NNCI Computation

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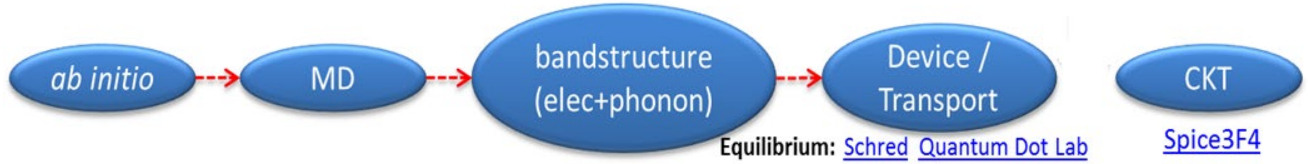
Objectives

- 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

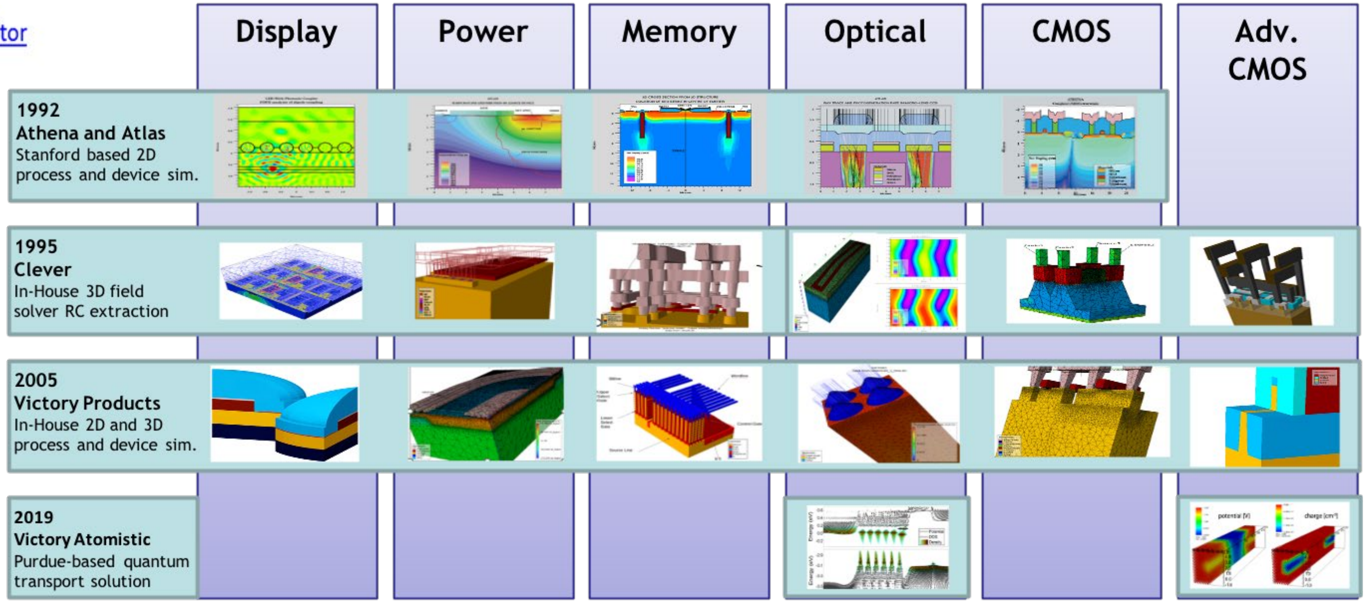
nanoHUB.org and Silvaco Victory as a Backend

nanoHUB Modeling Tools



- 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



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

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Short Course Developed – Needs Voicing only

