The Center for Computational Nanoscience
Mark van Schilfgaarde, Director

- A formal vehicle to forge links in research initiatives
  - Computational initiatives can be stronger when they can draw on a center
  - Facilitates finding areas of common interest, and links between ASU with outside interested in collaborative research or supporting research.
- A facility to invite visitors
  - Hope to draw leading experts as colloquium speakers
  - Possibly visitors can come for short states and collaborations
- Better communication among existing faculty
  - Internal seminars inform the rest about what interesting is going on at ASU
  - Integrate Education component in computational techniques
- Coordination with other centers, e.g. HPCI, Purdue Nanohub, IGERT, MRSEC

High-Performance Computing Initiative

ASU is fortunate to have an excellent center for high performance computing, initially sponsored by Ira Fulton.

Prof. Stanzione (director) has expanded the initial center into a 1000 processor facility.

Nodes are free up to a certain maximum, after which HPC charges $0.25/CPU hour --- enables large scale calculations at minimal cost.

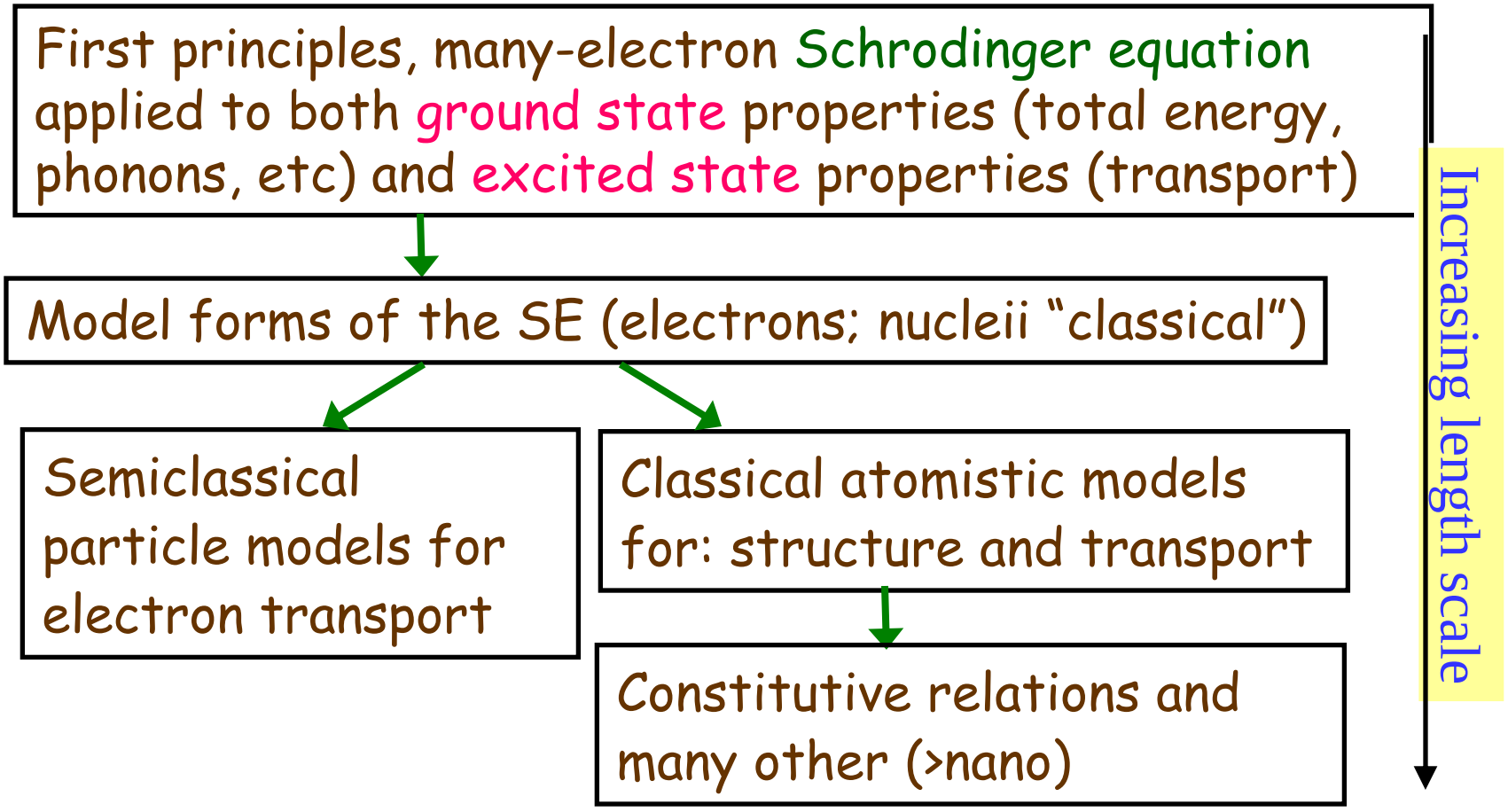
HPC supplies software support of standard computer and scientific packages (free) and custom support.

HPC offers classes on advanced programming techniques, e.g. code parallelization.

Enables faculty to extend range of research, and frees them from maintaining their own facilities.

Classification of Expertise by length scale

ASU's expertise in theory and computation spans many disciplines, ranging from atomic to the macroscopic scale:



Representative Faculty (many departments)

Ab initio SE, ground state: Adams (thermochemistry), Chizmeshya (carbon sequestration), Friesen (later), Rez (oxides), Seo (oxides)

Ab initio SE, excited state: : Kotani (later), Sankey (molecular and biological systems), van Schilfgaarde (Magnetism, GW)

Model SE , excited state: Ferry, Goodnick, Saraniti, Vasileska (later), Shumway (Quantum Monte Carlo, mostly dots)

Semiclassical electron transport: Ferry, Goodnick, Saraniti, Vasileska (later),

Classical atomistic methods: van der Vaart (later), Saraniti (later), Thorpe (rigid body dynamics of nano-bio molecules)

Grand Challenges for Computation:

Many ways to develop capacity to study new phenomena, or explain phenomena better. Three main classes:

1. Extend reliability of theory: At the most fundamental level, this is solving the SE to high accuracy. (Example GW theory, Kotani). As length scales increase approximations must, also. A significant challenge at any level.
2. Find alternatives that implement existing theories in more efficient ways.
3. Develop techniques that bridge length scales.

- The 3 most cited papers, and 6 of the 11 most cited papers in the Physical Review series (Phys. Rev. B, Phys. Rev. Lett., Rev. Mod. Physics) all have to do with *ab initio* approaches to solving the fundamental (Schrodinger) equation for the electrons.
- Walter Kohn won the Nobel Prize for Density Functional theory in 1998.
- Today, it is a major tool in almost every branch of science and engineering.
- Applicable to whole periodic table; however, its reliability is imperfect, and it is too expensive for even the mesoscale.

Table 1. *Physical Review* Articles with more than 1000 Citations Through June 2003

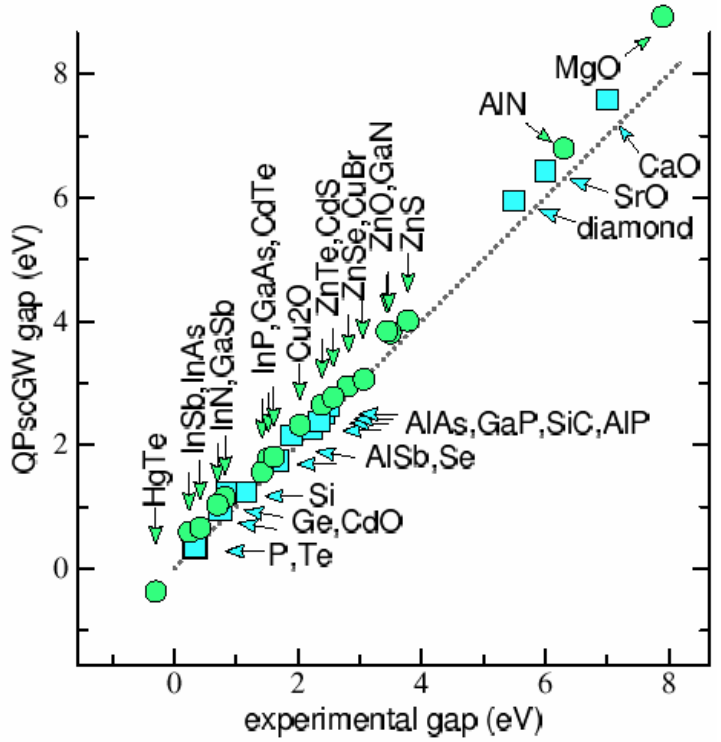
Publication	# cites	Av. age	Title	Author(s)	
PR **140**, A1133 (1965)	3227	26.7	Self-Consistent Equations Including Exchange and Correlation Effects	W. Kohn, L. J. Sham	←
PR **136**, B864 (1964)	2460	28.7	Inhomogeneous Electron Gas	P. Hohenberg, W. Kohn	←
PRB **23**, 5048 (1981)	2079	14.4	Self-Interaction Correction to Density-Functional Approximations for Many-Electron Systems	J. P. Perdew, A. Zunger	←
PRL **45**, 566 (1980)	1781	15.4	Ground State of the Electron Gas by a Stochastic Method	D. M. Ceperley, B. J. Alder	←
PR **108**, 1175 (1957)	1364	20.2	Theory of Superconductivity	J. Bardeen, L. N. Cooper, J. R. Schrieffer	
PRL **19**, 1264 (1967)	1306	15.5	A Model of Leptons	S. Weinberg	
PRB **12**, 3060 (1975)	1259	18.4	Linear Methods in Band Theory	O. K. Anderson	←
PR **124**, 1866 (1961)	1178	28.0	Effects of Configuration Interaction of Intensities and Phase Shifts	U. Fano	
RMP **57**, 287 (1985)	1055	9.2	Disordered Electronic Systems	P. A. Lee, T. V. Ramakrishnan	
RMP **54**, 437 (1982)	1045	10.8	Electronic Properties of Two-Dimensional Systems	T. Ando, A. B. Fowler, F. Stern	
PRB **13**, 5188 (1976)	1023	20.8	Special Points for Brillouin-Zone Integrations	H. J. Monkhorst, J. D. Pack	←

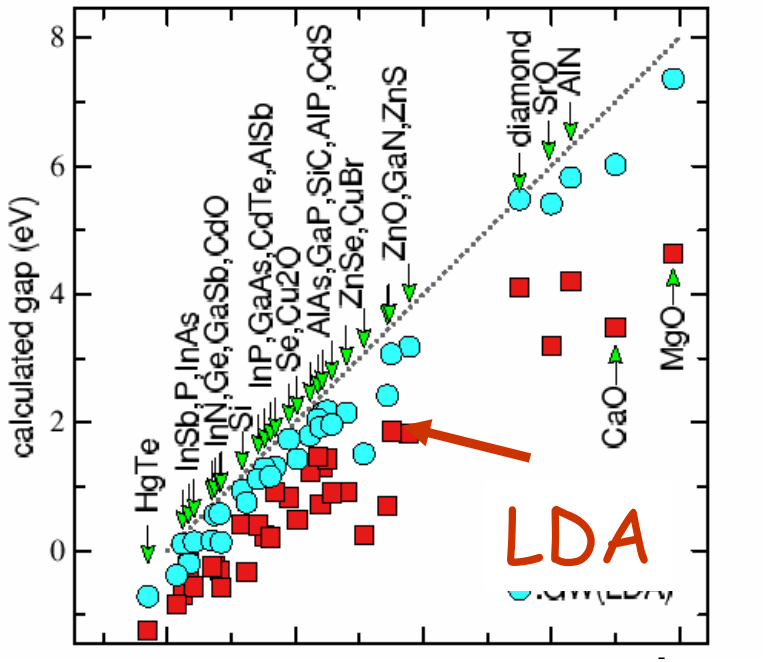
PR, Physical Review; PRB, Physical Review B; PRL, Physical Review Letters; RMP, Reviews of Modern Physics.

Success story: QSGW

Quasiparticle Self-Consistent GW (QSGW) is the most accurate and universally applicable *ab initio* theory yet developed for solids.

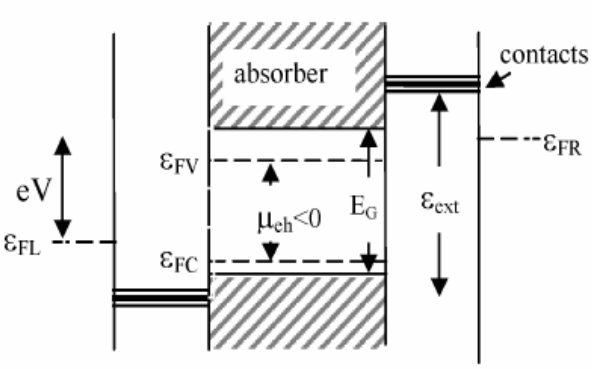
Example: semiconductor bandgaps predicted to ~0.2 eV of expt.



