NNCI Computation

Azad Naeemi
Georgia Institute of Technology
azad@gatech.edu

National Nanotechnology Coordinated Infrastructure

Objectives

- To facilitate access to the modeling and simulation capabilities and expertise
- To promote and facilitate the development of the new capabilities.
- To promote utilization of the computation resources.

https://www.nnci.net/computation-resources

nanoHUB.org and Silvaco Victory as a Backend

nanoHUB Modeling Tools

ab initio: ABINIT, SIESTA, ESPRESSO

MD: nanoMATERIALS (coarse grain MD)

bandstructure: Band Structure Lab, CNTbands (tight-binding)

Device / Transport:

Equilibrium: Schred Quantum Dot Lab

Non-Equilibrium:

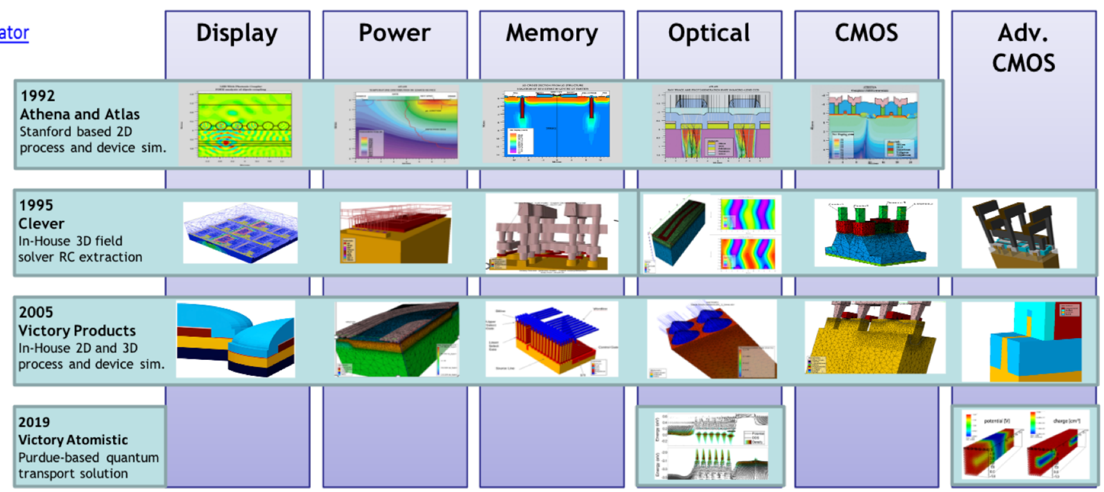
TCAD LAB (PADRE Drift-Diffusion)
nanoMOS (ballistic/mode space NEGF)
OMEN Nanowire (full-band/NEGF)
CNTFET Lab (ballistic/real-space NEGF)

Other:

Analytic Spin Precession Simulator
Nano Heatflow
CNIA (CNT interconnect)
Memristor