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

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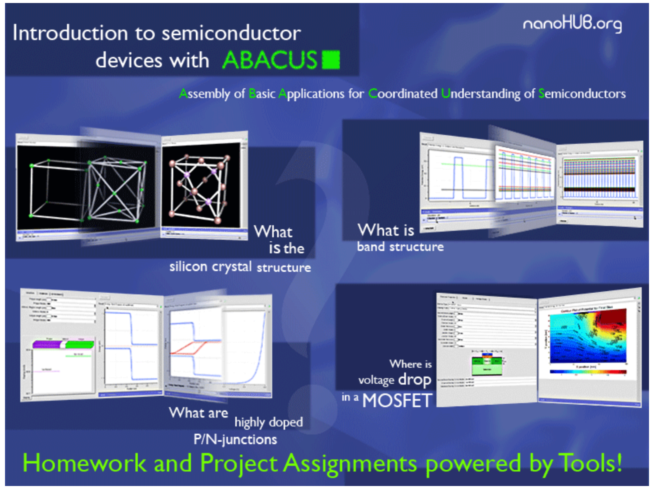
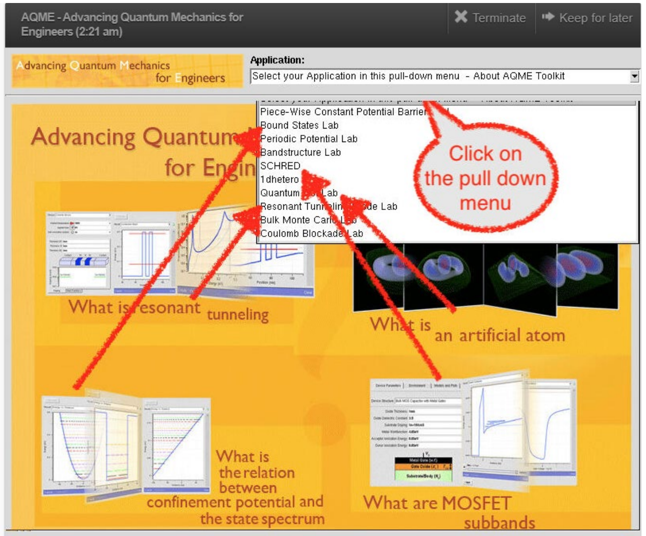
Tool-Based Curricula

- 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:

