NNCI Computation

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Objectives

- To facilitate access to the modeling and simulation capabilities and expertise
- To identify the strategic areas for growth
- To promote and facilitate the development of the new capabilities.

An inventory of available modeling and simulation resources and expertise has been complied and is posted on nanoHub.org.

8 supercomputers or major computing clusters are available in various sites.

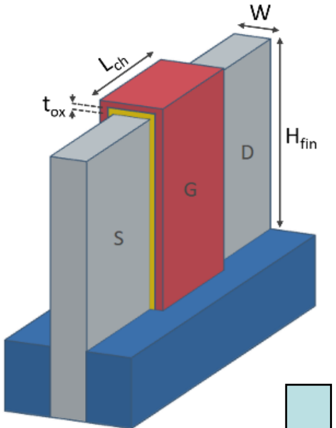
https://www.nnci.net/computation-resources

Computation @ NCI-SW (Porf. Dragica Vasileska)

- Research efforts:
  - **Low-power Silicon FinFET's:** Ballistic effects, Multi-Gate Granularity (MGG) and Hot-Carrier Degradation (HCD)
  - **High-power GaN MISFETs:** Low-Field Mobility Characterization

- Educational Activities:
  - Development of a **Short Course** on Device and Process Modeling using TCAD Tools.
    - *The short-course will have the format as the ones deployed on nanoHUB – U.*
  - Deployment of simulation software and educational material on nanoHUB.org

