

NNCI Computation

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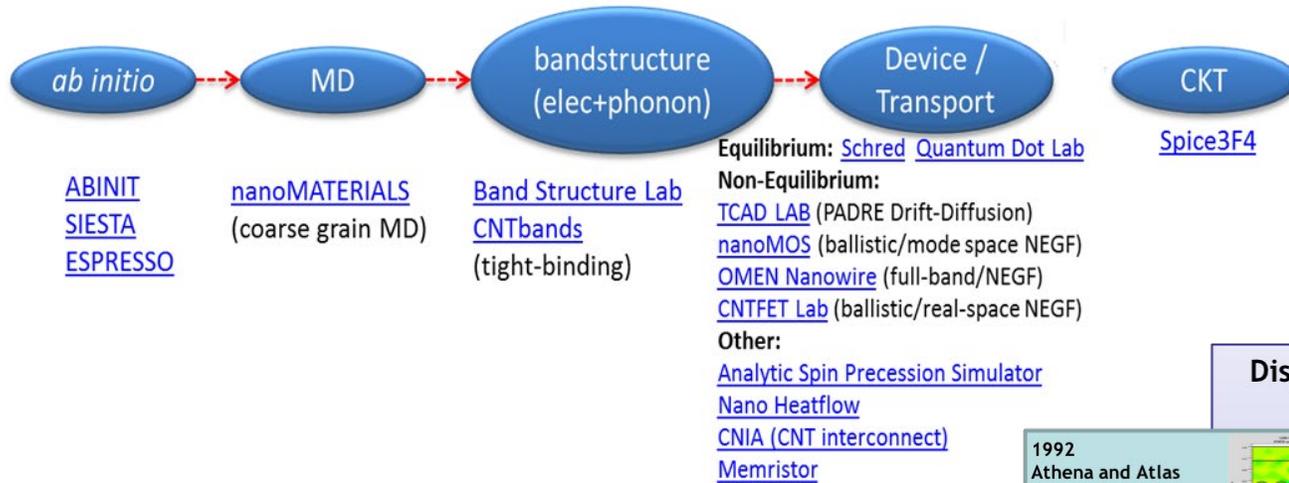
Objectives

- 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



Professor Vasileska's contribution in this new initiative:

- Educational materials for Silvaco Victory usage (ppt's and videos)
- Sample problems regarding device simulation ranging from low to room temperatures

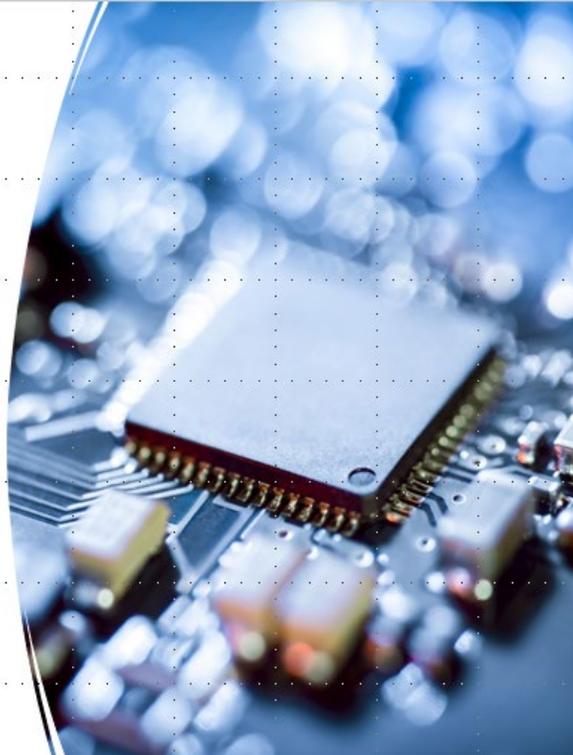
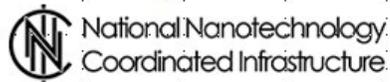
Silvaco Modeling Tools

	Display	Power	Memory	Optical	CMOS	Adv. CMOS
1992 Athena and Atlas Stanford based 2D process and device sim.						
1995 Clever In-House 3D field solver RC extraction						
2005 Victory Products In-House 2D and 3D process and device sim.						
2019 Victory Atomistic Purdue-based quantum transport solution						