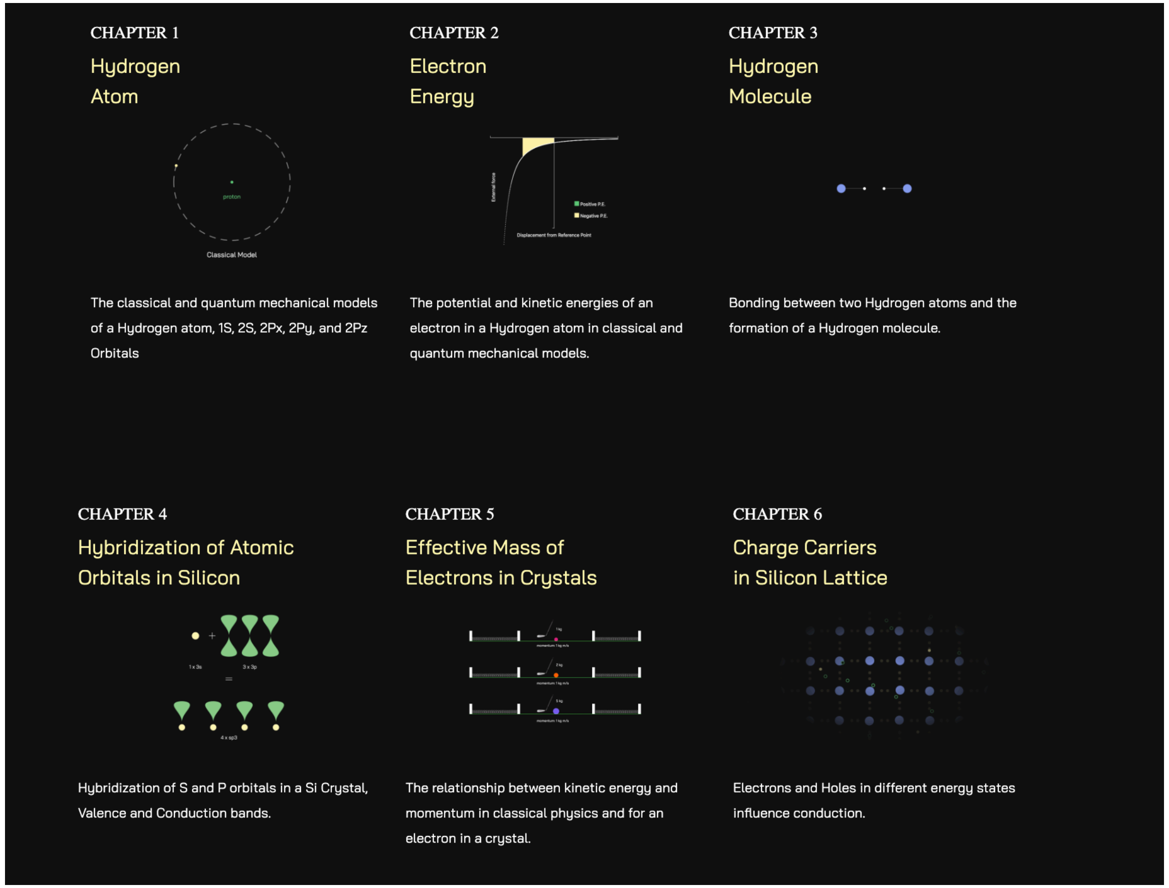
Tool-based curricula

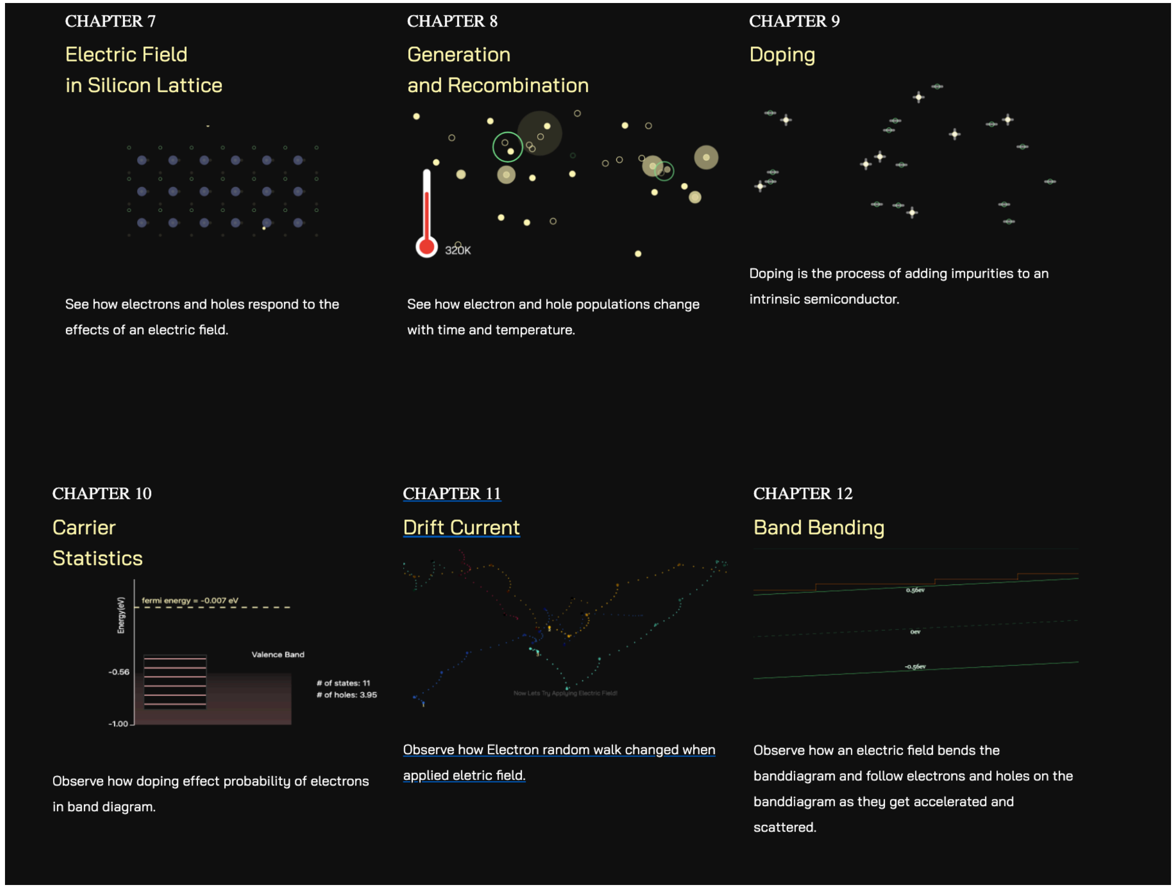
- Tool-based curricula consists of assembling a set of computational simulation tools with:
  - demos on how to use the tools,
  - the objectives of the tool and what can be learned with them,
  - assembly of solved problems,
  - homework assignments, and
  - challenge problems which are related to real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