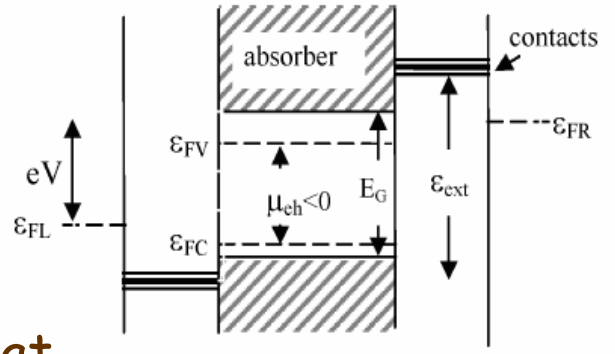


Example: Third-generation Photovoltaics

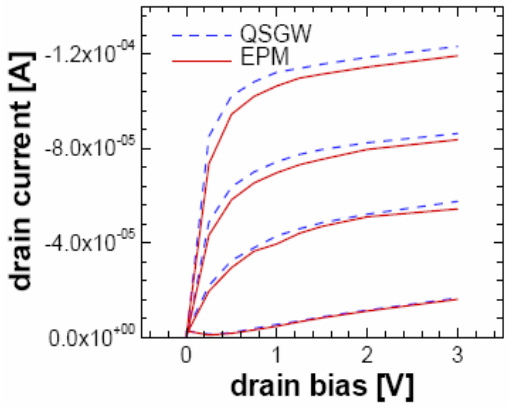
- Growing acceptance that the U.S. must reduce its reliance on oil.
  - Photovoltaics must be critical component of this, because their high conversion efficiencie
  - High conversion efficiencies and low cost are key barriers to practical realization today.
  - A collection of new ideas have been proposed t increase conversion efficiencies and surmount the standard Schockley-Quiesser limit. They are called "third-generation" technologies. They include:
    - "selective energy" contacts that collect electrons before thermalizing
    - Multiple e–h generation / incident photon through impact ionization
    - Multiple e–h generation / incident photon through impurity bands
  - Basic problem: none of these ideas has been realized in practice!
  - Are they even feasible?

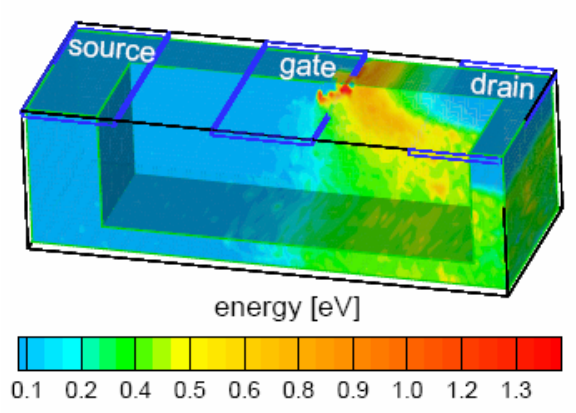


- Are 3rd generation proposals workable?
  - A hard question to answer experimentally.
  - Theoretical treatment so far has been too simple
  - Good modeling should: predict "best case" scenarios, and the effect of nonidealities that can occur under realistic conditions.



"Cellular Monte Carlo" simulator based on the Boltzmann equation (Saraniti and Goodnick). Models realistic devices with realistic parameters. The most sophisticated tool of its kind, it can potentially give a reasonable answer to those questions, before spending large resources on trying them.





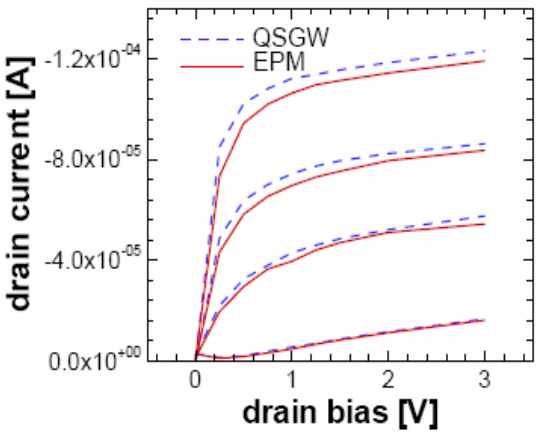
Example: GaAs MESFET

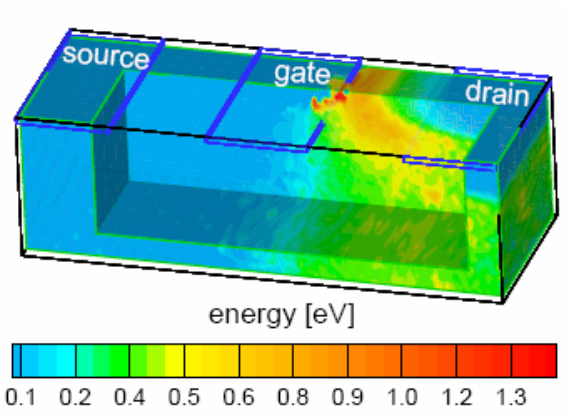
Bridging length scales

The CMC solves the Boltzmann equation for realistic devices. But it requires as input parameters such as energy bands and scattering matrix elements. If those inputs are good, the calculation should reliably predict device behavior. *Ab initio* theory such as QSGW can supply accurate inputs.

Example: MESFET in GaAs. Much experimental data; reliable model to generate inputs (EPM) can be developed from this data.

Alternatively, use QSGW. Doesn't rely on experiments! In this case, results almost identical. What about InN?





Ab initio Electrochemistry (Friesen)

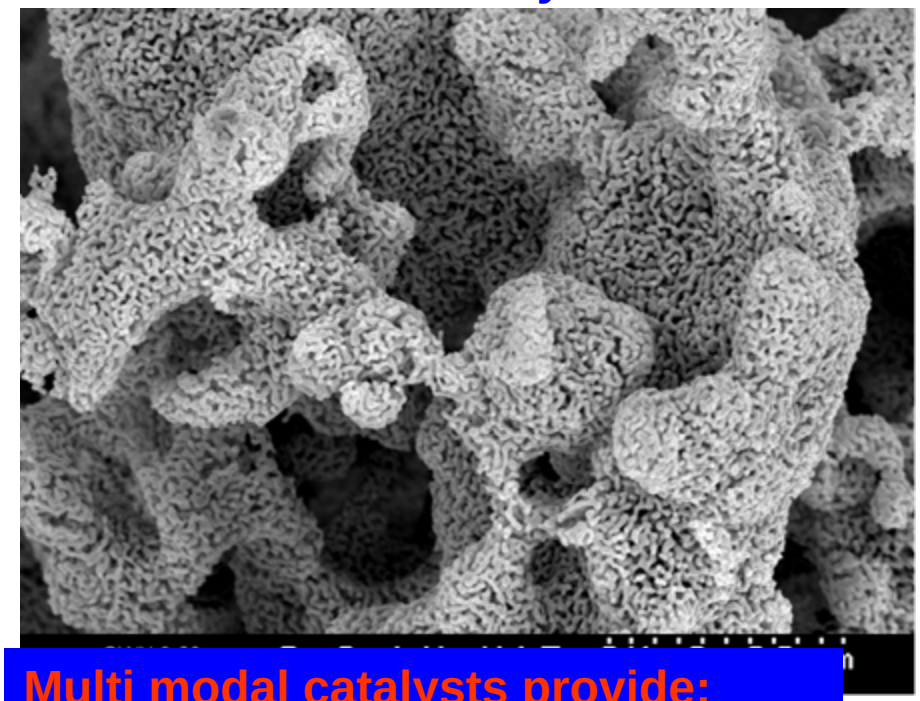
- A key loss mechanism in catalysts: The voltage required to generate a practically acceptable current (overpotential) is higher than the thermodynamic potential.
- This difference occurs through losses on the atomic scale as the ions cross the electrode/electrolyte interface.
- Details are poorly understood, particularly in protic ionic liquids (little-studied)
- Plan: use *ab initio* framework to model the electrodode, electrolyte, and interface; and the ion exchange mechanism.
- Challenge: interfaces are too big to realistically attack with good quality present-day modeling methods based on the local-density approximation to density-functional theory
- Project includes development of next-generation methods that will make this possible.

Friesen Research Group

School of Materials, Arizona State University

Renewable Energy Electrochemistry

Multi-modal, Bi-functional Electro-Catalysts

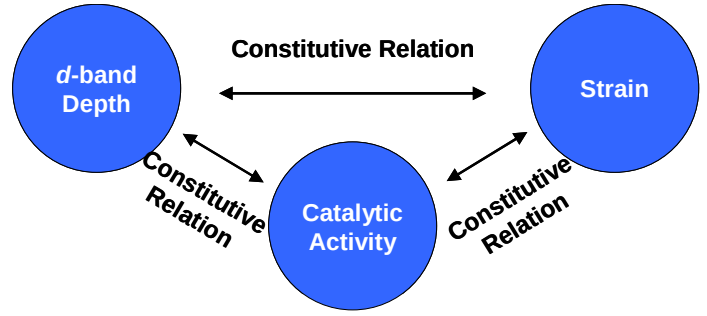


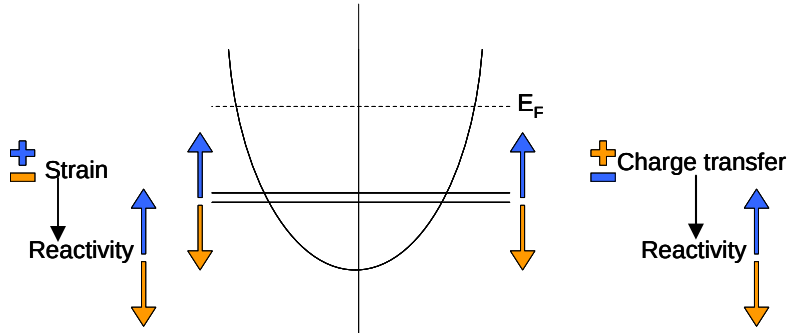
Multi modal catalysts provide:

-Enhanced transport kinetics

-High surface area

Tuning Activity





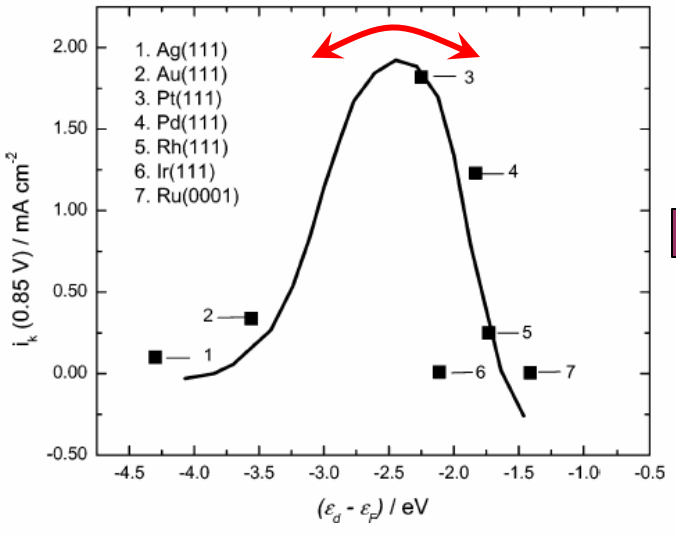
-Tune hybridization w/ Adsorbates

-strain

-eigenstrains

Tuning catalytic activity

Tune activity by applying Physical strain: Max ~1%



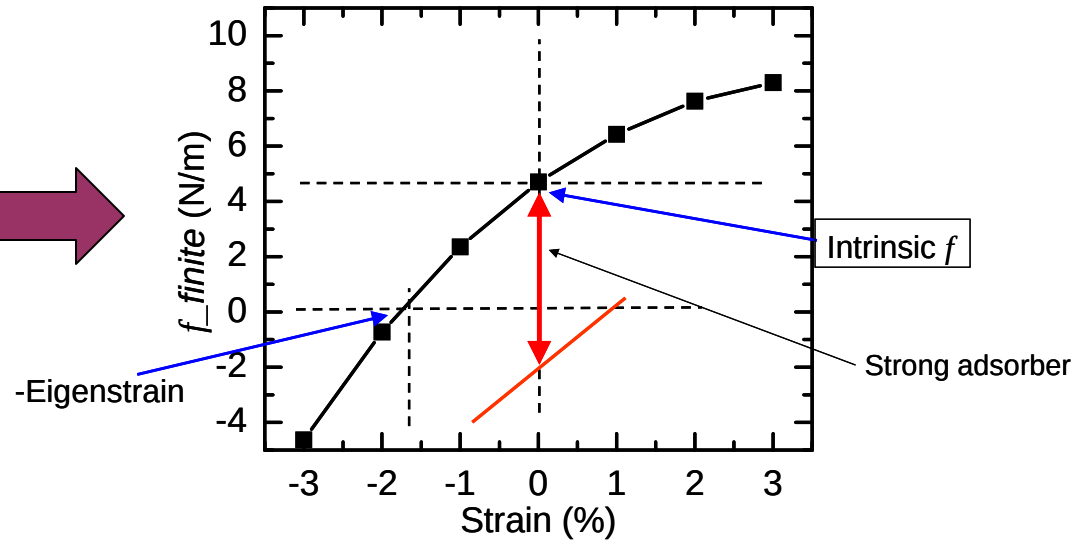
404 *J. Phys. Chem. C* 2007, *111*, 404−410

Catalytic Activity−d-Band Center Correlation for the O_2 Reduction Reaction on Platinum in Alkaline Solutions

F. H. B. Lima,† J. Zhang,‡ M. H. Shao,‡ K. Sasaki,‡ M. B. Vukmirovic,‡ E. A. Ticianelli,† and R. R. Adzic*,‡

Tune *sp-d* hybridization w/ physical strain.