Short Course Developed – Needs Voicing only

Semiconductor Device Modeling and Simulation

Dragica Vasileska
Arizona State University



Lectures
Quizzes
Short Projects

Outline of the Short Course

- **Computational Electronics**
- Crystallography and Bandstructure
- Semiconductor Transport Models
 - Drift-Diffusion Modeling
 - Hydrodynamic and Energy Balance Modeling
- Introduction to Silvaco Atlas (Device Simulation Platform)
- Use of Silvaco's Victory Device (ATLAS) to Modeling of Si-Based Devices
 - Classical Device Modeling
 - MOS Capacitors
 - MOSFETs
 - SOI Devices
 - Introduction of Quantum-Correction Models to Classical Device Modeling
 - Modeling of Self-Heating Effects in Nanoscale Devices

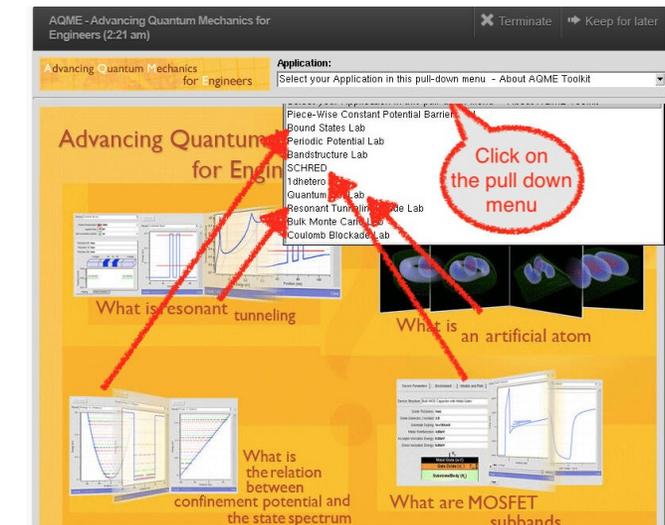
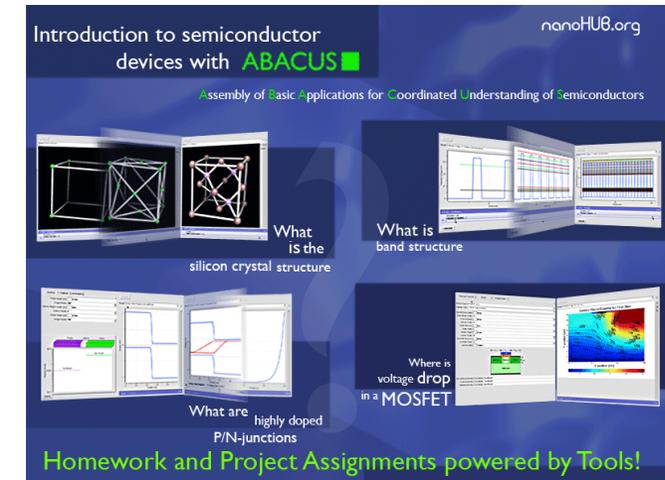
Basic Knowledge Required for Semiconductor Devices

Tool-Based Curricula

- New paradigms of learning are necessary for training students in the vibrant and constantly changing field of nanoelectronics.
- Prof. Vasileska (ASU) and Prof. Klimeck (Purdue) proposed a novel methodology:

Tool-based curricula

- Tool-based curricula consists of assembling a set of computational simulation tools with:
 - demos on how to use the tools,
 - the objectives of the tool and what can be learned with them,
 - assembly of solved problems,
 - homework assignments, and
 - challenge problems which are related to real world applications.



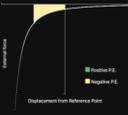
Immersive Virtual Worlds for Learning Semiconductor Physics

CHAPTER 1
Hydrogen Atom



The classical and quantum mechanical models of a Hydrogen atom, 1S, 2S, 2Px, 2Py, and 2Pz Orbitals

CHAPTER 2
Electron Energy



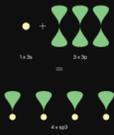
The potential and kinetic energies of an electron in a Hydrogen atom in classical and quantum mechanical models.

CHAPTER 3
Hydrogen Molecule



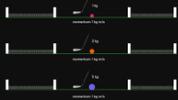
Bonding between two Hydrogen atoms and the formation of a Hydrogen molecule.

CHAPTER 4
Hybridization of Atomic Orbitals in Silicon



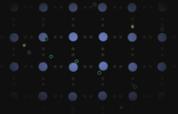
Hybridization of S and P orbitals in a Si Crystal, Valence and Conduction bands.