Immersive Virtual Worlds for Learning Semiconductor Physics





https://learnqm.gatech.edu

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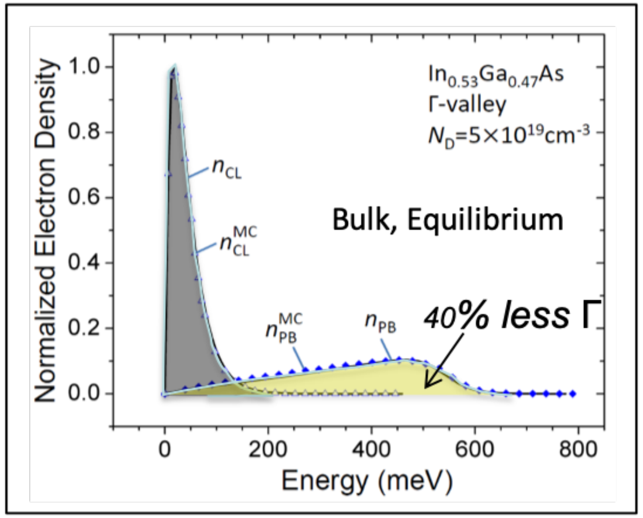
Georgia Institute of Technology 1885 Progress and Service

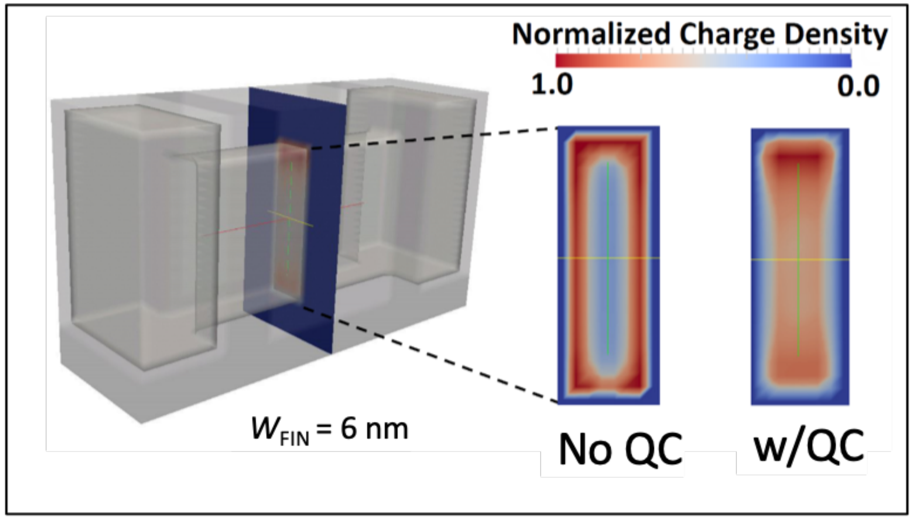
IEEE SSCS Solid-State Circuits Society™ IC Innovation

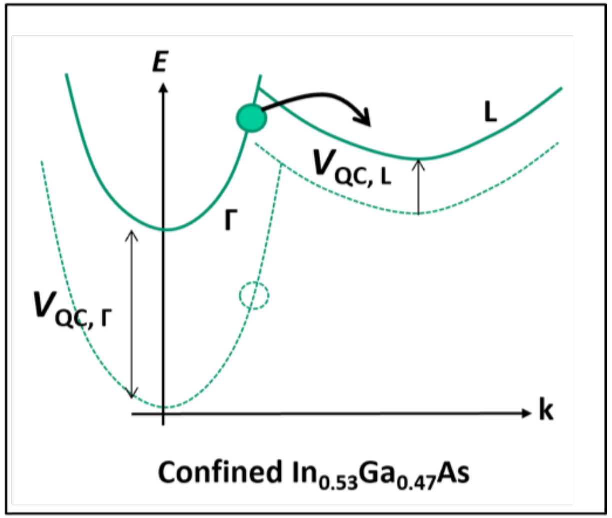
2022 SSCS Inaugural James D. Meindl Innovators Award