Tune activity by modifying Eigenstrain: >4% achievable through adsorption



Constitutive relations exist between surface stress, strain, eigenstrain, and d-band position.

Map d-band position as a function of surface stress change w/ adsorption to tune in real-time.

Electronic structure calculations allow for the direct analysis of surface stress (~eigenstrain) and d-band position changes in the presence of adsorbed species. Experiment can then directly monitor catalytic activity and surface stress changes in real-time.

Molecular Dynamics of Folding/Unfolding/Refolding Conformational Changes

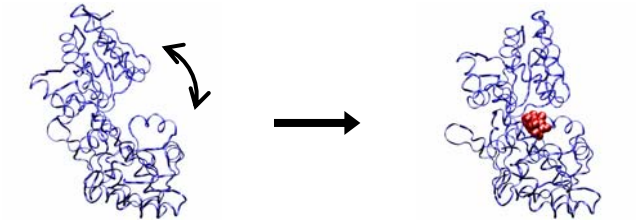
Arjan van der Vaart

Center for Biological Physics
Department of Chemistry and Biochemistry

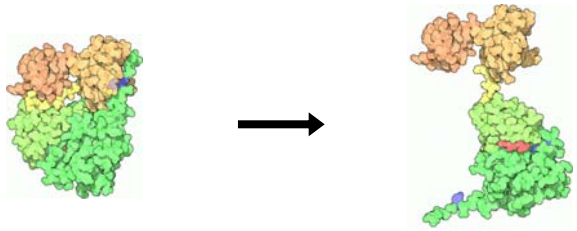
Conformational change = The change in shape of a biomolecule upon binding other molecules

Conformational changes are crucial for the functioning of many proteins

1. **transport proteins**
   e.g. maltose-binding protein

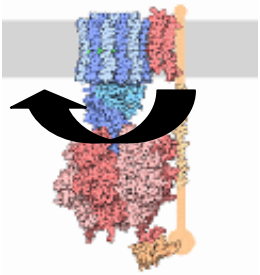


2. **kinases**
   transfer phosphate groups from high-energy donor molecules (e.g. ATP), to specific target molecules. Very common in the body.



Src tyrosine kinase

3. **molecular motors**
   e.g. F_OF_1-ATPase



4. **etc. etc.**

How do conformational changes work?

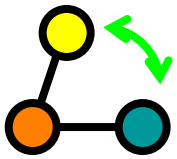
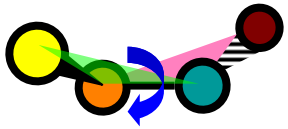
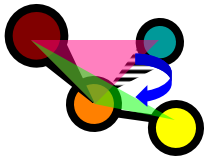
1. What interactions lead to the conformational behavior?
2. What are the pathways for the conformational change?
3. What is its biological function?
4. Can we block the conformational behavior?

Method: Atomistic Molecular Dynamics Simulations

1. High spatial resolution
2. All interactions are quantified
3. Thermodynamic properties can be calculated

Molecular Dynamics (MD)

Atoms treated as classical point-masses moving in a model potential

Bonded terms				Non-bonded terms	
Bonds	Angles	Dihedrals	Improper Dihedrals	Electrostatics	van der Waals
					
$k_b(r-r_0)^2$	$k_a(\theta-\theta_0)^2$	$k_d[1+\cos(n\phi-\phi_0)]$	$k_i(\omega-\omega_0)^2$	$(q_1q_2)/(\varepsilon r)$	$E[(r_m/r)^{12}-(r_m/r)^6]$

The model potential is fitted to experiments and quantum mechanical calculations

The potential must be transferable

Atomic motion propagated by classical (Newtonian) dynamics using a very small timestep (10^{-15} seconds)

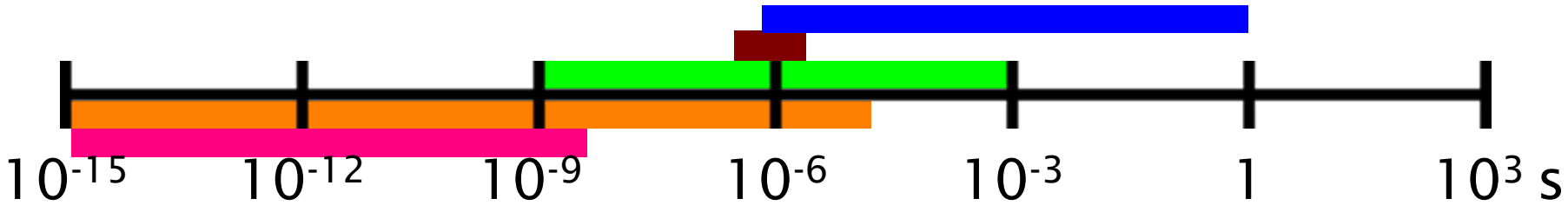
ASU

Problem: Timescales of conformational motion

protein domain motion

unwinding of DNA helix

protein folding



molecular dynamics large system

molecular dynamics small system

Thus: need to develop "smart" techniques!

Quasiparticle Self-consistentGW (QSGW) method

Takao Kotani , Mark van Schilfgaarde

Our questions are

- What defects reduce the performance of HfO_2?
- Spin-polarized current for MRAM, Fe/MgO/Fe
- Interpret EELS data to guess atomic structure
- New “thermo-power material”?

--- We have to know **electronic structure** ---

So many first-principle calculations are performed now.

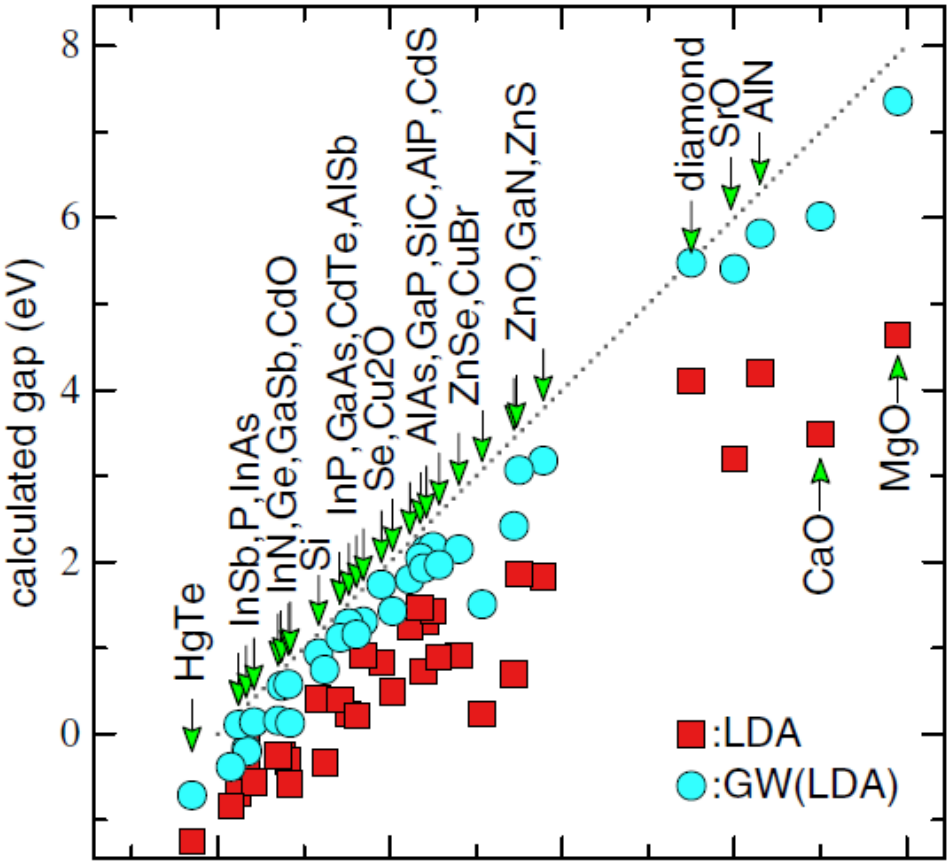
Difficulties in first-principle methods.

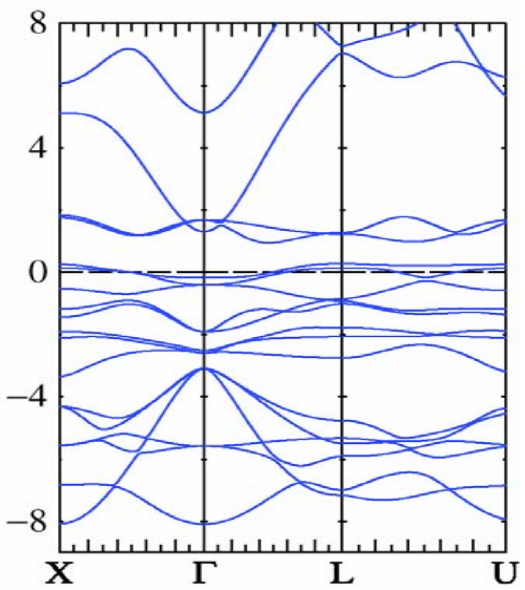
(1) Computational costs
(2)We can not evaluate quantities directly. E.g. Tc for High-Tc SC.
(3)Poorness of Standard approximations,

LDA (local density approx.) or so→ our QSGW method can solve this problem.

(3) is serious ---
"**reliability**" can be still problematic.

Poorness of standard approximations





CoO is insulator (gap ~4 eV);
LDA predicts metallic
LDA+U works. But what U?

Quasiparticle self-consistent GW method

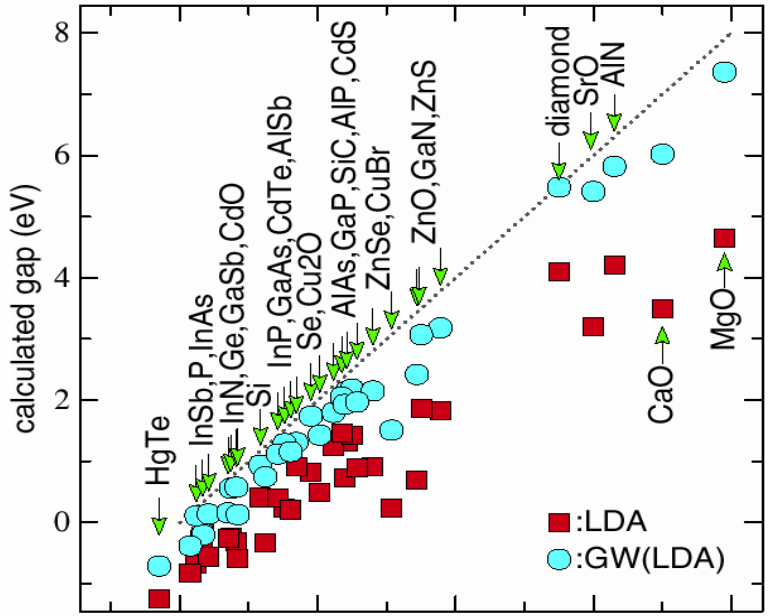
It looks like Hartree-Fock method, but it uses "Dynamical Screened Coulomb interaction *" instead of the bare Coulomb interaction .

*it is determined self-consistently.

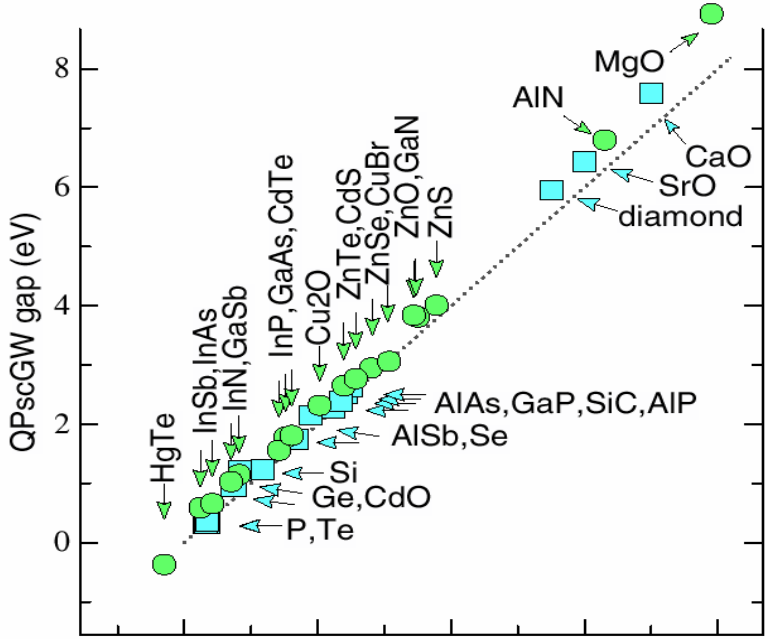
Optimum independent-particle picture.
Thus, ready to be used for device simulators.

