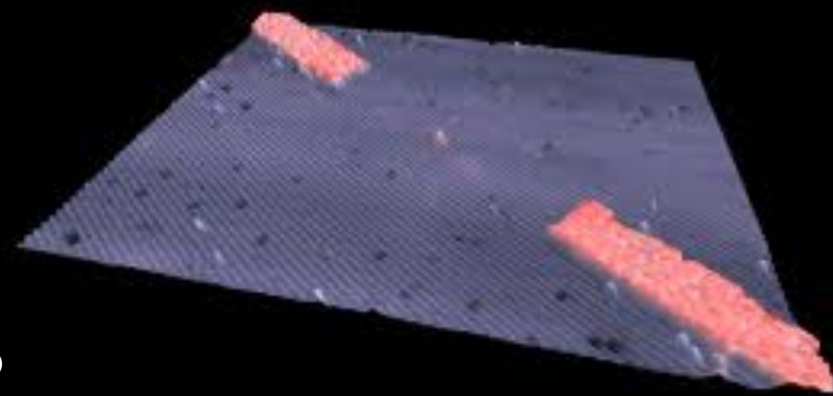
Inspired Modeling



Why?

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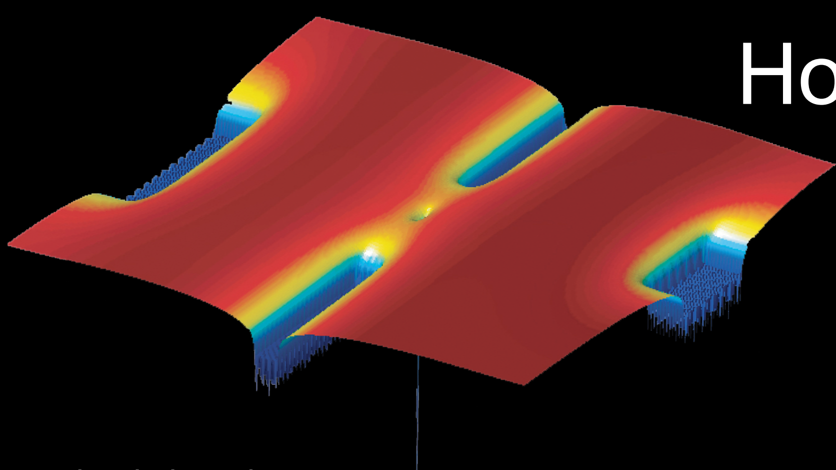

How to model this new world?

Where to study this?