CHAPTER 5
Effective Mass of Electrons in Crystals



The relationship between kinetic energy and momentum in classical physics and for an electron in a crystal.

CHAPTER 6
Charge Carriers in Silicon Lattice



Electrons and Holes in different energy states influence conduction.

CHAPTER 7
Electric Field in Silicon Lattice



See how electrons and holes respond to the effects of an electric field.

CHAPTER 8
Generation and Recombination



See how electron and hole populations change with time and temperature.

CHAPTER 9
Doping



Doping is the process of adding impurities to an intrinsic semiconductor.

CHAPTER 10
Carrier Statistics



Observe how doping effect probability of electrons in band diagram.

CHAPTER 11
Drift Current



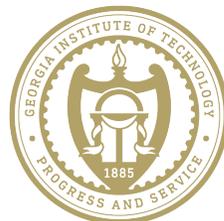
Observe how Electron random walk changed when applied electric field.

CHAPTER 12
Band Bending



Observe how an electric field bends the band diagram and follow electrons and holes on the band diagram as they get accelerated and scattered.

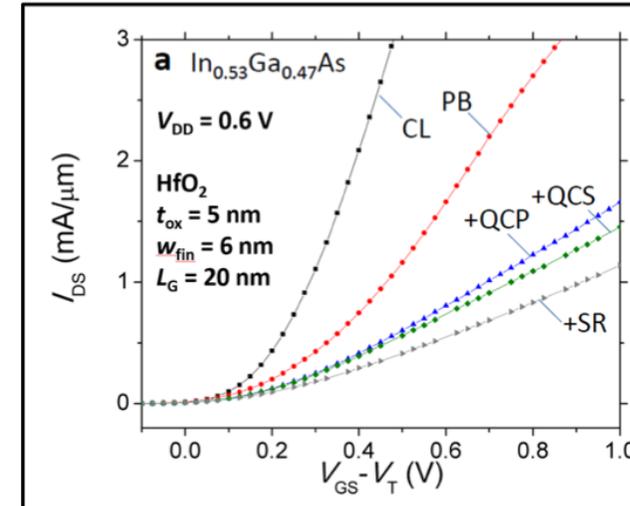
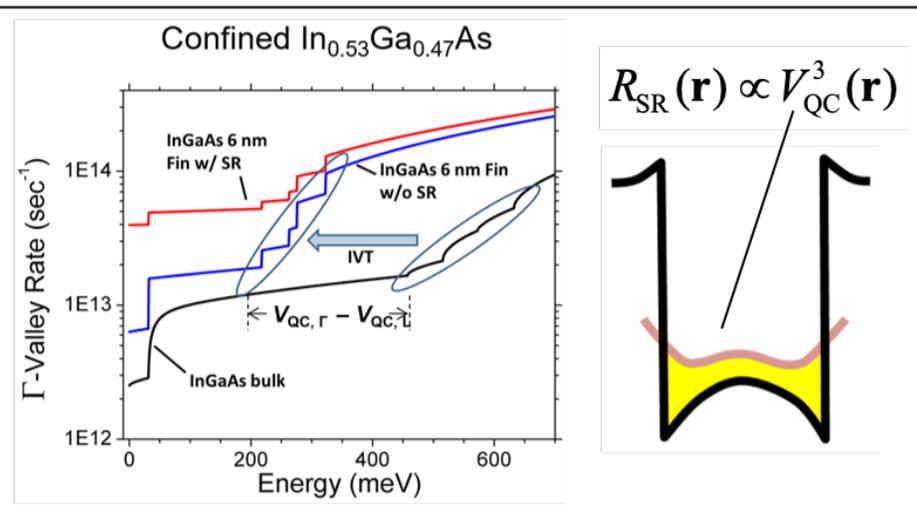
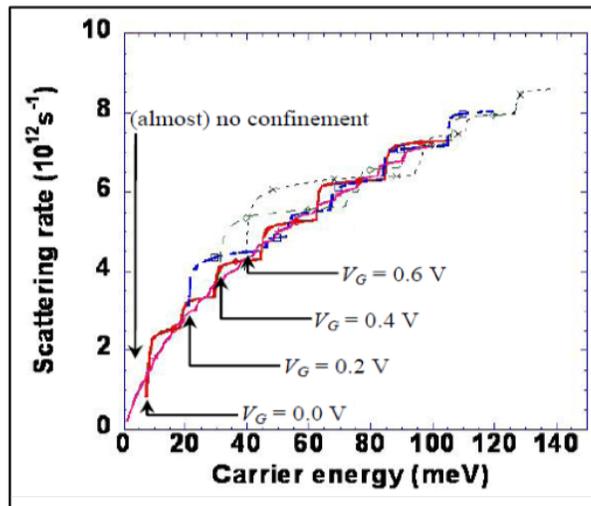
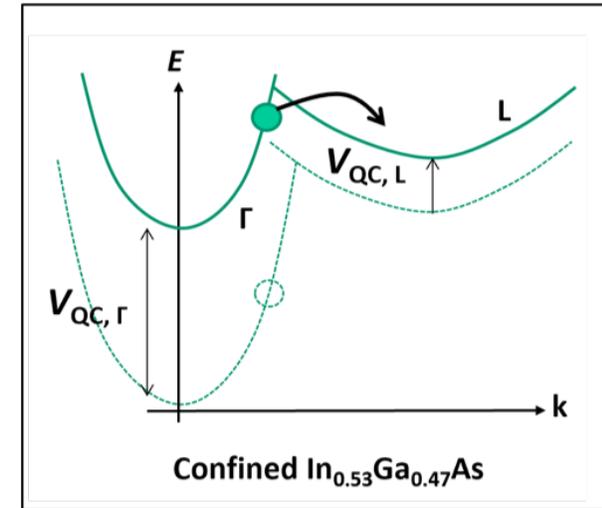
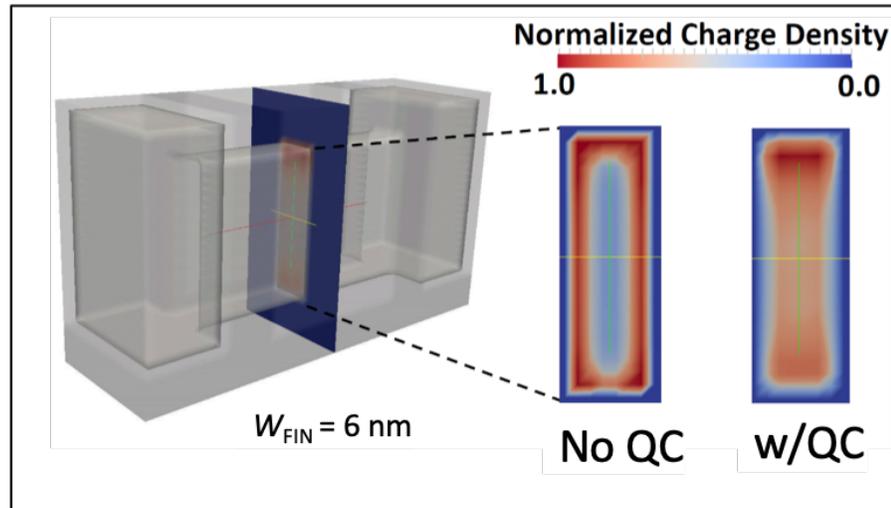
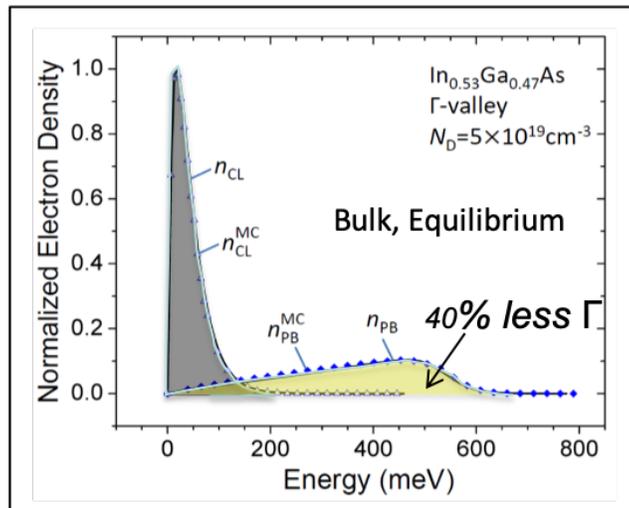
<https://learnqm.gatech.edu>