Our Result by QSGW

Experimental band gap vs. Calculated band gap



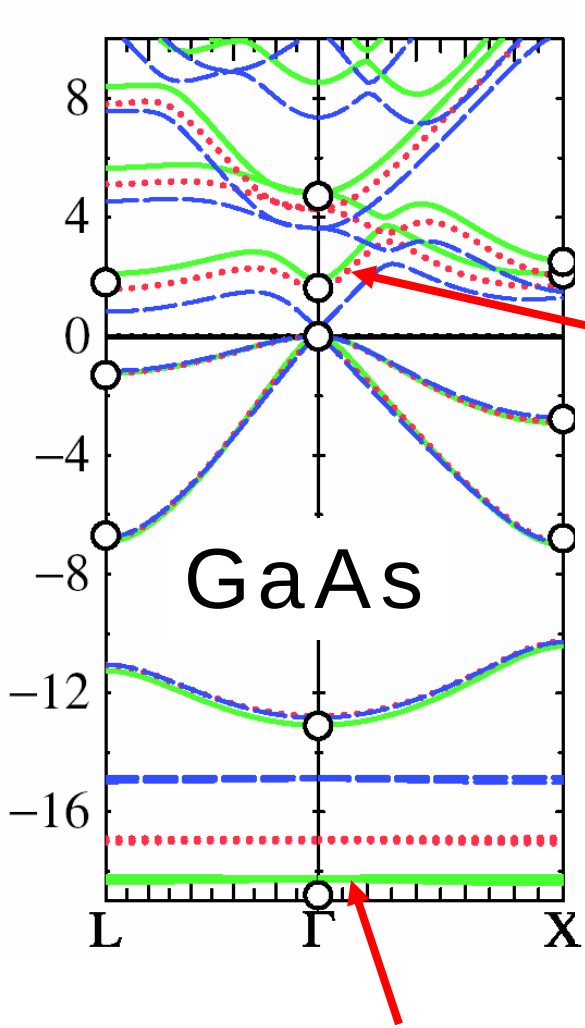
← LDA, GW



← QSGW: Good!

Almost along the diagonal line!

Typical case for semiconductor



QSGW: green

O: Experiment

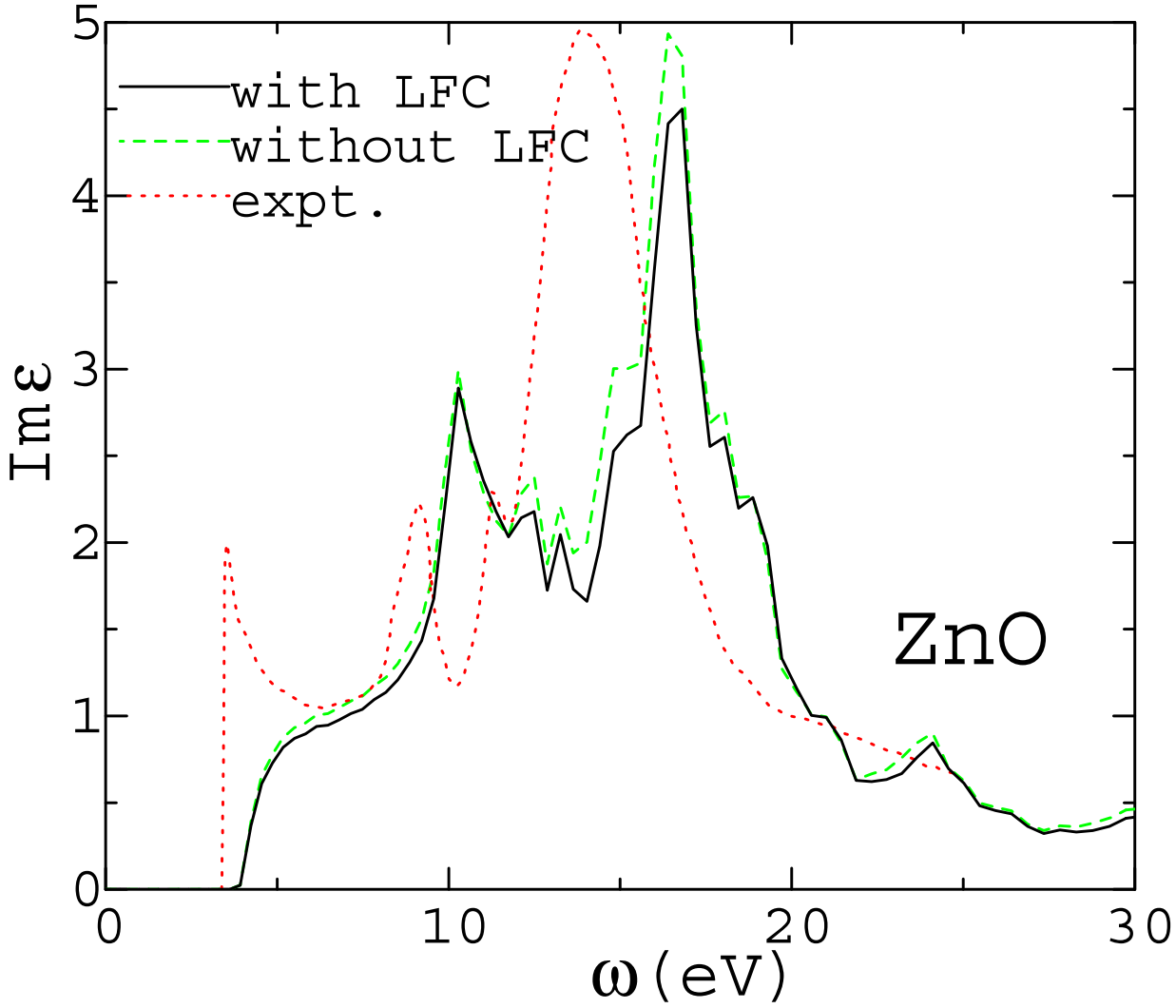
m^* (QSGW) = 0.073

m^* (LDA) = 0.022

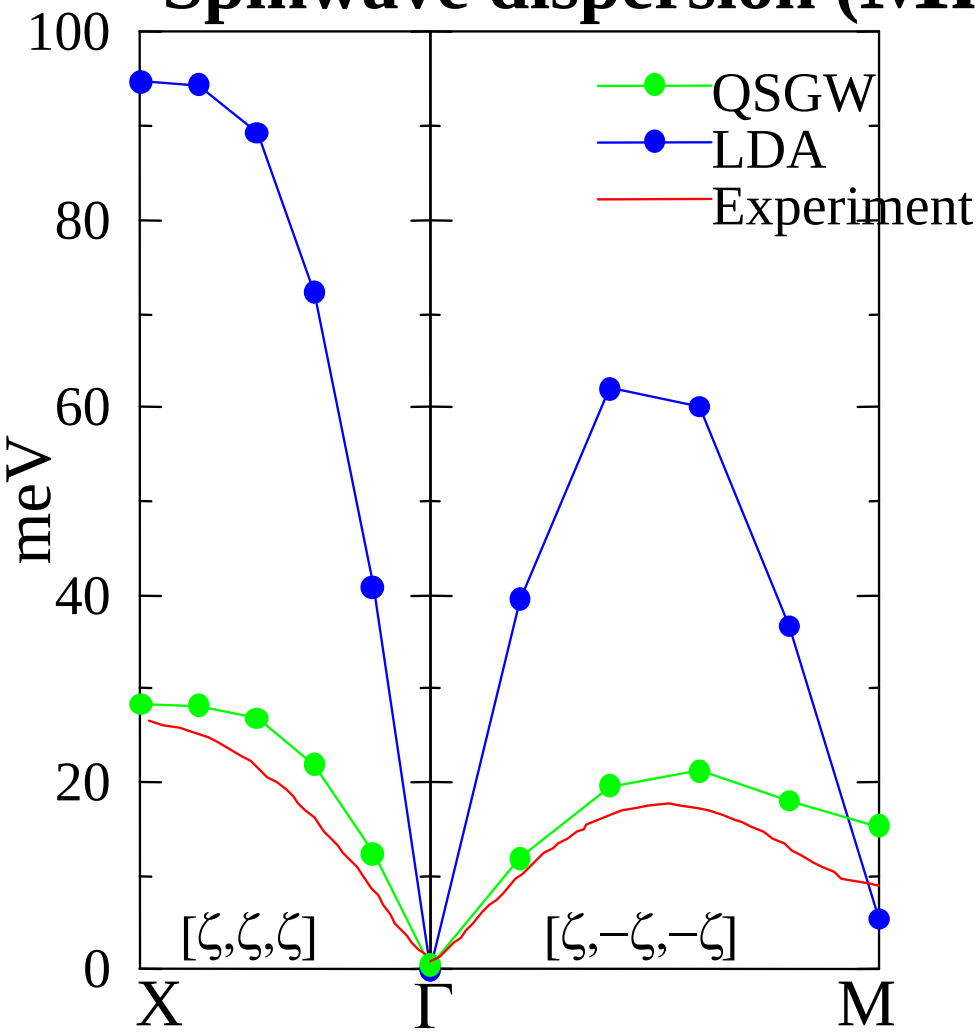
m^* (expt) = 0.067

Ga *d* level well described

ZnO dielectric



Spinwave dispersion (MnO AF-II)



*Energy bands, and optical properties are also described well.

Conclusions

- The QSGW method

  Self-consistent perturbation theory

  - optimum independent-particle picture.

  - wide range of materials.

  - no parameters like LDA+U.

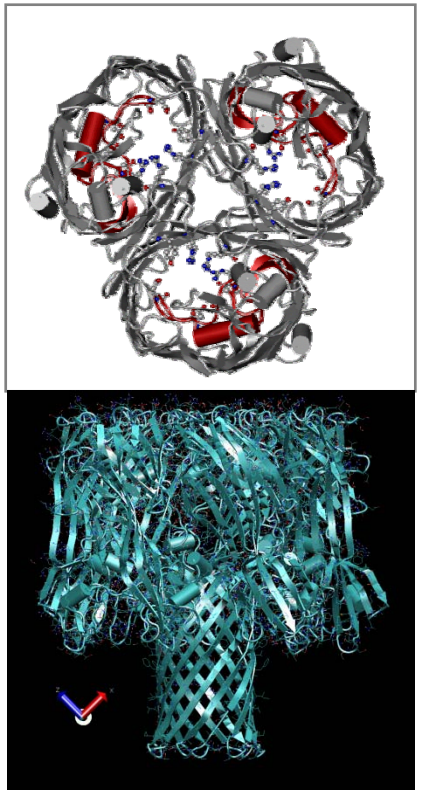
  QSGW is the very basis for next-generation electronic structure calculation.

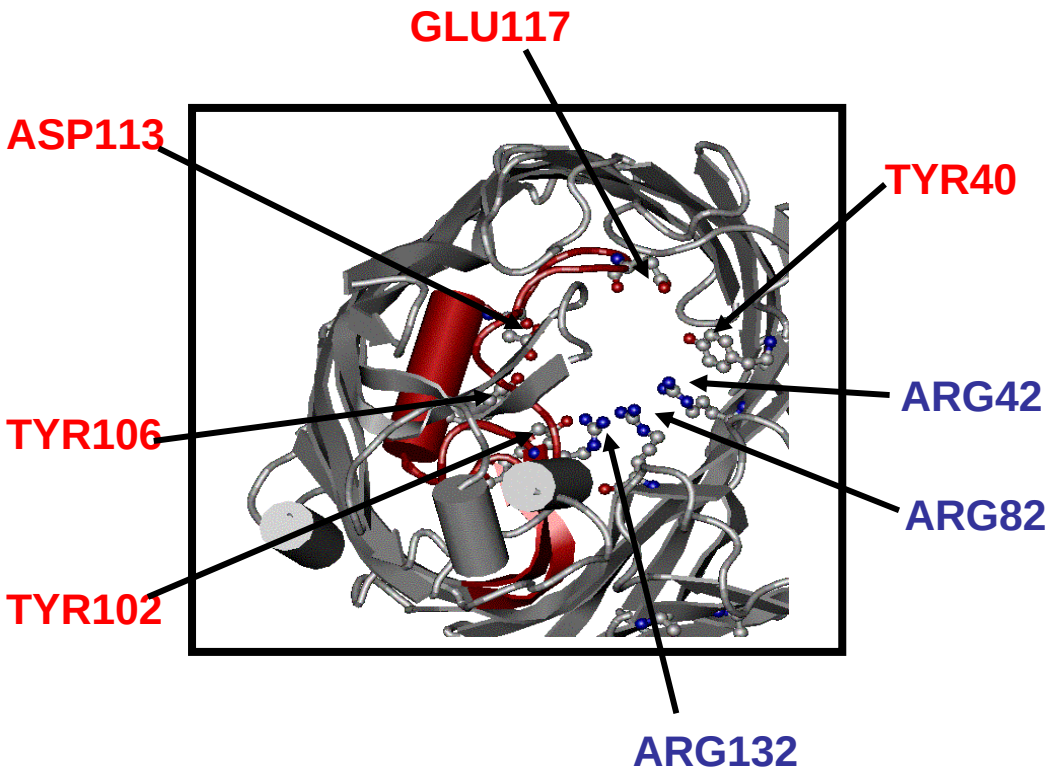
---

* How to make speed up?
* Phonon should be included.
* Make it more accurate.