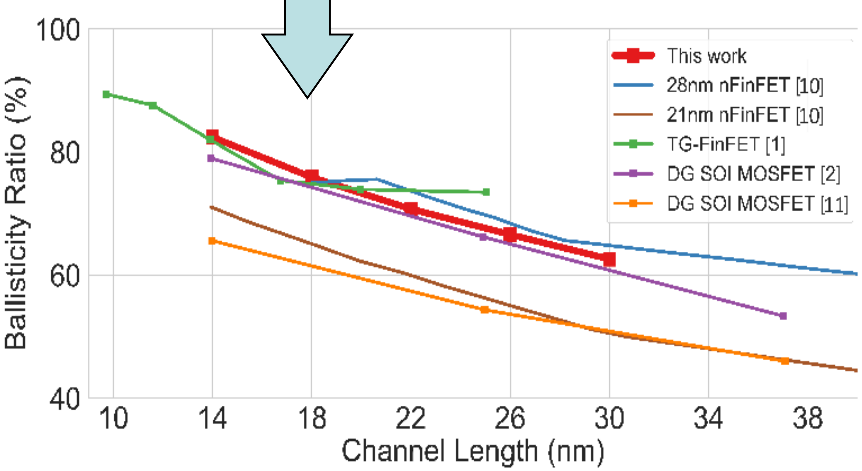
Device Simulation – Silicon FinFETs

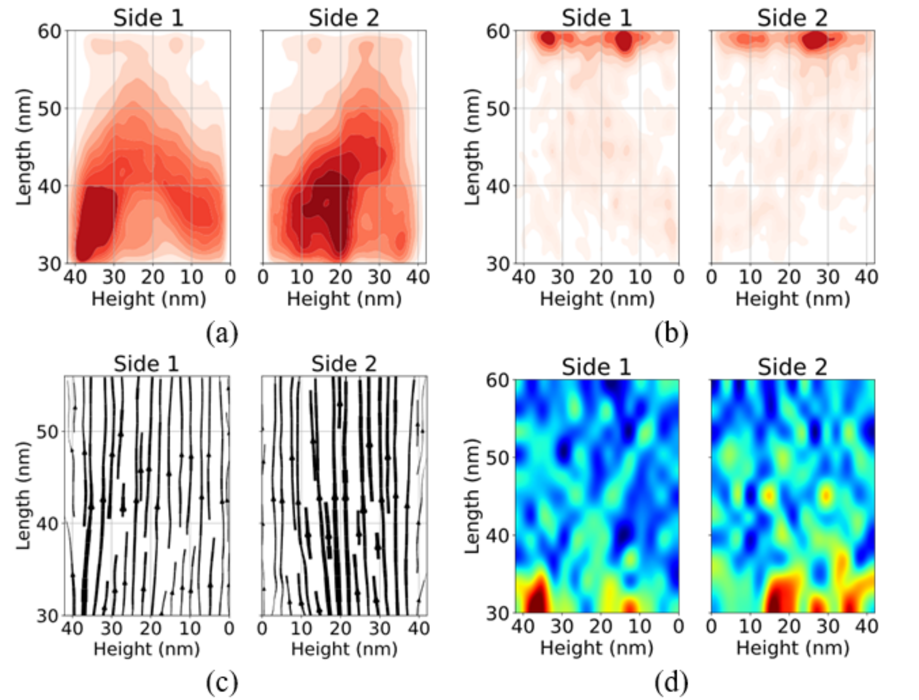


Metal Gate Granularity

Hot Carrier Degradation

Ballistic Transport





Evaluating MGG impact on the carriers' interaction with $Si\text{-}SiO_2$ interface through the evaluation of the KDE for the electrons that have energy above (a) 0.25 eV and (b) 1.25 eV, on percolation paths (c), and on a charged trap impact on the drain current according to its location in the $Si\text{-}SiO_2$ interface (d). In all cases, the left and right figures depict the two side channels of the FinFET device.

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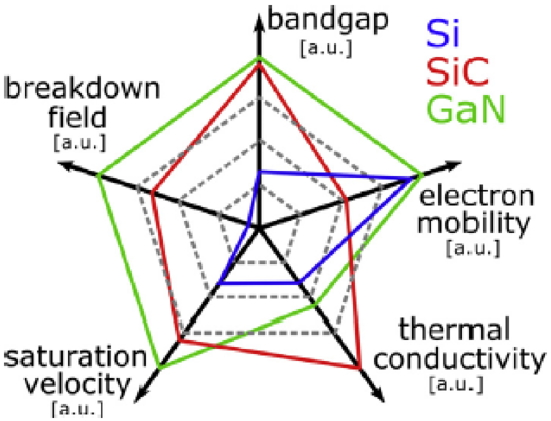
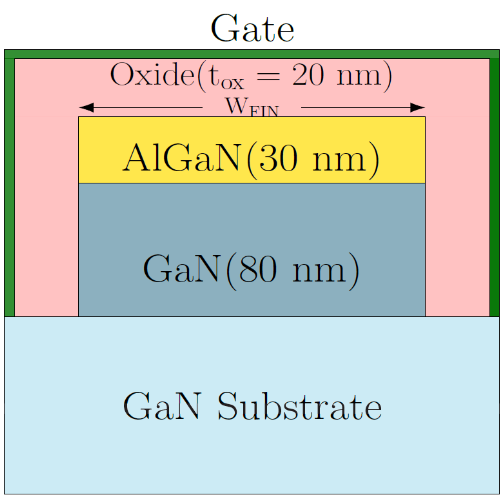
Gabriela F. Furtado, Vinícius V. A. Camargo, Dragica Vasileska, and Gilson I. Wirth, "Evaluating the Ballistic Transport in nFinFETs: A Carrier Centric Perspective", IEEE Transactions on Nanotechnology.

Device Simulation – GaN MISFETs

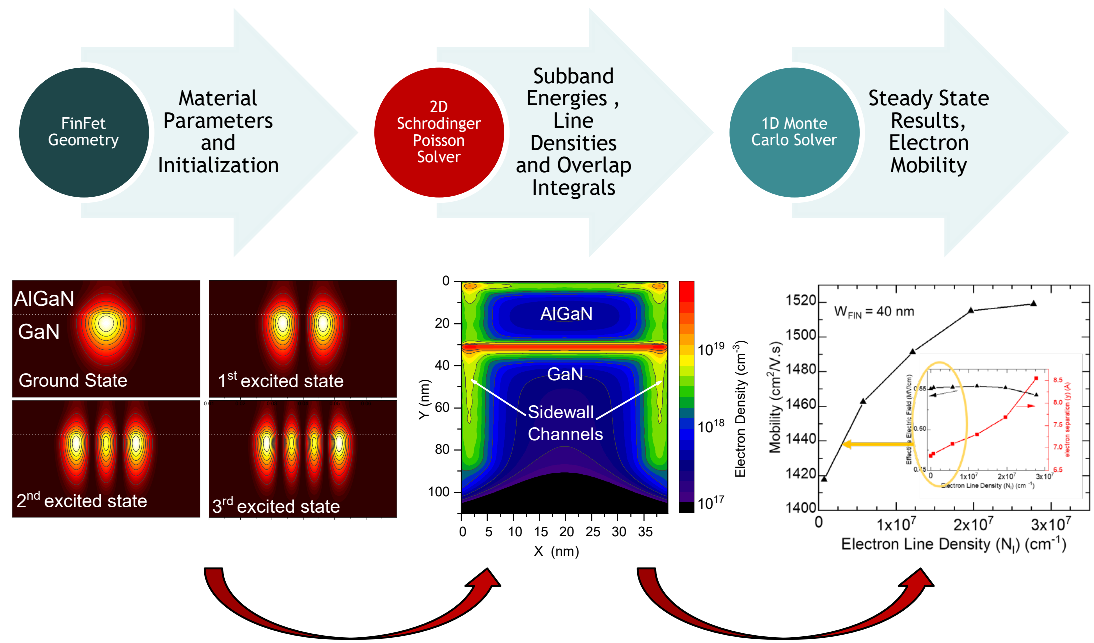


- High electron mobility and saturation drift velocity compared to SiC ➔ *RF device applications*.
- Wide bandgap and a high breakdown field lead to high reverse blocking capability ➔ *power device applications*.