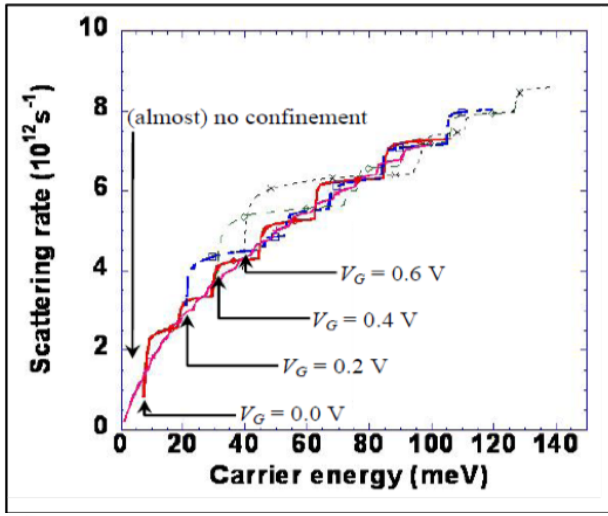
SRC®

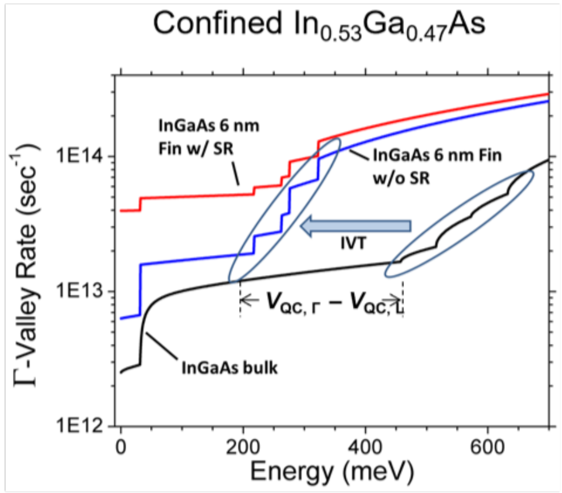
Impact of Quantum Confinement in Ultra-Scaled Devices