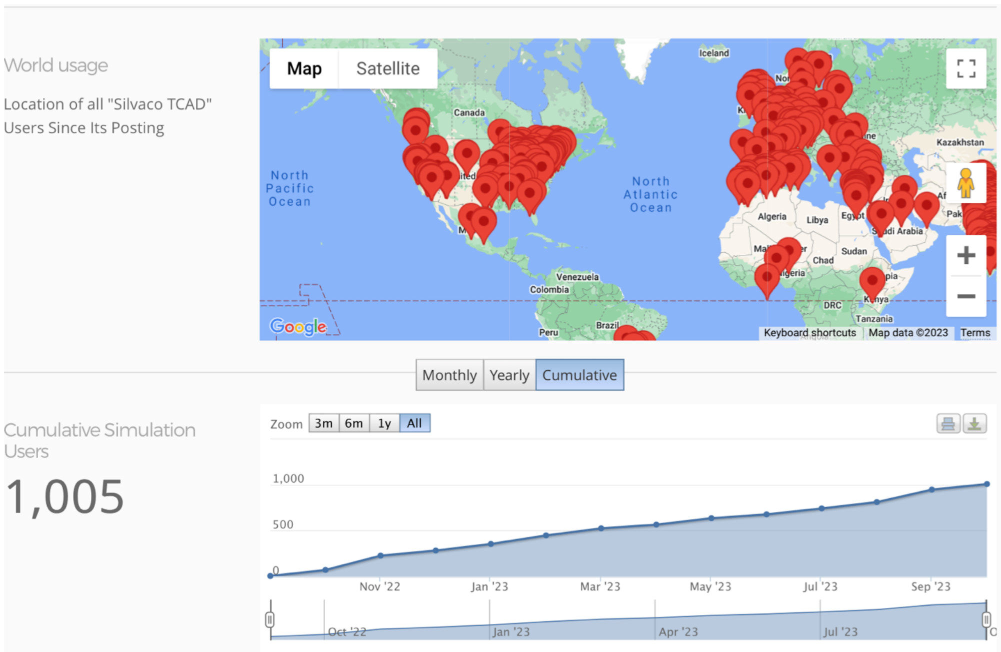
CKT: Spice3F4

Silvaco Modeling Tools



National Nanotechnology Coordinated Infrastructure

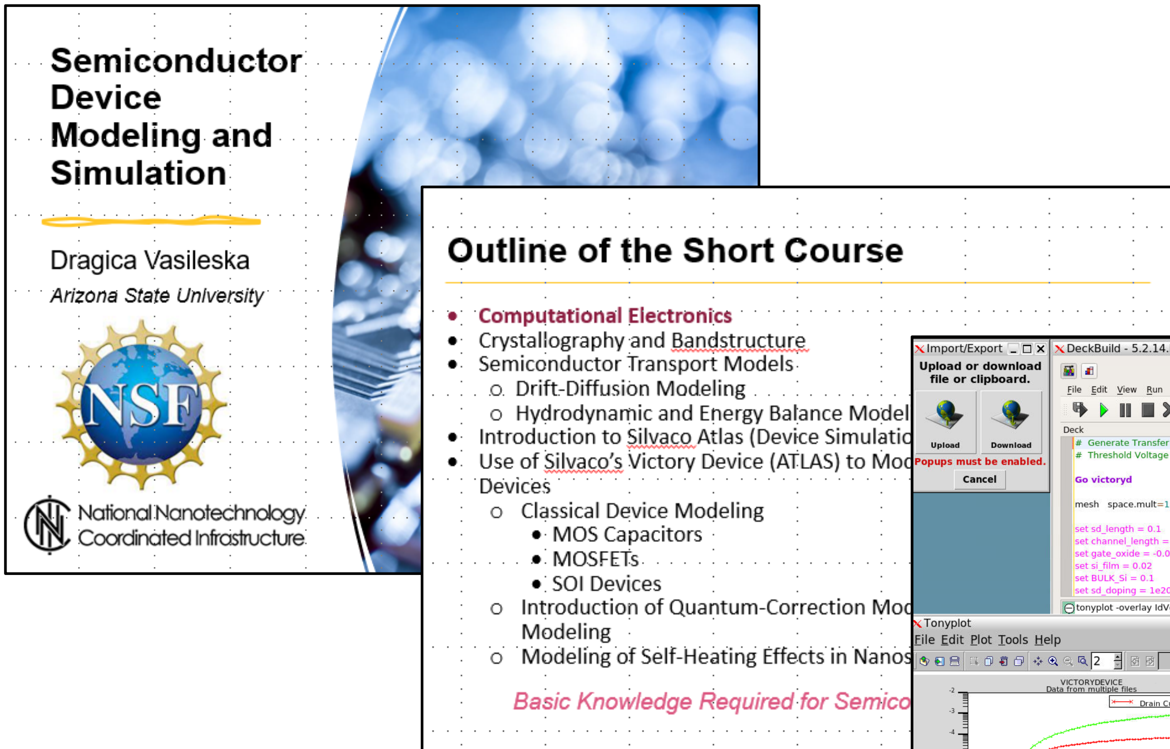
Silvaco TCAD Tool Usage

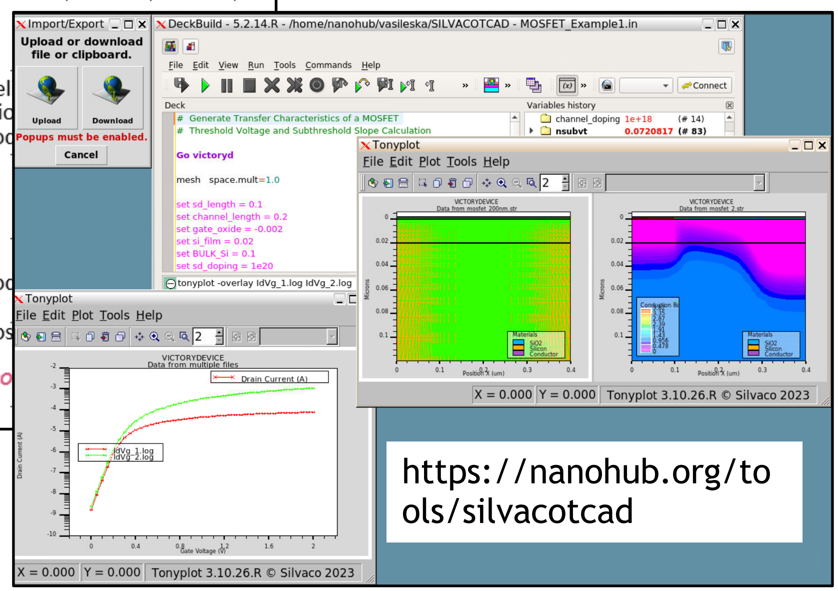


National Nanotechnology Coordinated Infrastructure

Short Course on Device Modeling and Simulation

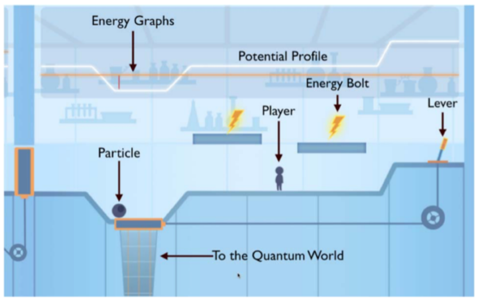
Short Course is in Production Stage!

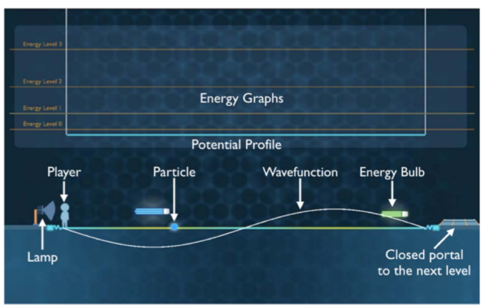