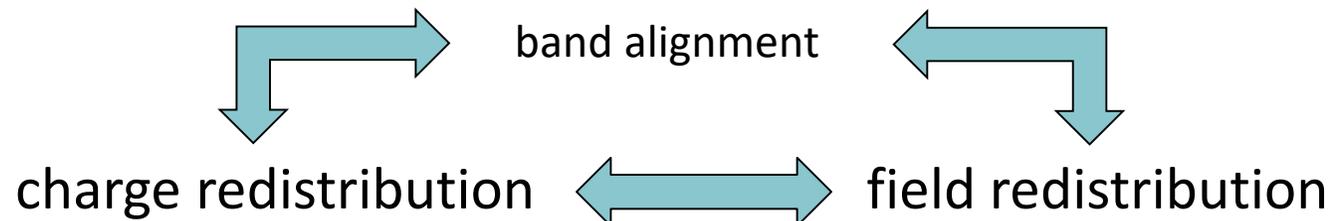
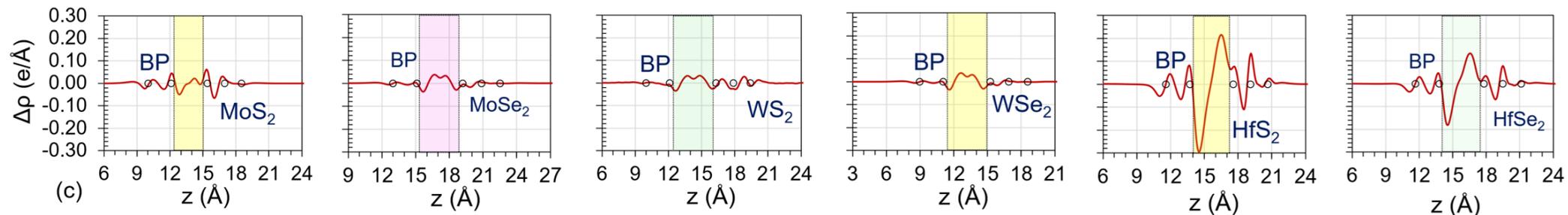
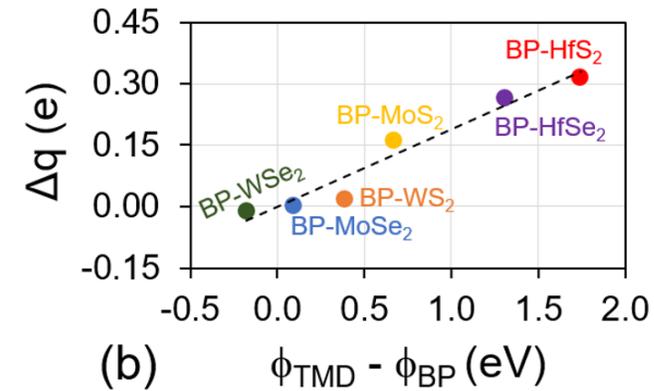
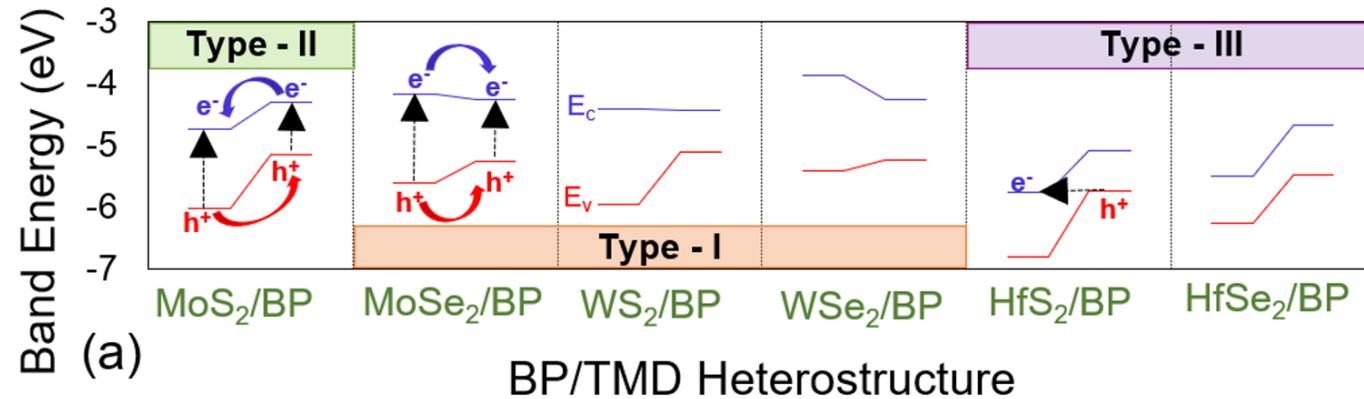
2022 SSSC Inaugural James D. Meindl Innovators Award