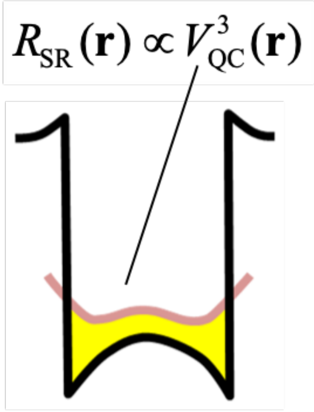


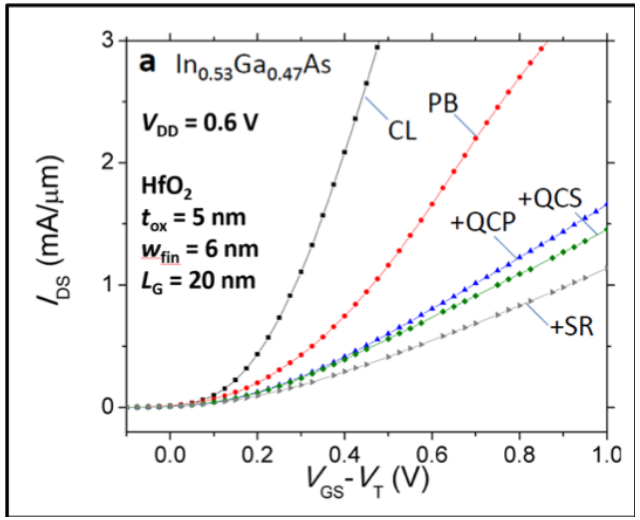




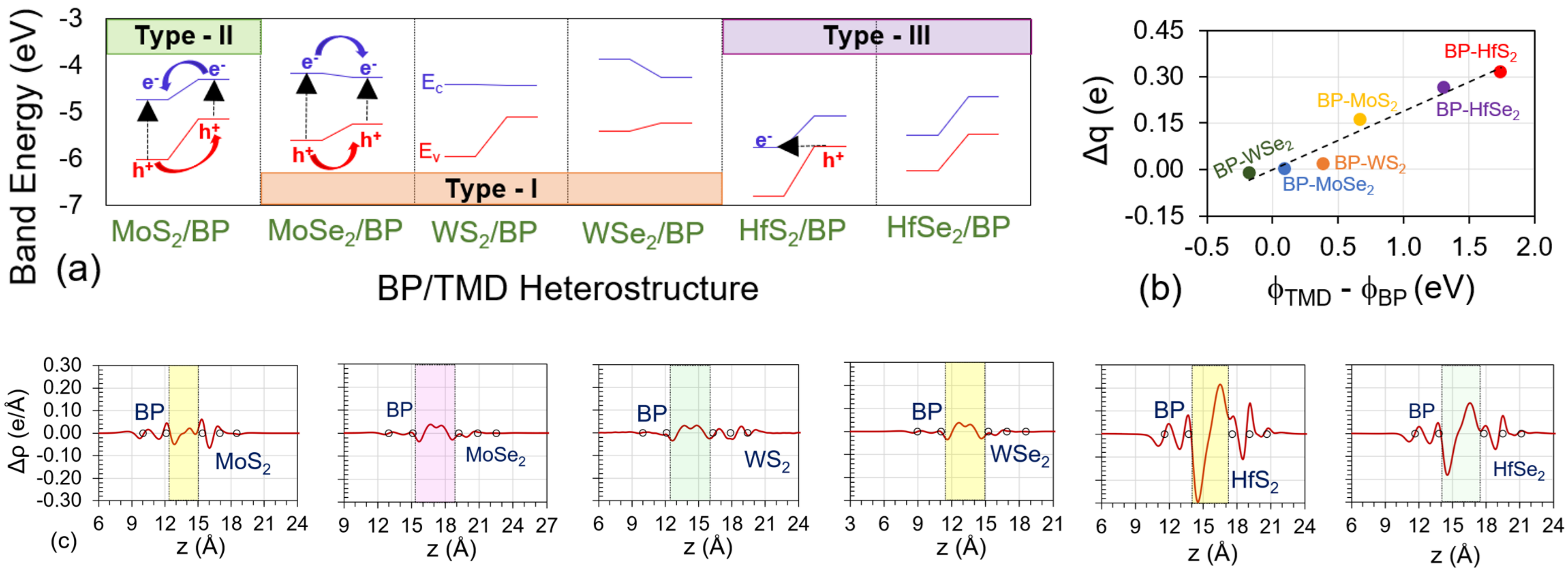








Band Alignment in BP/TMD Heterostructures vs. Electron Affinity Rule



band alignment

charge redistribution ⟷ field redistribution

NNCI, B. Archer, <u>N. Navlakha</u>, L F Register, S.K. Banjerjee

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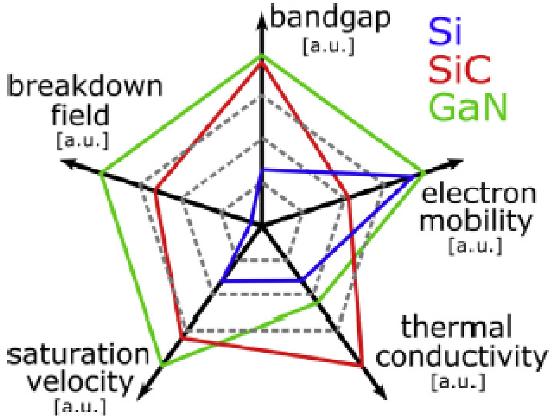
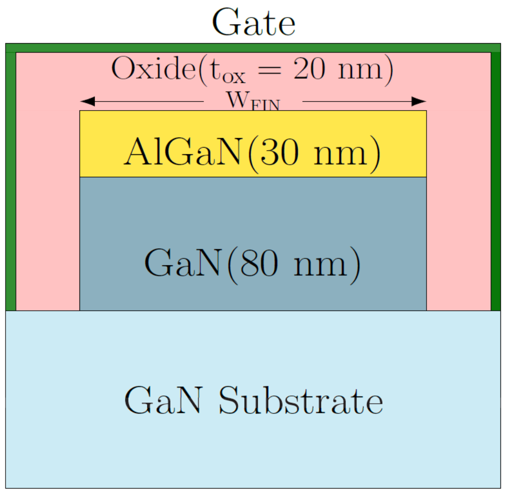
Device Simulation – GaN MISFETs