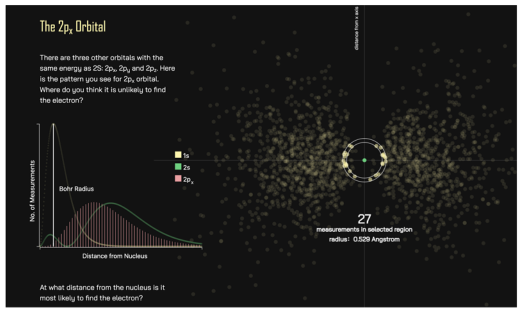
National Nanotechnology Coordinated Infrastructure

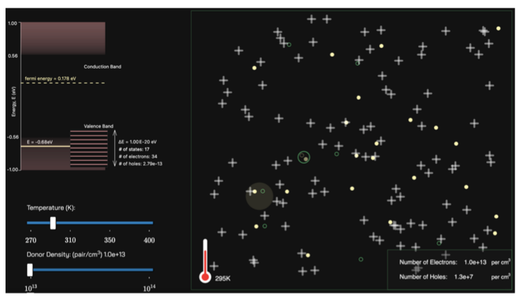
Immersive Virtual Worlds for Experiential Learning of Microelectronics



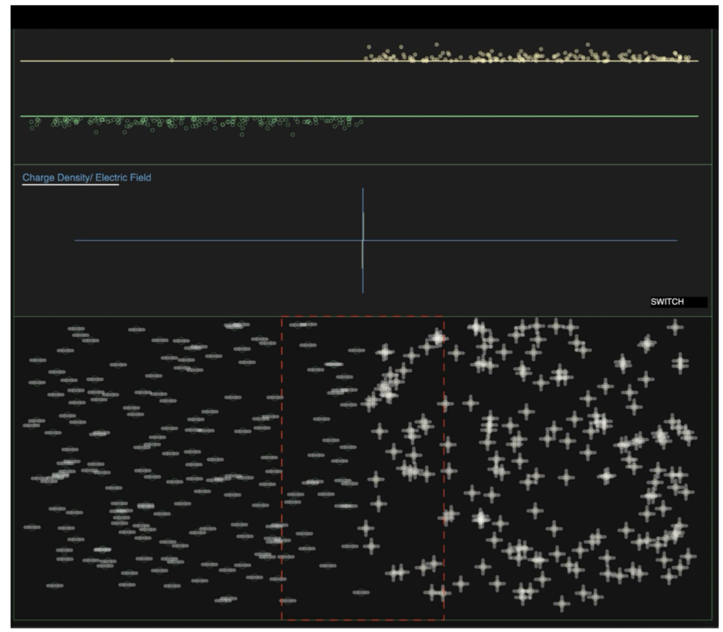


Immersive Games from Classic to Quantum Worlds





Interactive Visualizations from Hydrogen Atom to Carrier Statistics in Si



Interactive Visualizations and Virtual Reality for Semiconductor Devices (Under Development)