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*, ISBN: 978-89-89453-30-7, p. 103-104.

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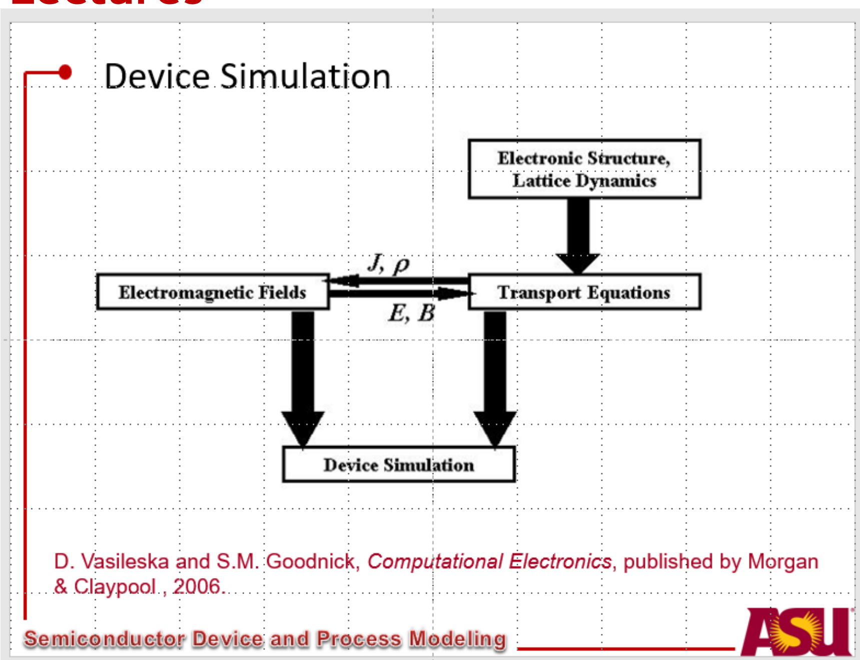
Education: *Device and Process Simulation Course*

Self-Paced Short Course (5 weeks – equivalent to 1 credit hour)

Similar structure like nanoHUB-U courses

Lectures



Quizzes

Projects:

- Band-Structure Calculation Lab
- 1D DD Solver for pn-Diodes
- Silvaco TCAD:
    - MOSFETs Modeling: Scaling and Ballistic Effects
    - SOI Devices: Self-Heating Effects
    - Quantum Corrections to Semi-Classical Approaches – BQP
    - GaN HEMTs and Polarization Charges
    - Multi-Junction Solar Cells and BBT
    - Victory Process Modeling