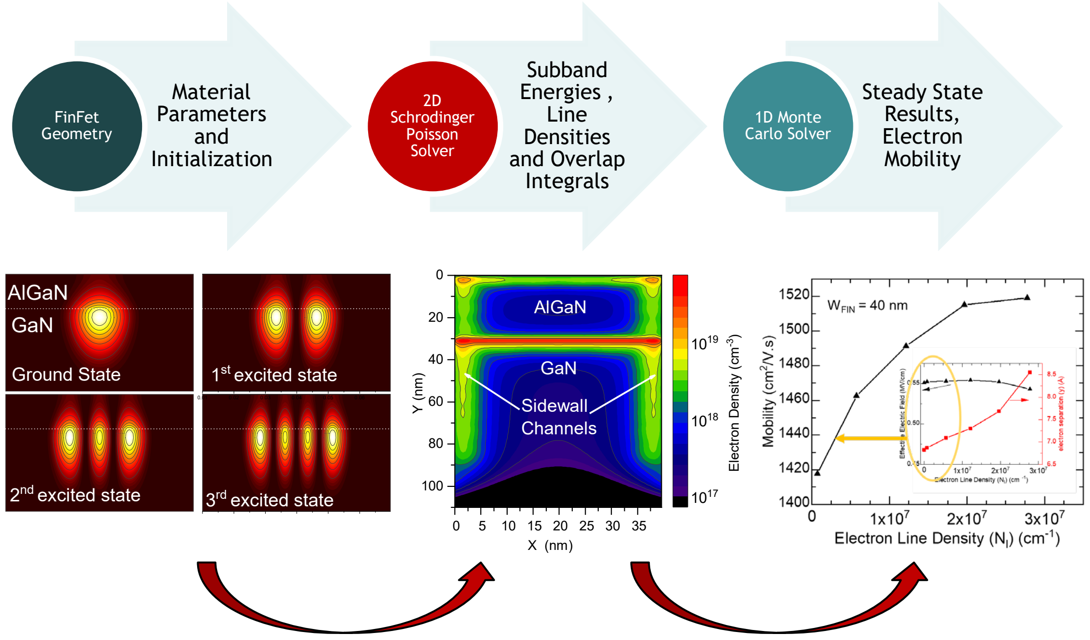


- High electron mobility and saturation drift velocity compared to SiC ➔ *RF device applications*.
- Wide bandgap and a high breakdown field lead to high reverse blocking capability ➔ *power device applications*.



GaN MISFET for RF applications

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



Naveen Kumar, Pranay Baikadi, Dragica Vasileska, Michael Povolotskyi, in *Proceedings of IWCN 2021*, p. 103-104.

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

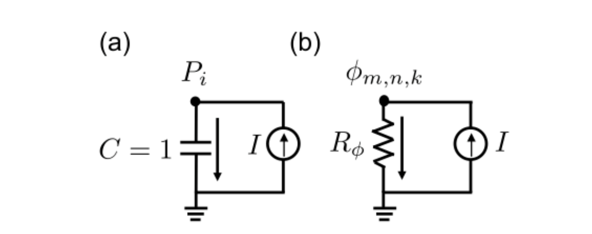
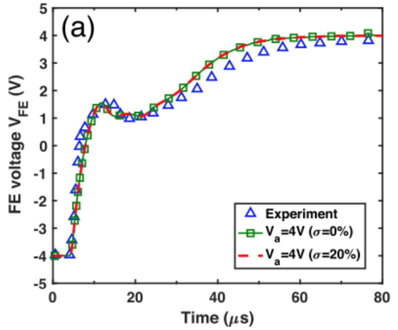
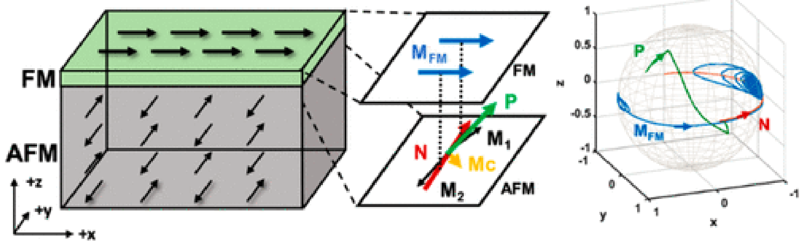


Fig. 1. SPICE equivalent circuit diagrams of (a) TDGL equation, wher
$i = 1, 2, 3$. (b) Poisson's equation.



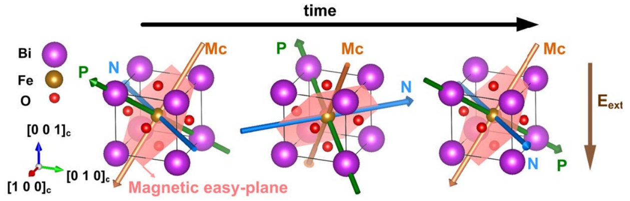
Physics-Based Circuit Models for Phase-Field FE Simulations