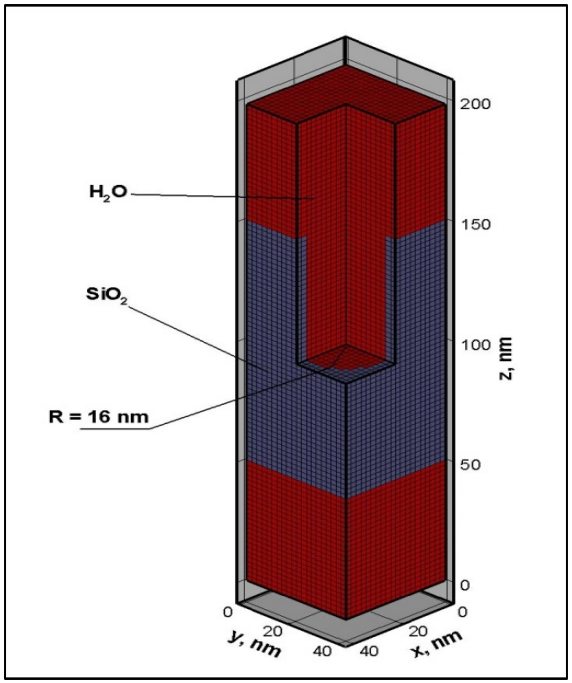
Modeling and Design of Biomimetic Nanoconductors

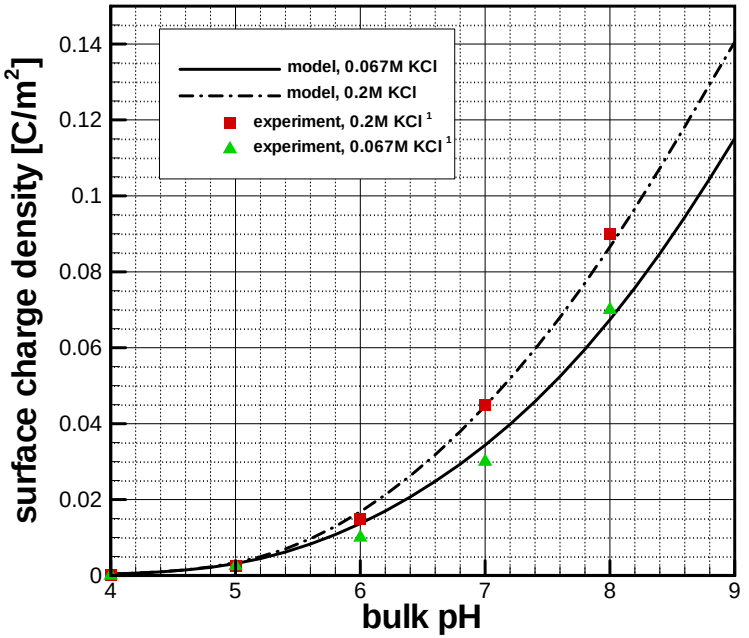
Marco Saraniti, Sasha Smolyanitsky, and Prathibha Ramaprasad





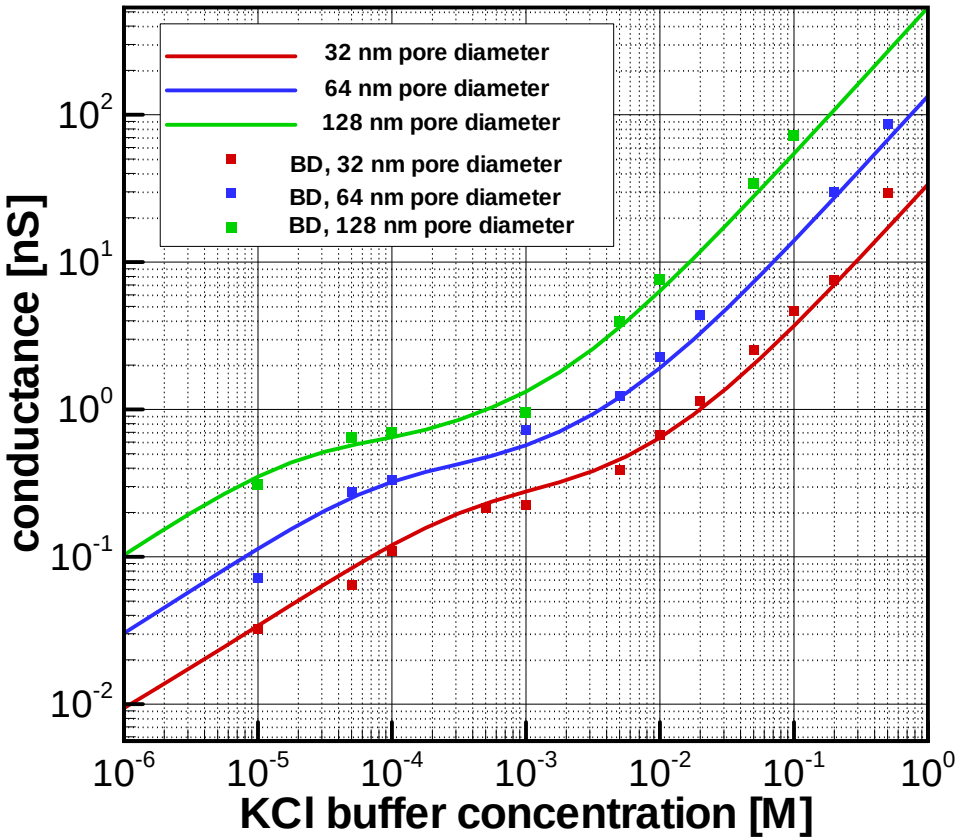
Surface Charge Density on SiO_2 Pores





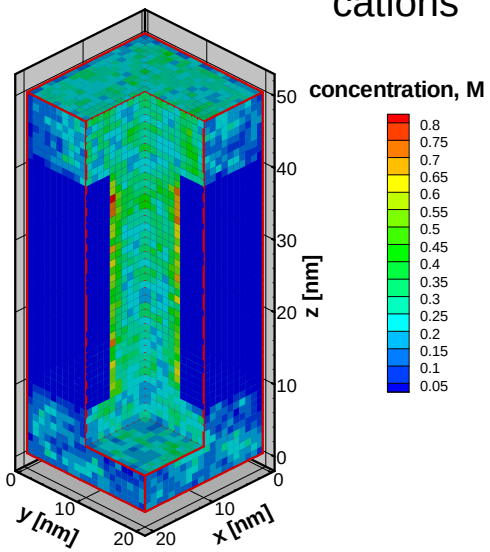
1. Patricia M. Dove and Colin M. Craven. *Surface charge density on silica in alkali and alkaline earth cloride electrolyte solutions*. Geochimica et Cosmochimica Acta, 69(21), 2005.

Conductance (pH=7)

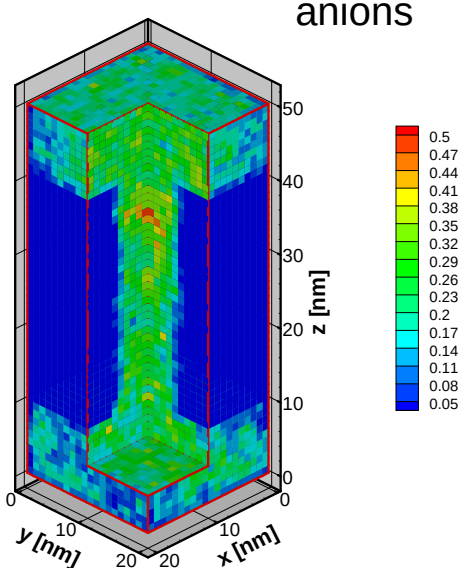


3D Brownian Dynamics Simulation

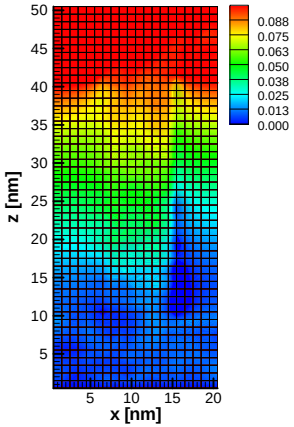
cations

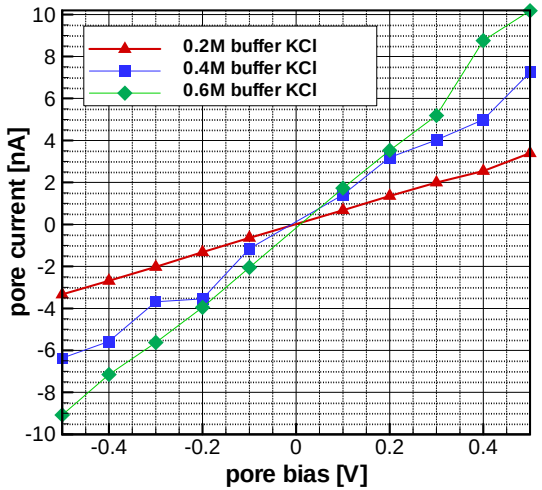


anions



potential [V] (slice at y = 10.5 nm)

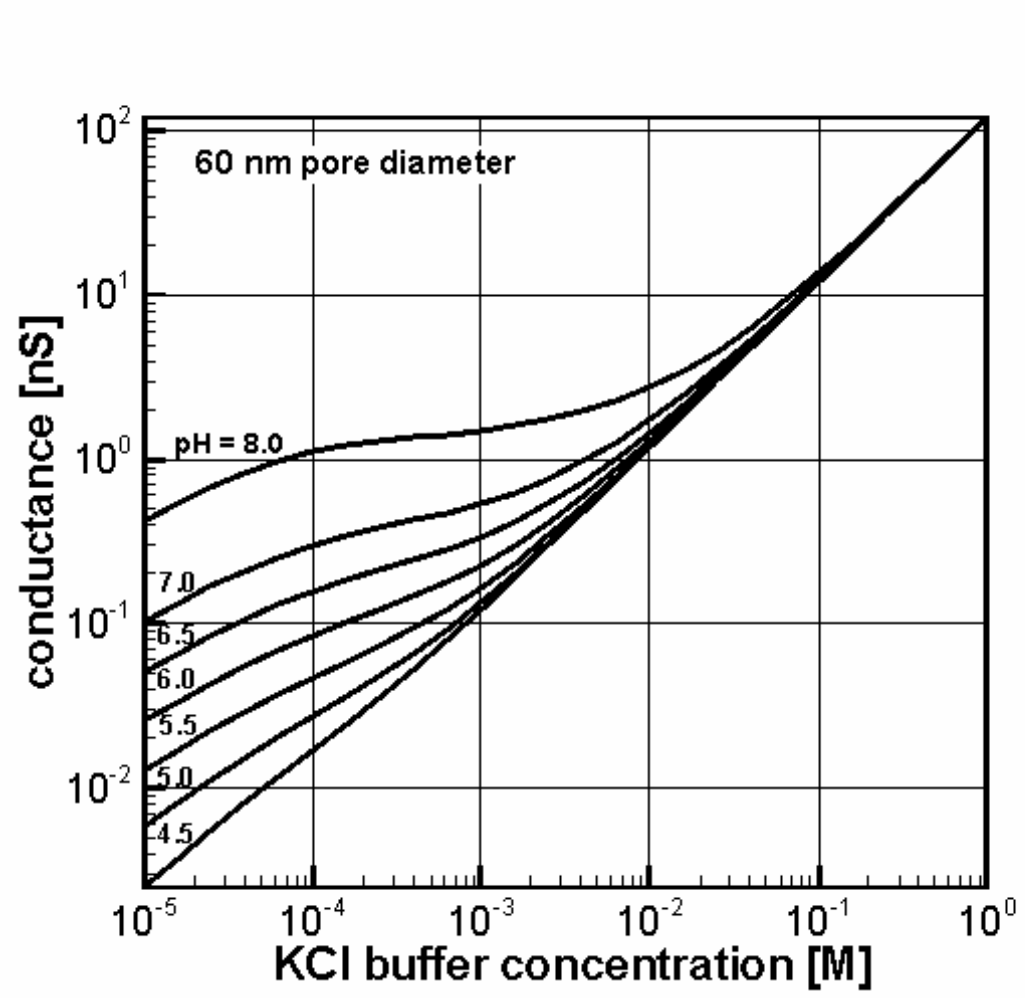




National Center for Design of Biomimetic Nanoconductors
http://www.nanoconductor.org