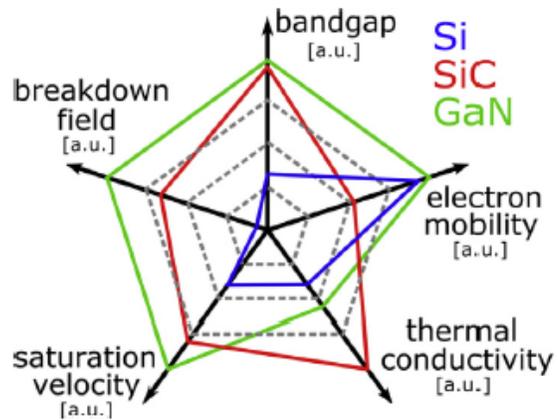
Impact of Quantum Confinement in Ultra-Scaled Devices



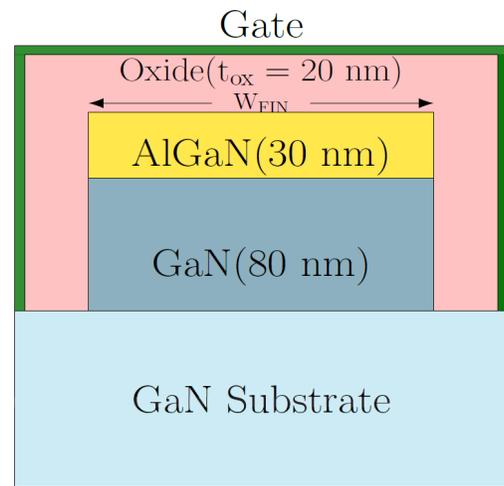
Band Alignment in BP/TMD Heterostructures vs. Electron Affinity Rule



Device Simulation – GaN MISFETs

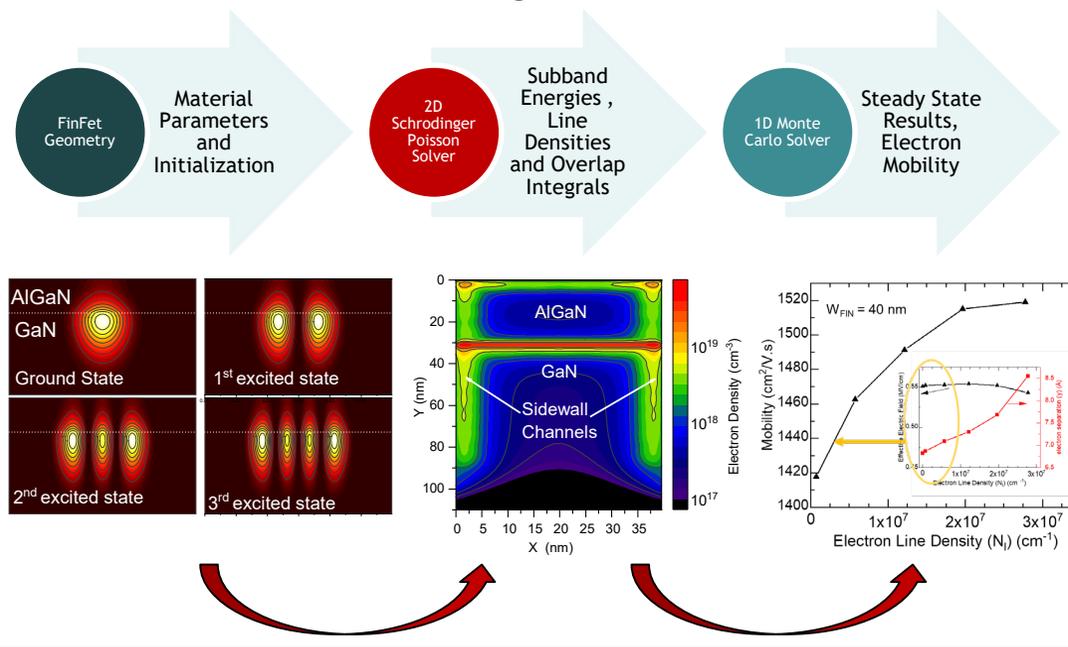


- High electron mobility and saturation drift velocity compared to SiC → *RF device applications*.
- Wide bandgap and a high breakdown field lead to high reverse blocking capability → *power device applications*.