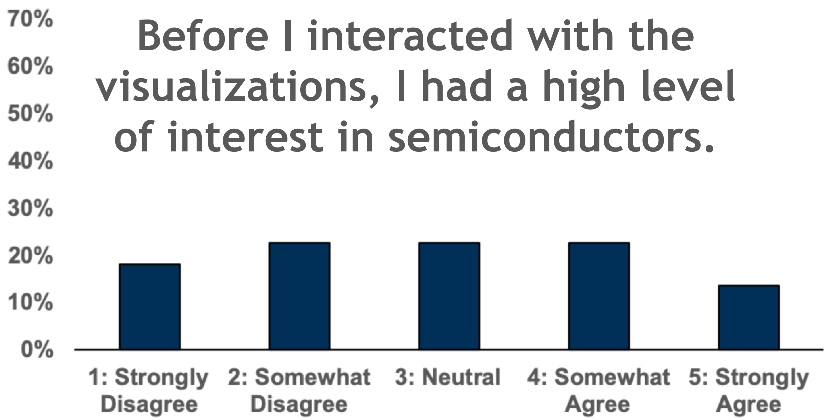
National Nanotechnology Coordinated Infrastructure

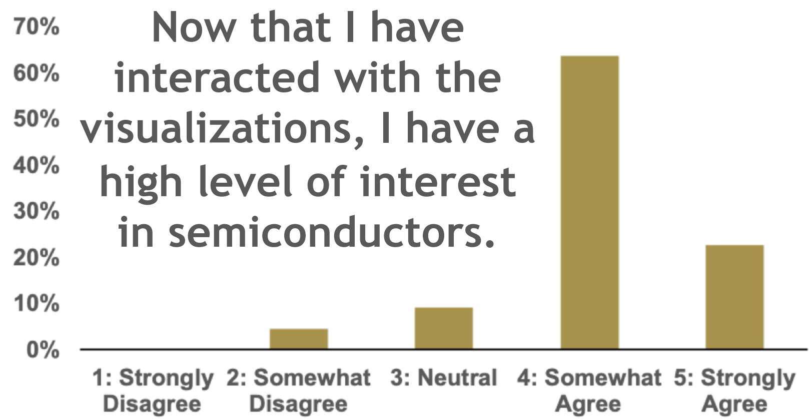
NSF

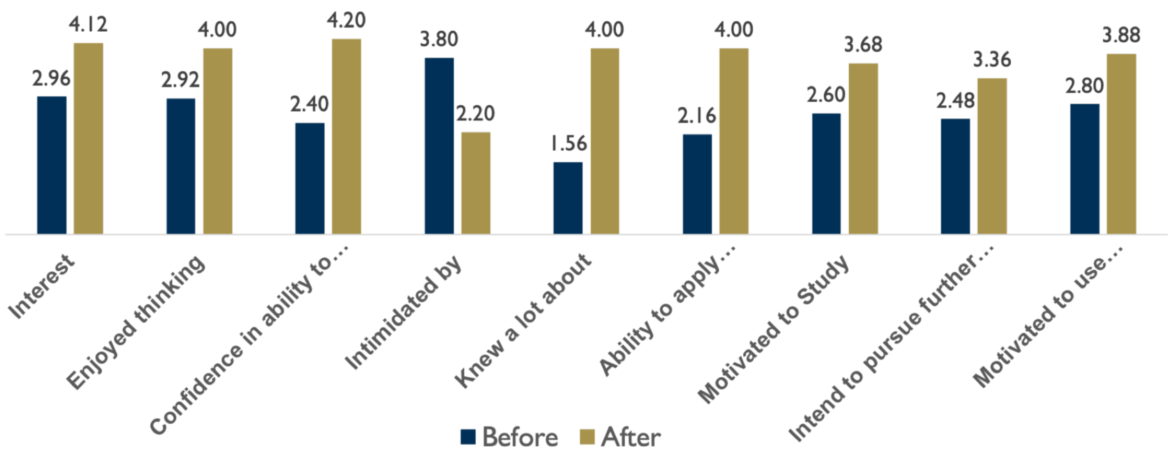
https://learnqm.gatech.edu

Georgia Tech

Significant Improvement in Students' Attitude



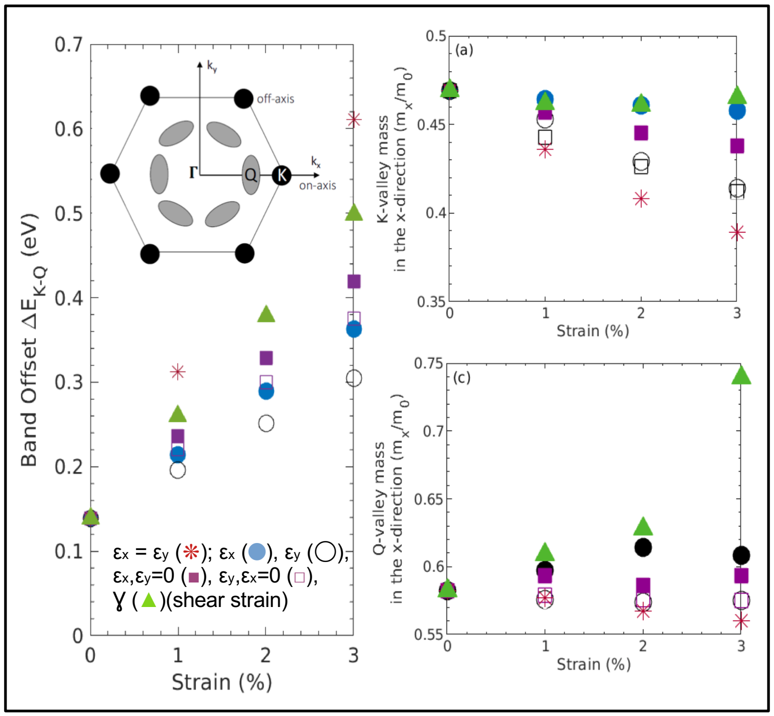




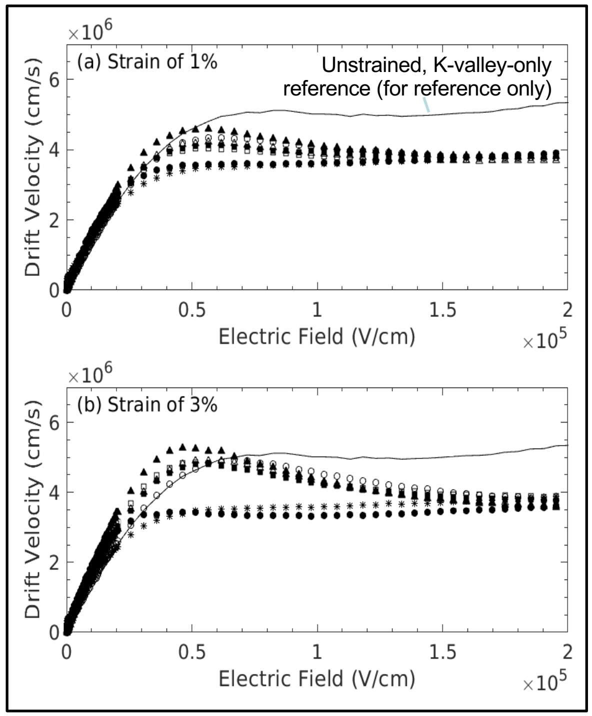
National Nanotechnology Coordinated Infrastructure