ASU ARIZONA STATE UNIVERSITY

pH-Dependent Conductance

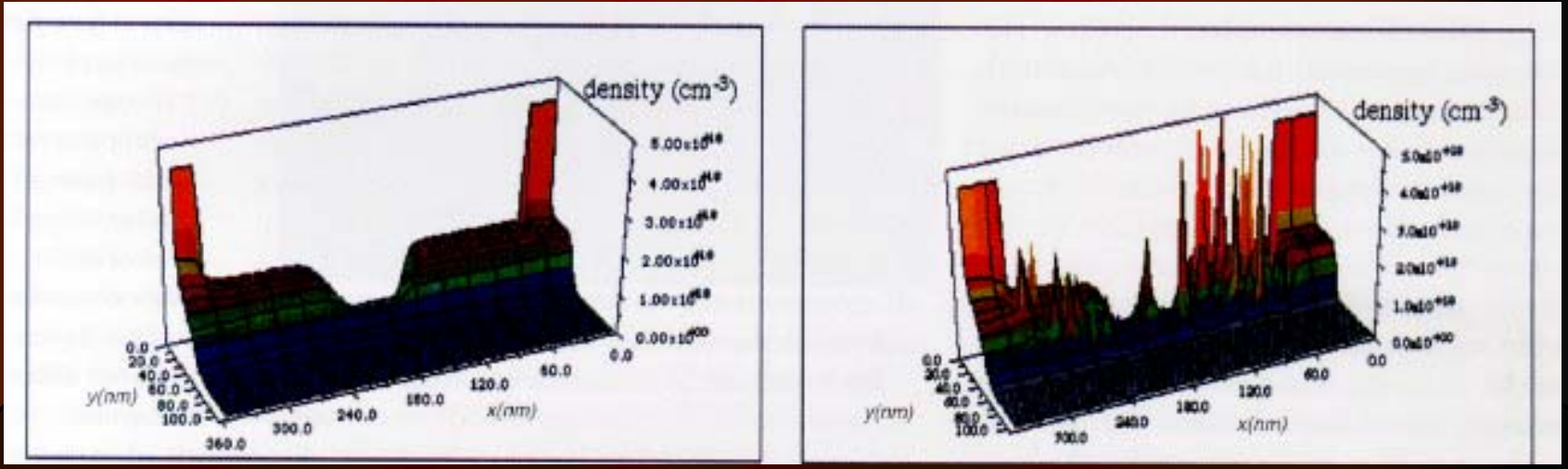


Computational Electronics

Dragica Vasileska
Professor
Arizona State University

Pre-1990 Simulation Efforts

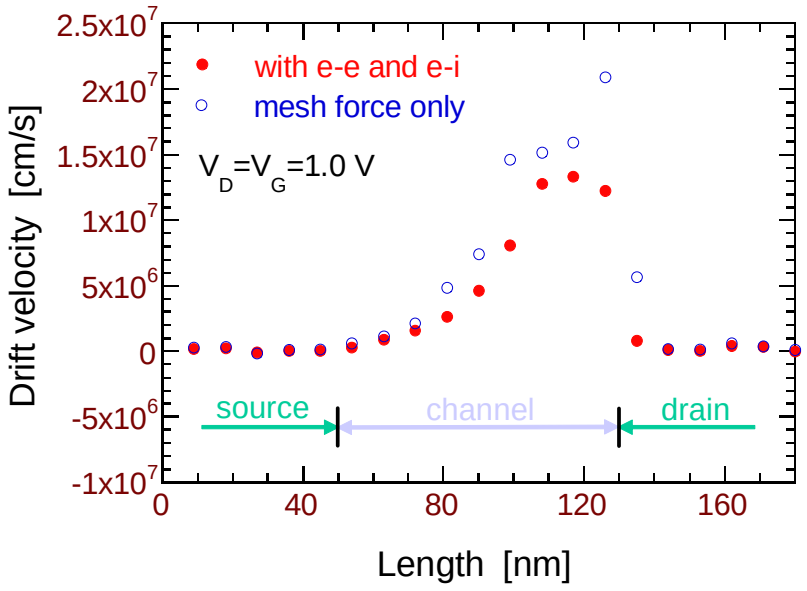
- Semiclassical:
  - Monte Carlo-Molecular Dynamics Simulations (Ferry-Lugli)
- Quantum:
  - Wigner Function Simulations (Kluksdahl, Ringhofer, Ferry)
  - Quantum Hydrodynamic simulations without and with inclusion of discrete impurity effects (JR Zhou)

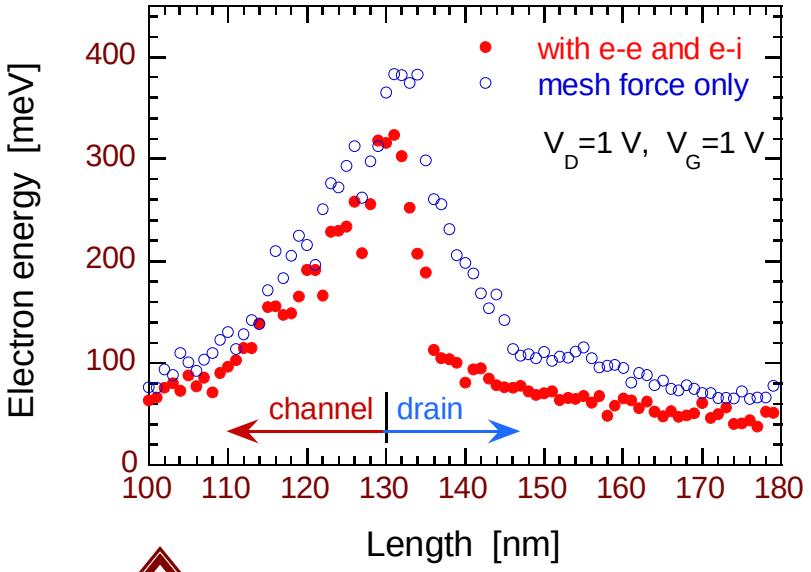


Post-1990 Simulation Efforts

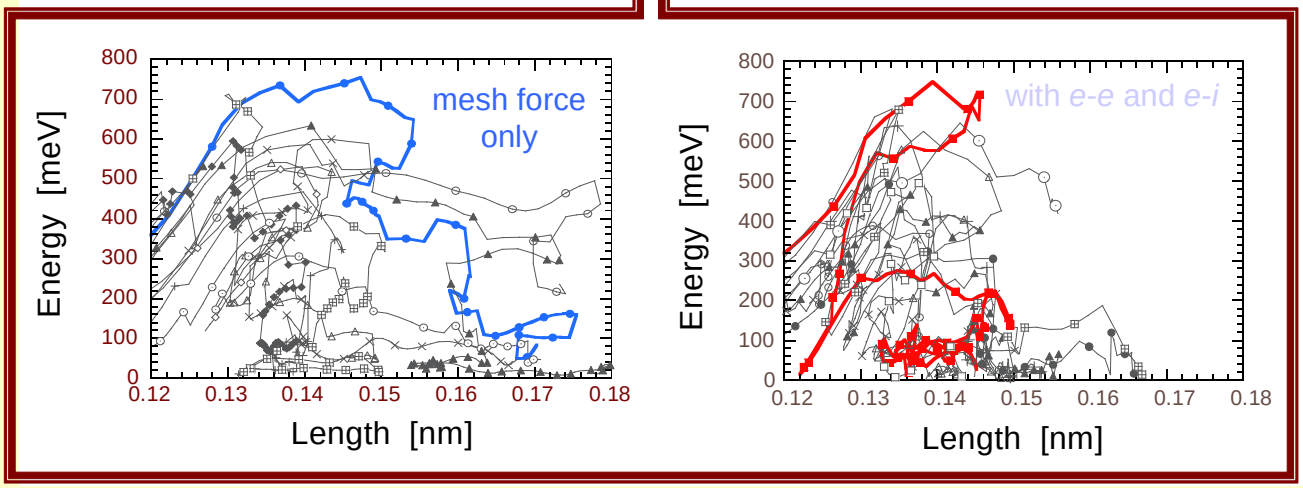
- Semiclassical
  - 3D Drift-diffusion simulations for discrete impurity effects examination in 50 nm MOSFET devices (Vasileska-1996)
  - **First 3D Monte Carlo device simulation code with a real space treatment of the short range electron-electron and electron-impurity interactions (Gross, Vasileska, Ferry-1997)**
  - Development of a variety of 3D Efficient Poisson Equation Solvers (Wigger, Speyer, Vasileska, Goodnick, Saraniti-1997)
  - **Development of a full-band CA Monte Carlo device simulation code (Saraniti, Wigger, Goodnick-1997)**
  - Inclusion of the effective potential in semiclassical Monte Carlo device simulation schemes (Vasileska, Ferry, Ringhofer-2000)
  - **Development of the first 2D thermal device simulation code (Raleva, Vasileska, Goodnick-2007)**

MOSFETs - Role of the *E-E* and *E-I*





Individual electron trajectories over time



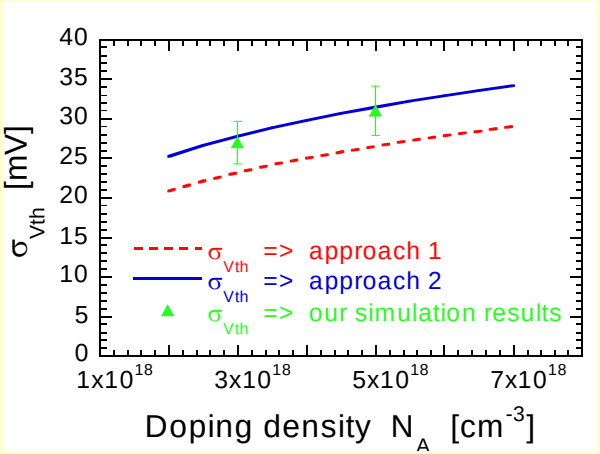
MOSFETs - Discrete Impurity Effects

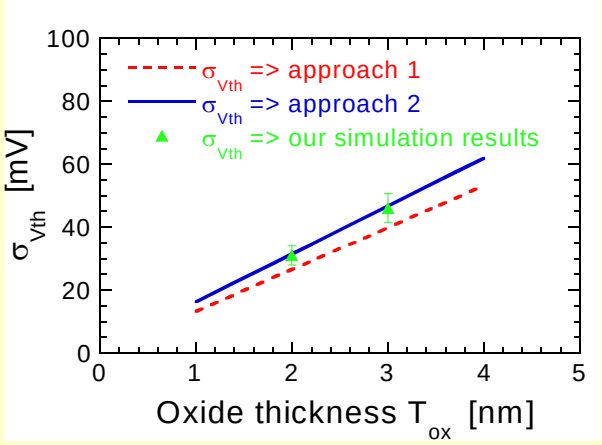
Approach 1 [1]: $\sigma_{Vth} = \frac{\sqrt[4]{q^3 \varepsilon_{Si} \phi_B}}{\sqrt{2}} \frac{T_{ox}}{\varepsilon_{ox}} \frac{\sqrt[4]{N_A}}{\sqrt{L_{eff} W_{eff}}}$; $\phi_B = \frac{k_B T}{q} ln\left(\frac{N_A}{n_i}\right)$

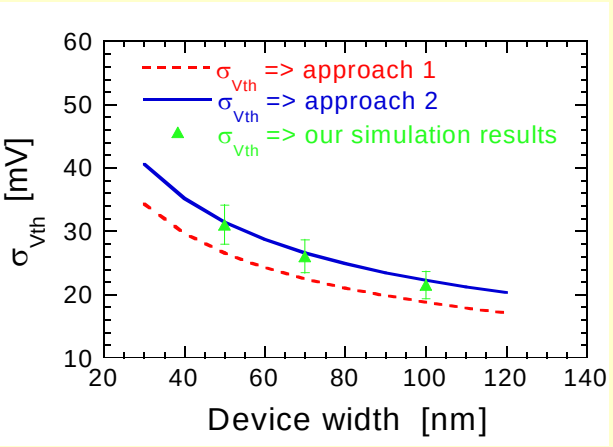
Approach 2 [2]: $\sigma_{Vth} \approx \frac{\sqrt[4]{4q^3 \varepsilon_{Si} \phi_B}}{\sqrt{3}} \left[\frac{k_B T / q}{\sqrt{4q\varepsilon_{Si}\phi_B N_A}} + \frac{T_{ox}}{\varepsilon_{ox}}\right] \frac{\sqrt[4]{N_A}}{\sqrt{L_{eff} W_{eff}}}$

[1] T. Mizuno, J. Okamura, and A. Toriumi, *IEEE Trans. Electron Dev.* **41**, 2216 (1994).

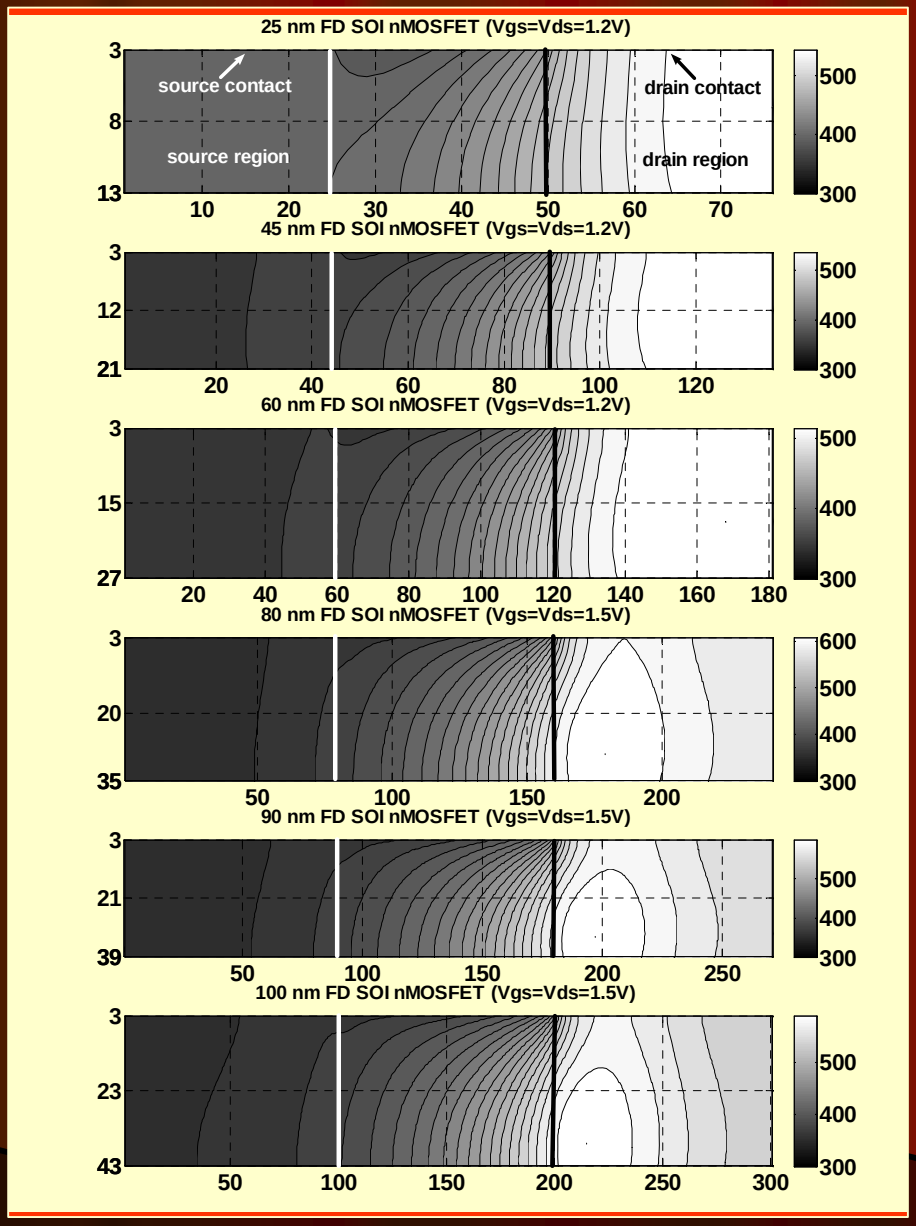
[2] P. A. Stolk, F. P. Widdershoven, and D. B. Klaassen, *IEEE Trans. Electron Dev.* **45**, 1960 (1998).