GaN MISFET for RF applications

3D Poisson-2D Schrödinger-1D Monte Carlo Solver



Modeling @ GT (Ferroelectrics, Antiferromagnets, Multiferroics, Magnets & their Heterojunctions)

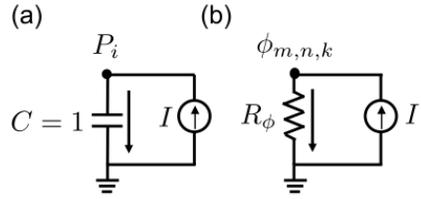
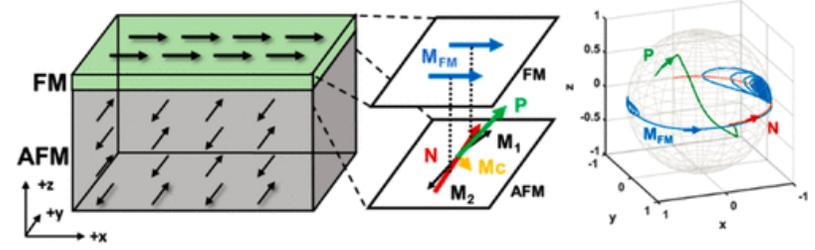
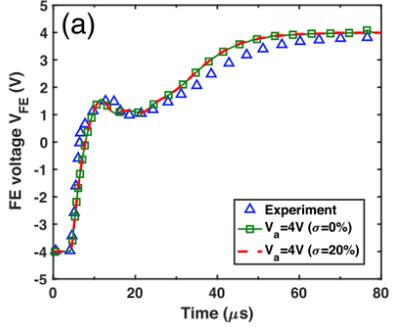
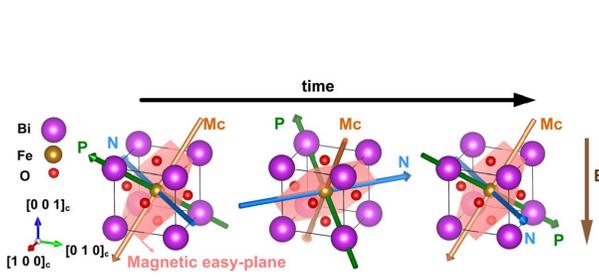


Fig. 1. SPICE equivalent circuit diagrams of (a) TDGL equation, when $i = 1, 2, 3$. (b) Poisson's equation.



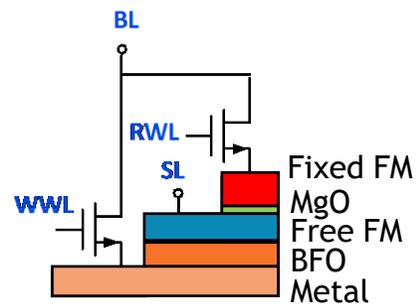
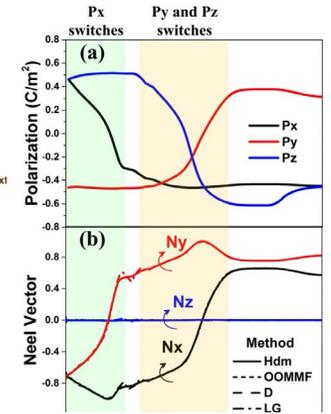
Dynamic Response of BFO/CoFe Heterostructure
 Nano Letters, 2020

Physics-Based Circuit Models for Phase-Field FE Simulations IEEE-Trans. Electron Devices, 2020

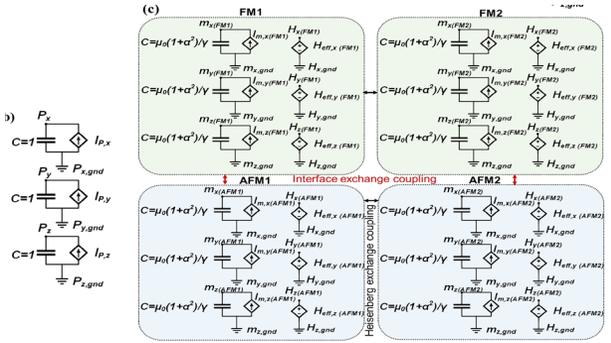


Magnetization Dynamics of a Single-Domain BiFeO₃ Nanoisland

IEEE-Trans. Magnetism, 2020



Magnetoelectric MRAM



SPICE-compatible compact models

IEEE-TED 2021, IEEE JXCDC 2021

SPICE Subcircuits publicly available:
<https://doi.org/10.1109/JXCDC.2022.3143130>