DFT Band Structure + Semiclassical Monte Carlo Based Study of Transport in Stained MoS_2

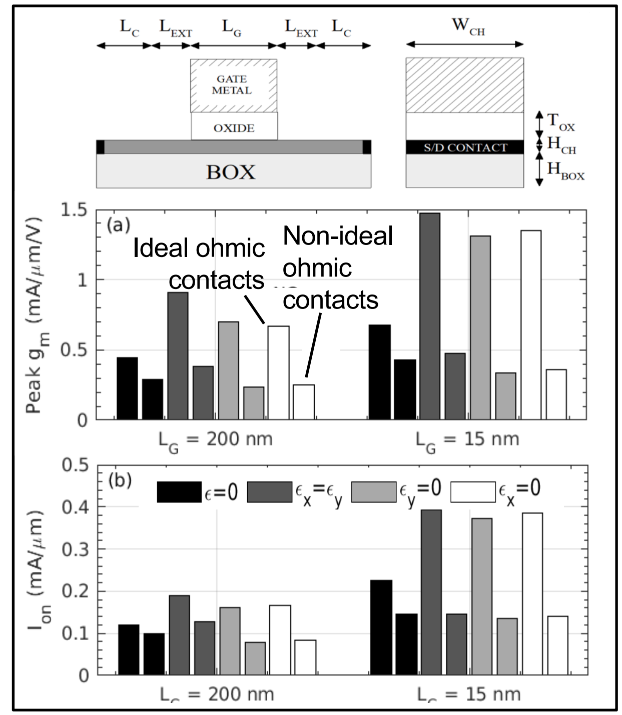
band structure



(2D) bulk transport



device performance



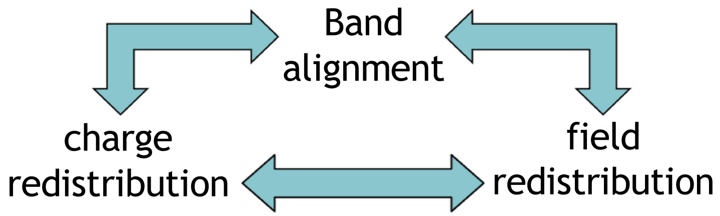
National Nanotechnology Coordinated Infrastructure

A.A. Bhatti, B.T. Archer, N. Navlakha, L.F. Register, S.K. Banerjee—UT-Austin

(to be published in Journal of Applied Physics with minor revisions)