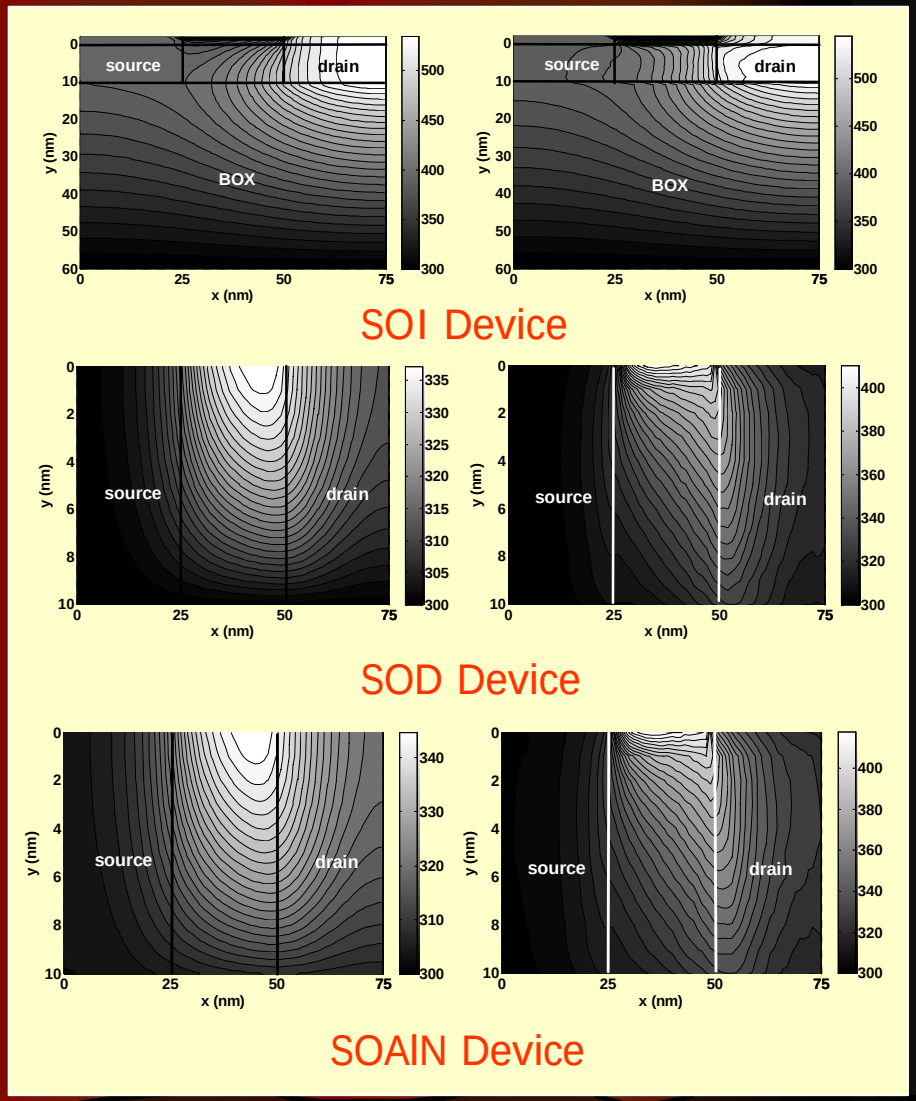




Lattice Heating and Scaling of Transistor Dimensions



Conventional SOI Transistors vs. SOD transistors with different boundary condition for the temperature on the gate



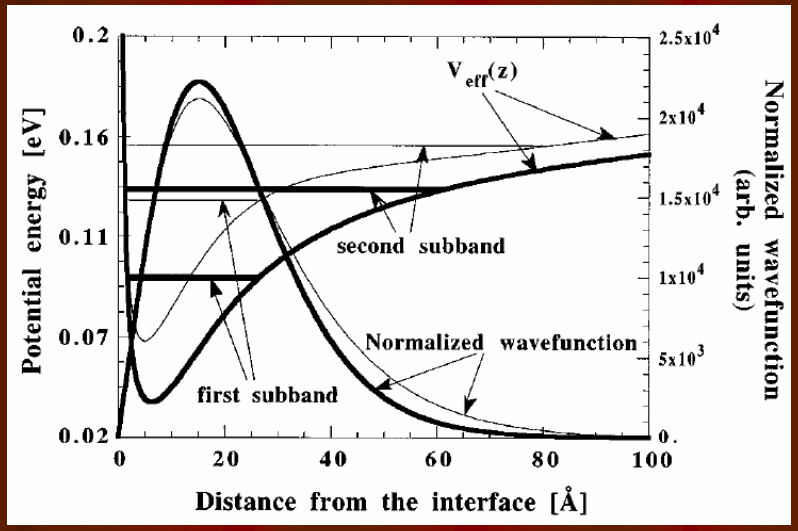
Notice better heat spread in the SOD and the SOAIN devices.

Post-1990 Simulation Efforts

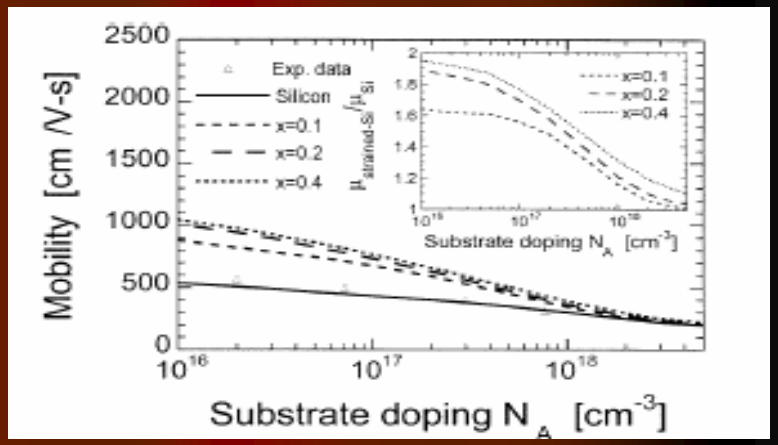
- Quantum
  - Green's function codel for the low-field mobility calculation (1993-Vasileska, Ferry) – **For the first time we have included self-consistent Born approximation in realistic transport calculation**
  - **Development of SCHRED (Vasileska-1997)**
  - Development of a variety of 2D/3D Schrodinger Poisson solvers for simulations of quantum dots in Si and GaAs technology (Vasileska, Ahmed - 1999)
  - Effective potential inclusion in semiclassical simulators (Vasileska, Ferry, Ahmed, Ringhofer - 2002)
  - **2D Poisson-1D Schrodinger full-band simulator for transport in p-channel Si/SiGe devices (Krischnan, Vasileska, Fischetti – 2005)**
  - **Development of 2D/3D Contact block reduction method for quantum transport of nanoscale devices (Khan, Mamaluy, Vasileska)**

Green's Functions

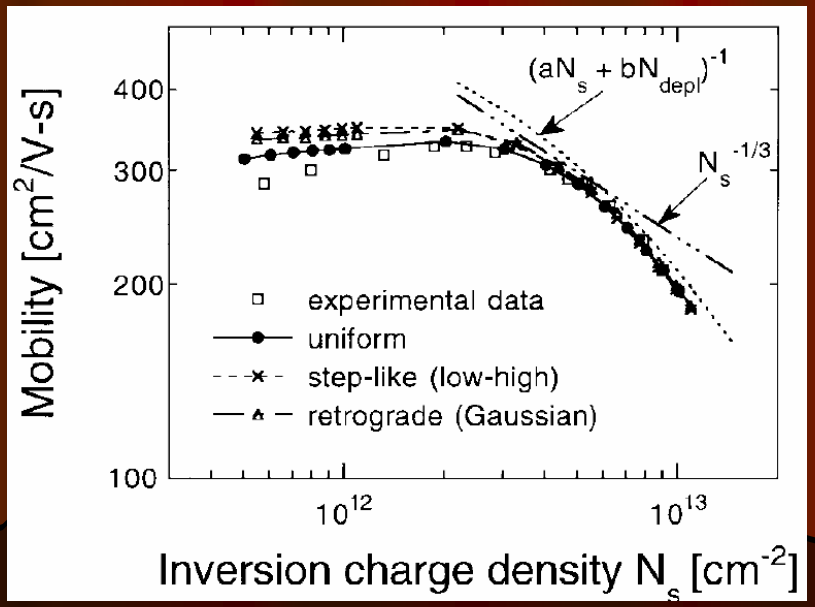
Exchange-correlation effects

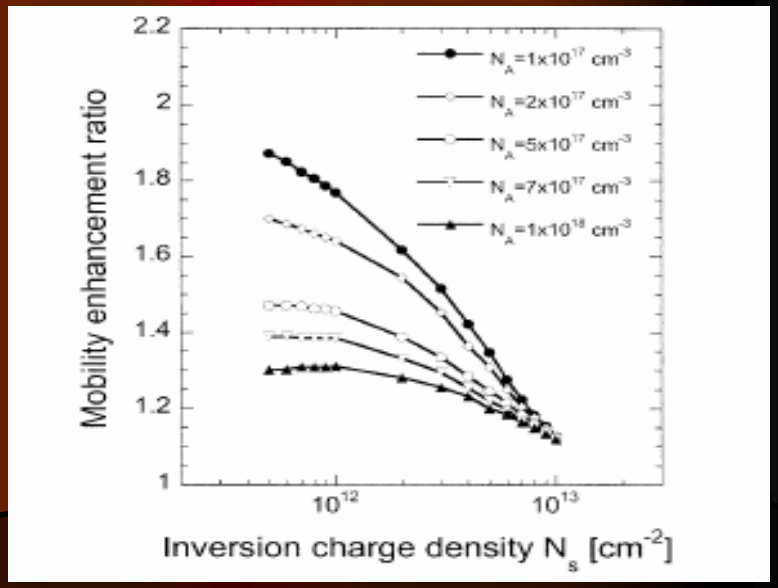


Starined-Si inversion layers

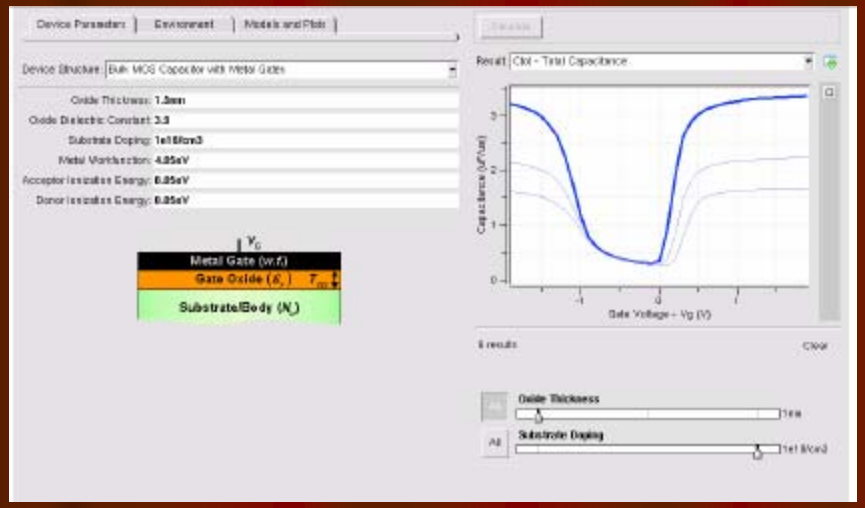


Universal mobility exploration in conventional Si inversion layers.