Computation Webinar Series

NNCI Seminar Series
PLEASE NOTE NEW DATE
May 5, 2021 | 4PM - 5PM EDT

COMPUTATION TALK: SIMULATION SOFTWARE NEXT DOOR

Abstract: Advancement in technology is propelling the growth of the semiconductor industry like never before. Semiconductor trends that drive growth within the industry include the introduction of the 5G technology, the increased demand for Artificial Intelligence (AI) chips and AI applications, and Internet of Things (IoT). With more advanced IoT products within the market, starting from industrial automation systems to connected devices powered by semiconductors, IoT is about to supply diversified possibilities to semiconductor organizations.

In this talk, I will present a summary of the available simulation methodologies and products that can be useful to the NNCI community. In particular, I will focus on the capabilities of TCAD tools (such as Silvaco Victory, Synopsys Sentaurus, Comsol, etc.), tools available free of charge on nanohub.org, and few examples of in-house simulation tools that have not yet been adopted by the TCAD community.

Dragica Vasileska
Professor | Electrical Engineering
Arizona State University

Access the Event @ | <https://tinyurl.com/NNCISeminarVasileska>

NNCI Seminar Series
June 23, 2021 | 4PM - 5PM EDT

COMPUTATION TALK: A CASE STUDY OF ESSENTIAL PHYSICS AND TECHNOLOGY CHALLENGES AS REVEALED THROUGH MODELING: QUANTUM-CORRECTED SEMICLASSICAL MONTE CARLO SCALING STUDY OF Si, Ge, AND INGAAs FINFETS

Abstract: This presentation will address material options, channel orientations, contact geometries, and the effects of scaling on n-channel FinFETs. However, the emphasize will be on the role and requirements of modeling and what we can learn from it in a complex system as much or more so than the system itself. How prior knowledge of possible essential physics in the system(s) of interest informs the model choice—a quantum-corrected semiclassical Monte Carlo method in this case—and how the model integrates that essential physics to produce perhaps unexpected results will be considered.

Prof. Leonard F. Register
Dept. of Electrical and
Computer Engineering
University of Texas at Austin

Access the Event @ | <https://tinyurl.com/NNCISeminarRegister>

WWW.NNCI.NET

 National Nanotechnology
Coordinated Infrastructure

NNCI Computation Webinar
November 10, 2021 | 4PM - 5PM ET

THE EVOLUTION OF PROCESS TCAD IN SEMICONDUCTOR R&D AND MANUFACTURING

Shela Aboud, Ph.D. | Sr. Product Marketing Manager, Synopsys



 National Nanotechnology
Coordinated Infrastructure

NNCI Webinar: Education and Computation
August 31, 2022 | 4:00 p.m. - 5:00 p.m. ET

VIRTUAL IMMERSIVE WORLDS FOR EXPERIENTIAL LEARNING OF QUANTUM AND SEMICONDUCTOR PHYSICS

Professor Azad Naeemi | School of Electrical and Computer Engineering, Georgia Tech

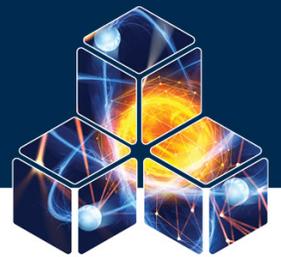


 National Nanotechnology
Coordinated Infrastructure

NNCI Webinar: Education and Computation
September 28, 2022 | 4:00 p.m. - 5:00 p.m. ET

THEORETICAL EXPLORATION OF ENERGY EFFICIENT SPINTRONICS DEVICES

**Professor Tony Low | Department of Electrical and Computer Engineering
University of Minnesota**



Looking Ahead

- The goal is to promote wider use of process and device simulation tools.
- Work closely with Prof. Vasileska (NCI-SW) and Prof. Register (TNF).
- Offer “Device and Process Simulation Course” developed by Prof. Vasileska at the network level.
- Invited e-seminars on various modeling and simulation topics:
 - Simulation approaches for various research areas
 - Emerging modeling and simulation trends
 - Examples of collaborations among theorists and experimentalists
- Promote and help public release of internally developed modeling/simulation tools.

Example: Drift Velocity and Band Bending