Band Alignments in Equilibrium and under Externally Applied Electric Field and Strain

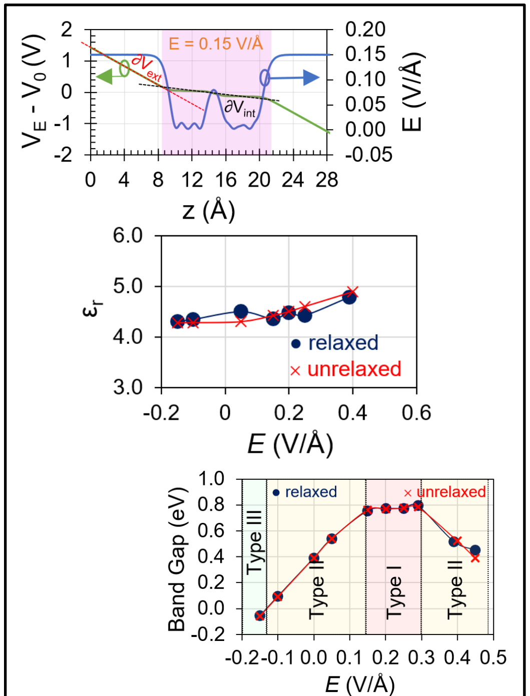
band alignment: BP/**various** TMDs



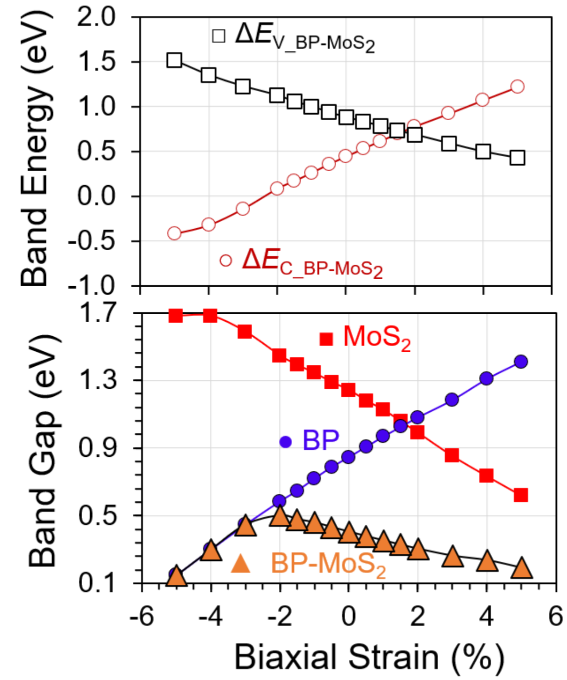
(Units of eV)		Electron Affinity Rule (based on isolated monolayers)					Simulated heterostructure (layer projected)						
Stack	Layer	E_c	E_v	ΔE_c	ΔE_v	E_g	E_c	E_v	ΔE_c	ΔE_v	E_g	$E_{g\,(Het)} - E_{g\,(EAR)}$	
MoS_2/BP	MoS_2	-4.79	-6.14	0.30	1.04	0.31	-4.74	-6.04	0.44	0.89	0.40	0.09	TYPE II
	BP	-4.49	-5.1				-4.30	-5.15					
$MoSe_2$/BP	$MoSe_2$	-4.16	-5.60	-0.17	0.36	0.92	-4.17	-5.61	-0.08	0.36	0.99	0.07	TYPE I
	BP	-4.33	-5.248				-4.26	-5.251					
WS_2/BP	WS_2	-4.43	-5.97	-0.08	0.86	0.61	-4.41	-5.95	-0.03	0.84	0.67	0.06	
	BP	-4.5	-5.111				-4.44	-5.114					
WSe_2/BP	WSe_2	-3.84	-5.38	-0.49	0.14	0.91	-3.87	-5.41	-0.40	0.17	0.98	0.07	
	BP	-4.33	-5.238				-4.26	-5.241					
HfS_2/BP	HfS_2	-6.09	-7.06	1.51	1.99	-1.01	-5.78	-6.74	0.7	1.07	-0.11	0.9	TYPE III
	BP	-4.59	-5.08				-5.09	-5.67					
$HfSe_2$/BP	$HfSe_2$	-5.70	-6.57	1.26	1.36	-0.49	-5.49	-6.29	0.82	0.81	-0.01	0.48	
	BP	-4.44	-5.21				-4.67	-5.48					