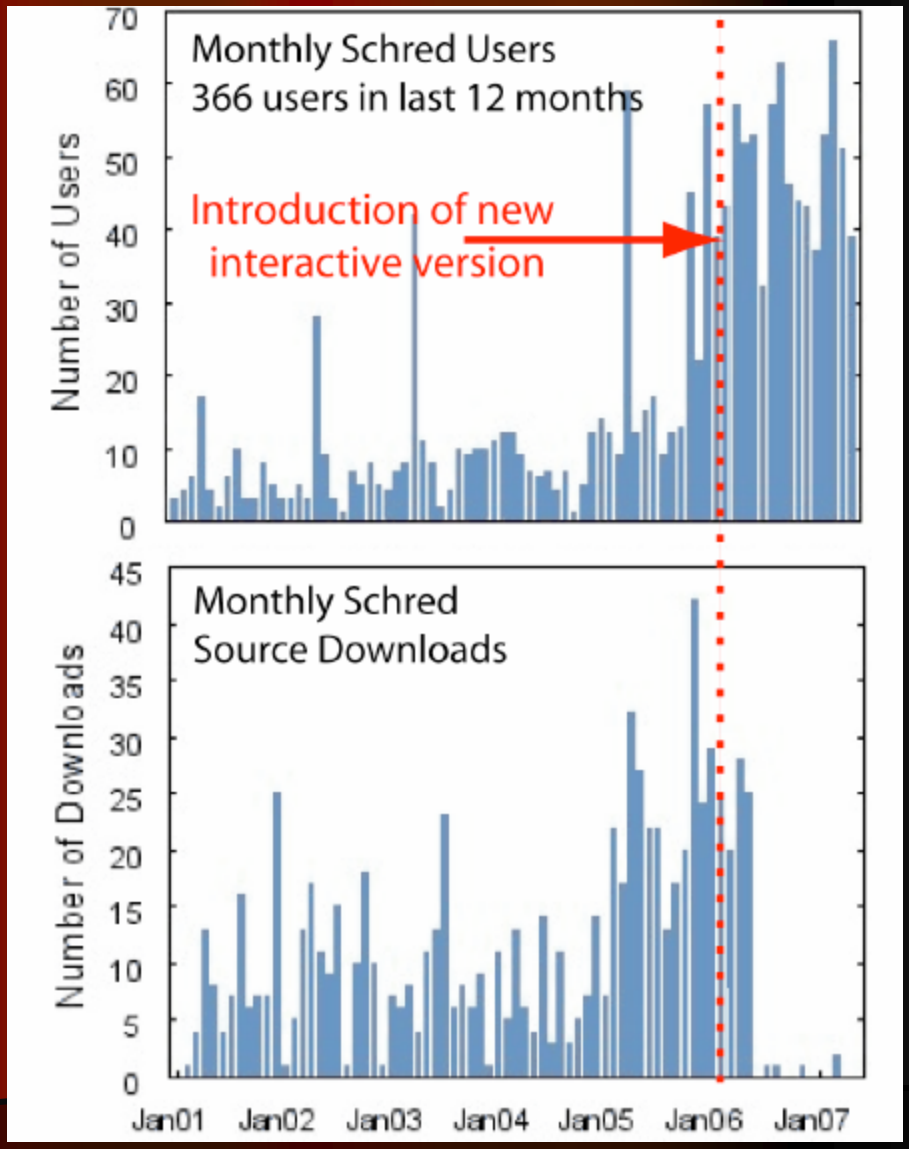




SCHRED



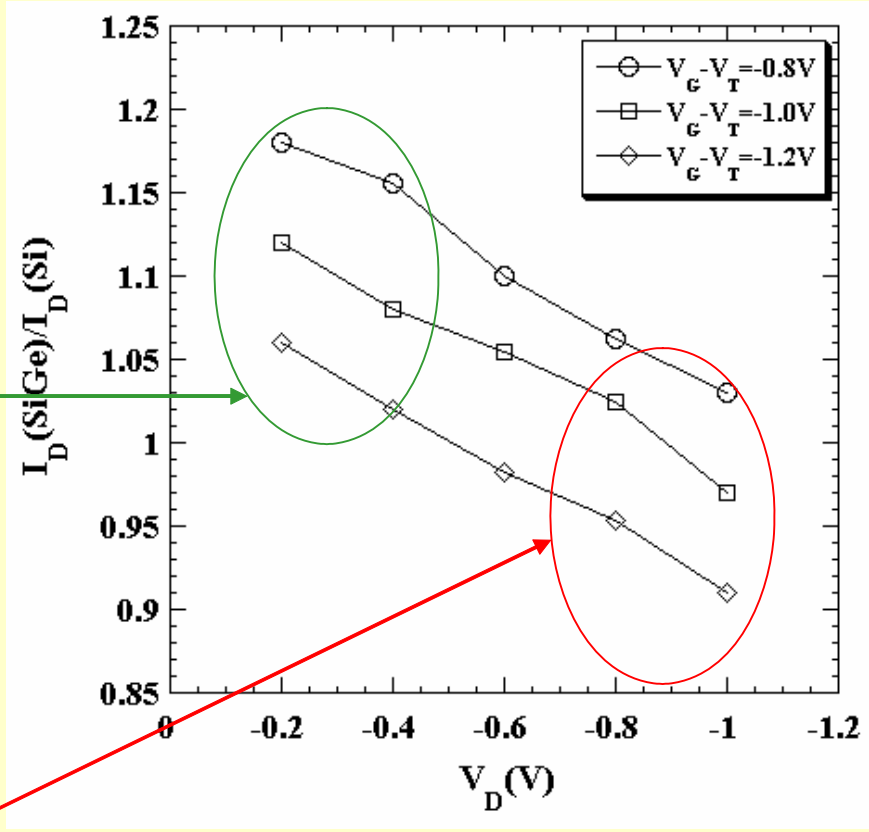
SCHRED was one of the first tools that was installed on PUNCH (nanoHUB) and is the most used non-comercial simulation module.



Modeling p-channel SiGe Devices

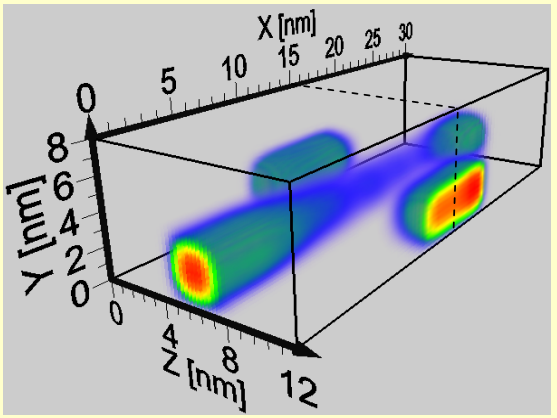
- We developed **the first** full-band self-consistent MC device simulator that takes both band-structure and quantum-mechanical size quantization effects into account.

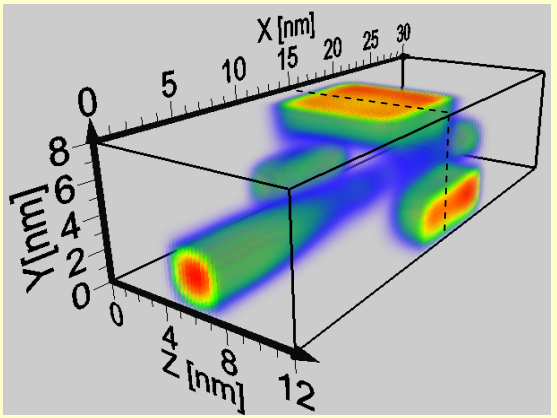
- We find that at **low applied bias there is an improved performance of *p*-channel strained SiGe devices due to the mobility enhancement**.
- The improvement becomes **degradation effect at high gate biases due to increased importance of surface-roughness and alloy disorder scattering**.

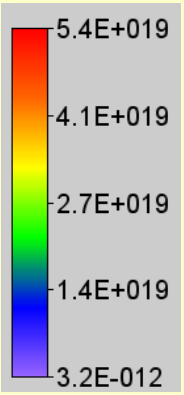


CBR – FinFET Simulation

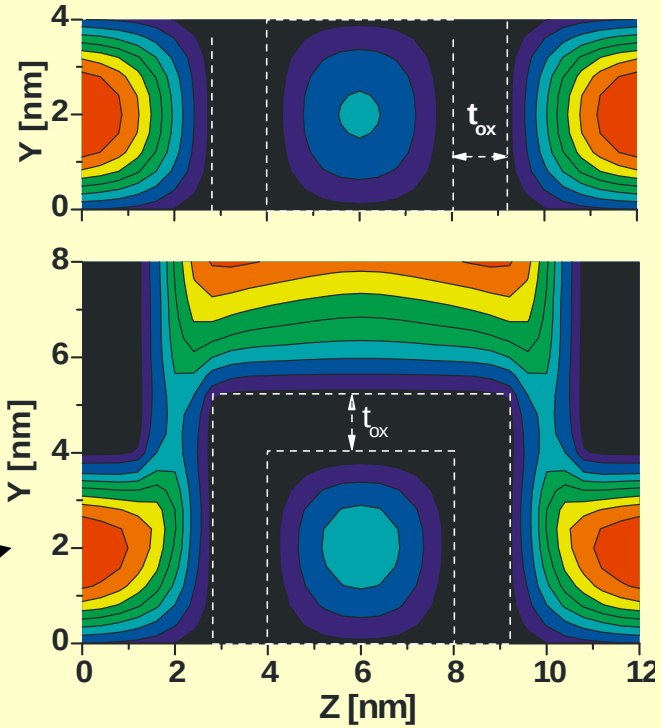
ELECTRON DENSITY: DG VS. TG





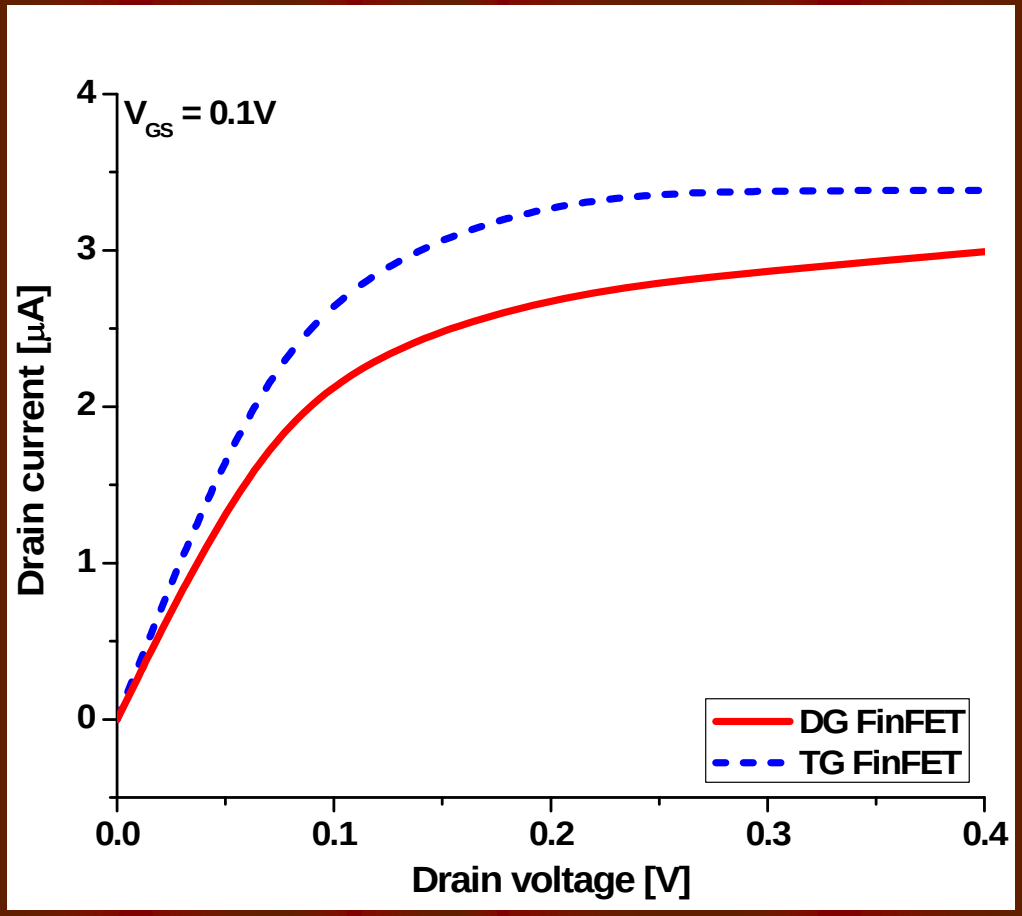


ON-state Electron density along the dotted line



V_{GS}=0.2, V_{DS}=0.4V

Electron density (TG) > electron density (DG)



- TG FinFET⇨ stronger control of gates ⇨pronounced saturation
- High output resistance compared to DG structure

Future Work

- On the semiclassical arena:
  - MC device simulator for modeling Solar Cells
  - Coupled MC simulators for electrons and phonons to model heating effects in nanoscale devices
- On the quantum arena:
  - Coupled 3DCBR and NEMO3D code for modeling quantum dot photodetectors and third generation quantum-dot solar cells
  - Extend 3DCBR to include magnetic domains and model spin currents.