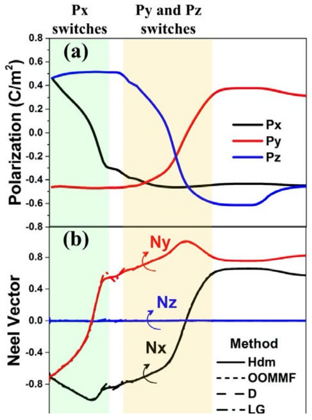
IEEE-Trans. Electron Devices, 2020



Dynamic Response of BFO/CoFe Heterostructure

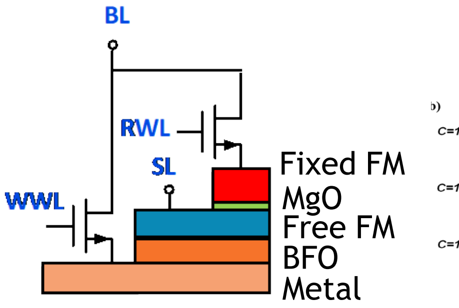
Nano Letters, 2020



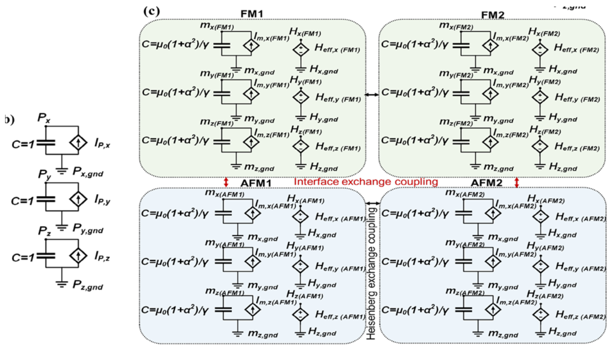


Magnetization Dynamics of a Single-Domain BiFeO3 Nanoisland

IEEE-Trans. Magnetism, 2020



Magnetoelectric MRAM



SPICE-compatible compact models

IEEE-TED 2021, IEEE JXCDC 2021

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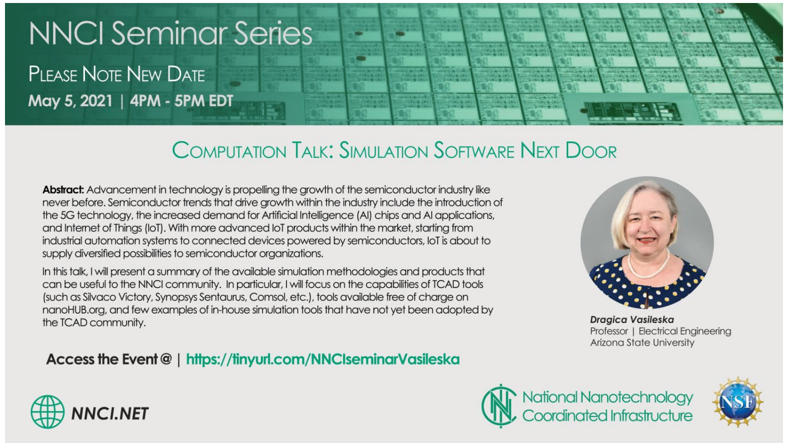
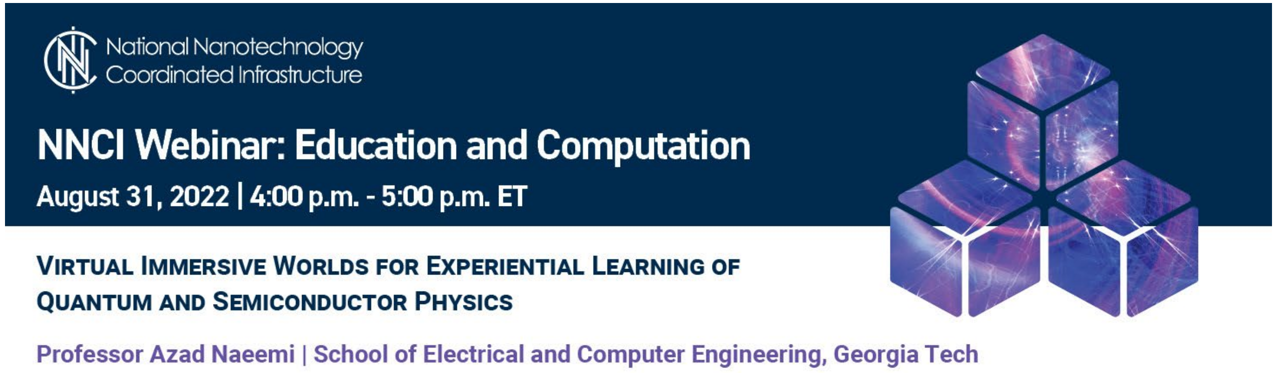
SPICE Subcircuits publicly available:
https://doi.org/10.1109/JXCDC.2022.3143130

Computation Webinar Series





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

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

https://learnqm.gatech.edu/Semiconductor-Physics-Visualization/index.html