Completion of study begun during last reporting

BP/MoS_2 + electric field



BP/MoS_2 + strain



National Nanotechnology Coordinated Infrastructure

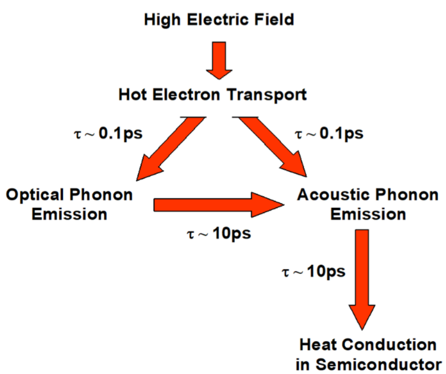
N. Navlakha, L.F. Register, S.K. Banerjee—UT-Austin

Modeling Self-Heating in Nanoscale Devices

$$\left(\frac{\partial}{\partial t}+v_e(\mathrm{k})\cdot\nabla_r+\frac{e}{\hbar}E(\mathrm{r})\cdot\nabla_k\right)f=\sum_{\mathrm{q}}\left\{W_{e,\mathrm{q}}^{\mathrm{k+q}\to\mathrm{k}}+W_{a,-\mathrm{q}}^{\mathrm{k+q}\to\mathrm{k}}-W_{e,-\mathrm{q}}^{\mathrm{k}\to\mathrm{k+q}}-W_{a,\mathrm{q}}^{\mathrm{k}\to\mathrm{k+q}}\right\}$$

$$\left(\frac{\partial}{\partial t}+v_p(q)\cdot\nabla_r\right)g=\sum_{\mathrm{k}}\left\{W_{e,\mathrm{q}}^{\mathrm{k+q}\to\mathrm{k}}-W_{a,\mathrm{q}}^{\mathrm{k}\to\mathrm{k+q}}\right\}+\left(\frac{\partial g}{\partial t}\right)_{p-p}$$

ASU Approach:
Energy Balance Model [1,2]

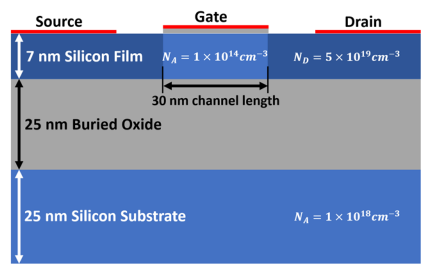


$$C_{LO}\frac{\partial T_{LO}}{\partial t}=\frac{3nk_B}{2}\left(\frac{T_e-T_L}{\tau_{e-LO}}\right)+\frac{nm^*v_d^2}{2\tau_{e-LO}}-C_{LO}\left(\frac{T_{LO}-T_A}{\tau_{LO-A}}\right),$$

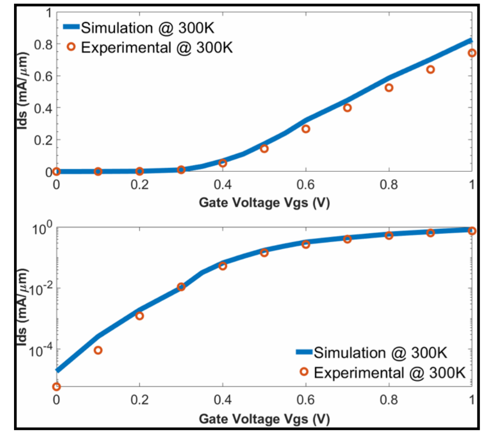
$$C_A\frac{\partial T_A}{\partial t}=\nabla\cdot\left(k_A\nabla T_A\right)+C_{LO}\left(\frac{T_{LO}-T_A}{\tau_{LO-A}}\right)+\frac{3nk_B}{2}\left(\frac{T_e-T_L}{\tau_{e-L}}\right).$$

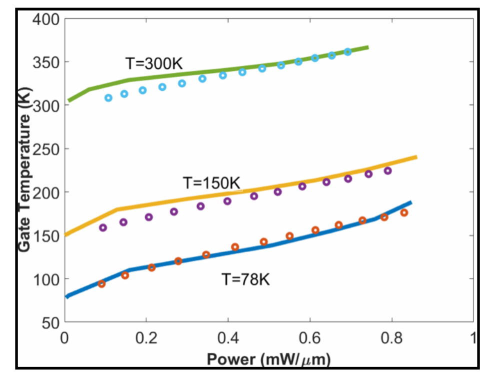
[1] J. Lai and A. Majumdar, "Concurrent thermal and electrical modeling of submicrometer silicon devices", J. Appl. Phys., Vol. 79, 7353 (1996).
[2] K. Raleva, D. Vasileska, S. M. Goodnick and M. Nedjalkov,"Modeling Thermal Effects in Nanodevices", IEEE Transactions on Electron Devices, vol. 55, issue 6, pp. 1306-1316, June 2008.

Model Validation



Simulation Results





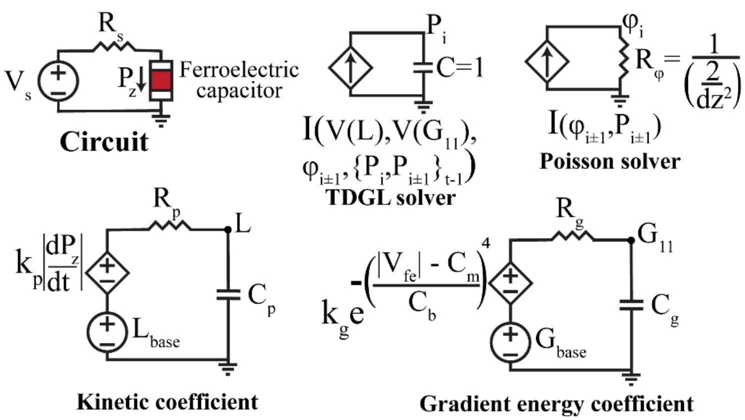
Experimental data:
M. Casse et al., "FDSOI for cryoCMOS electronics: device characterization towards compact model", IEDM (2022)

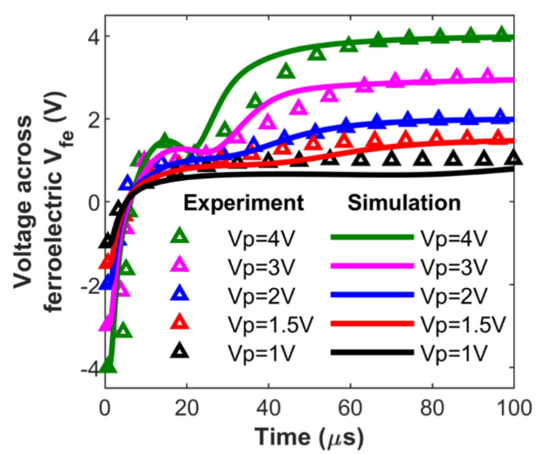
National Nanotechnology Coordinated Infrastructure

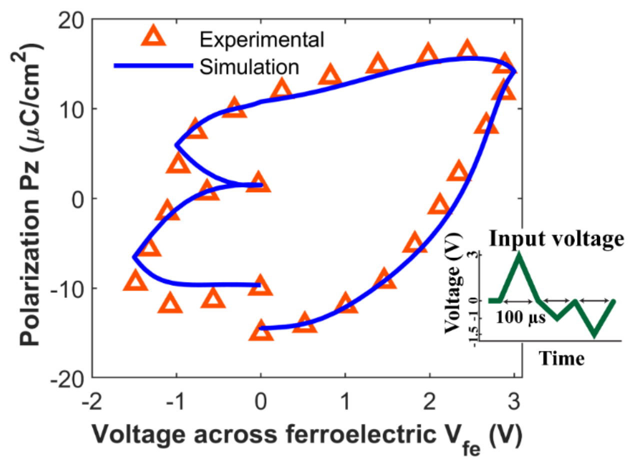
NSF

ASU

Ferroelectric Device Modeling Framework







Phase-Field Based Compact Models for FE Capacitors, IEEE-T-ED 2023

30,000X Speed up compared to prior phase-field simulations with no loss of accuracy.

Models to be released on nanoHub

National Nanotechnology Coordinated Infrastructure

Naeemi, GT

Computation Webinar Series

National Nanotechnology Coordinated Infrastructure

NNCI Webinar

February 15, 2023 | 4:00 p.m. - 5:00 p.m. ET

Antiferromagnetic Tunnel Junctions for Spintronics

Evgeny Tsymbal | Department of Physics and Astronomy, University of Nebraska-Lincoln

NNCI Computational Webinar

April 27, 2022 | 3PM - 4PM ET

Semiconductor Workforce Development through Immersive Simulations on nanoHUB.org

Gerhard Klimeck, Tanya Faltens, Daniel Mejia, Alejandro Strachan, Lynn Zentner, Michael Zentner*
Network for Computational Nanotechnology, Purdue University
*San Diego Supercomputing Center, UCSD

NNCI Computation Webinar

August 23, 2023 | 4:00 p.m. - 5:00 p.m. ET

Silvaco Technology CAD, Background, Overview, and Future

Eric Guichard | SVP and GM of TCAD, Silvaco, Inc.

National Nanotechnology Coordinated Infrastructure

NSF

https://www.youtube.com/channel/UCN1IaymO8KcA_fMEB1FhPgQ

Next Computation Webinar

National Nanotechnology Coordinated Infrastructure

NNCI Webinar

November 16, 2023 | 3:00 p.m. - 4:00 p.m. ET

Particle Based Simulation of Weidebandgap Devices

Stephen Goodnick | Department of Electrical Engineering at Arizona State University