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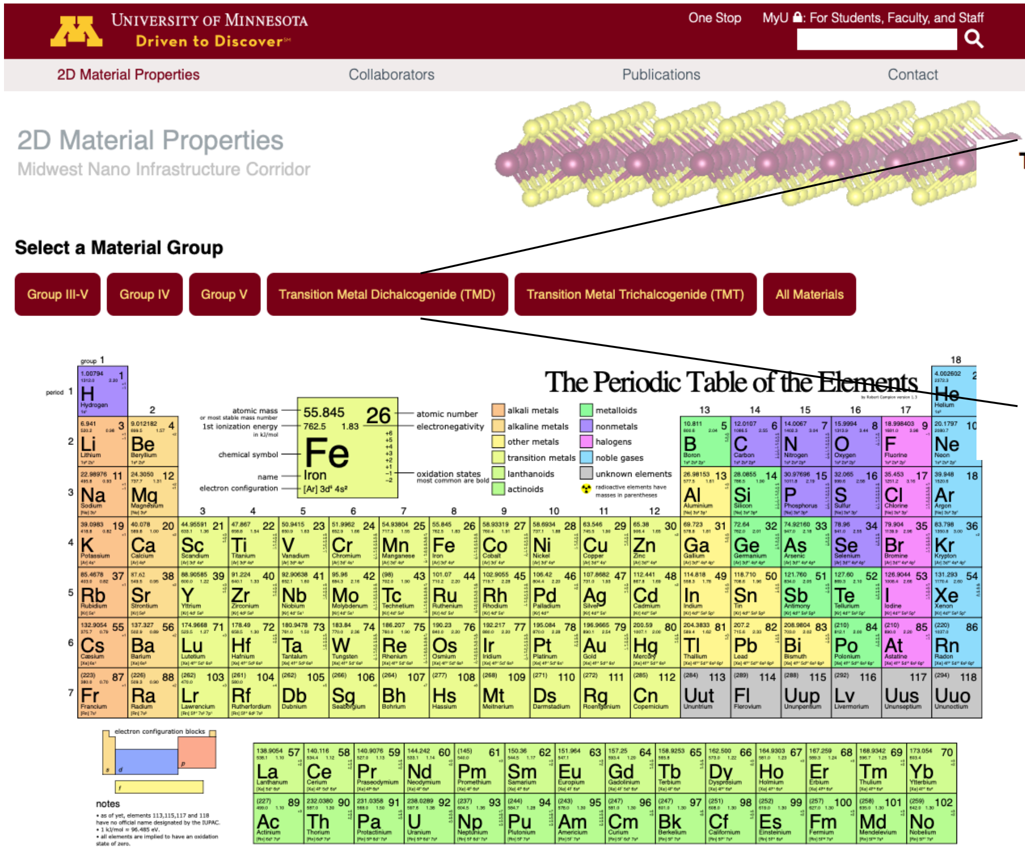
2D Materials Database on MNIC Website



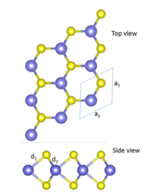
Transition Metal Dichalcogenide (TMD) – Select a Material for Details

- HfS2 (Hafnium disulfide)
- HfSe2 (Hafnium diselenide)
- MoS2 (Molybdenum disulfide)
- MoSe2 (Molybdenum diselenide)
- MoTe2 (Molybdenum ditelluride)
- ReS2 (Rhenium disulfide)
- ReSe2 (Rhenium diselenide)
- SnS2 (Tin disulfide)
- SnSe2 (Tin diselenide)
- WS2 (Tungsten disulfide)
- WSe2 (Tungsten diselenide)
- WTe2 (Tungsten ditelluride)

WSe2 – Tungsten diselenide – Transition Metal Dichalcogenide (TMD)

Experimental Properties Table

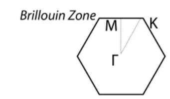
Crystal Structure



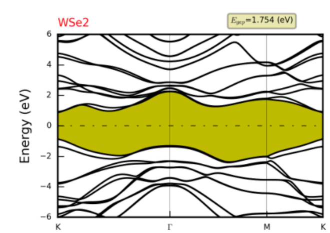
WSe2 Crystal Structure

a_1	3.32 Å
a_2	3.32 Å
d_1	2.55 Å
d_2	4.19 Å

Bandstructure



WSe2 Brillouin Zone



WSe2 Band Plot (HSE)

	PBE	HSE
Valence Band Maximum	-4.70 eV	-5.12 eV
Conduction Band Minimum	-3.47 eV	-3.37 eV
Band Gap	1.23 eV	1.75 eV

Includes more than 45 2D materials.

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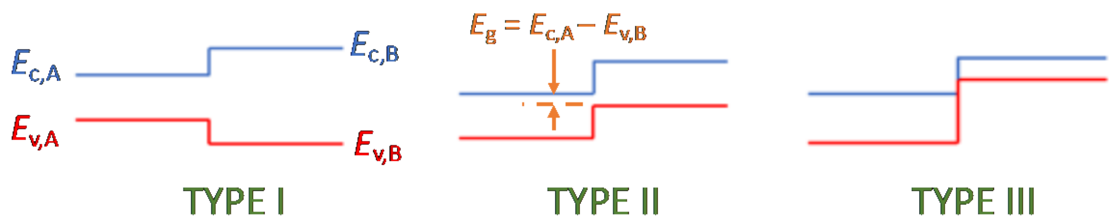
http://apps.minic.umn.edu/2D/search.php

2D Heterostructures @TNF (Prof. Frank Register)

- Vertical stacked
  - *van der Waals interaction*
  - *no dangling bonds* → *reduced interface* traps
- Optoelectronics
  - improved scalability,
  - controllability,
  - tunability,
  - flexibility
- Band tuning
  - strain Engineering
  - layer Engineering
  - electric Field
  - material Engineering



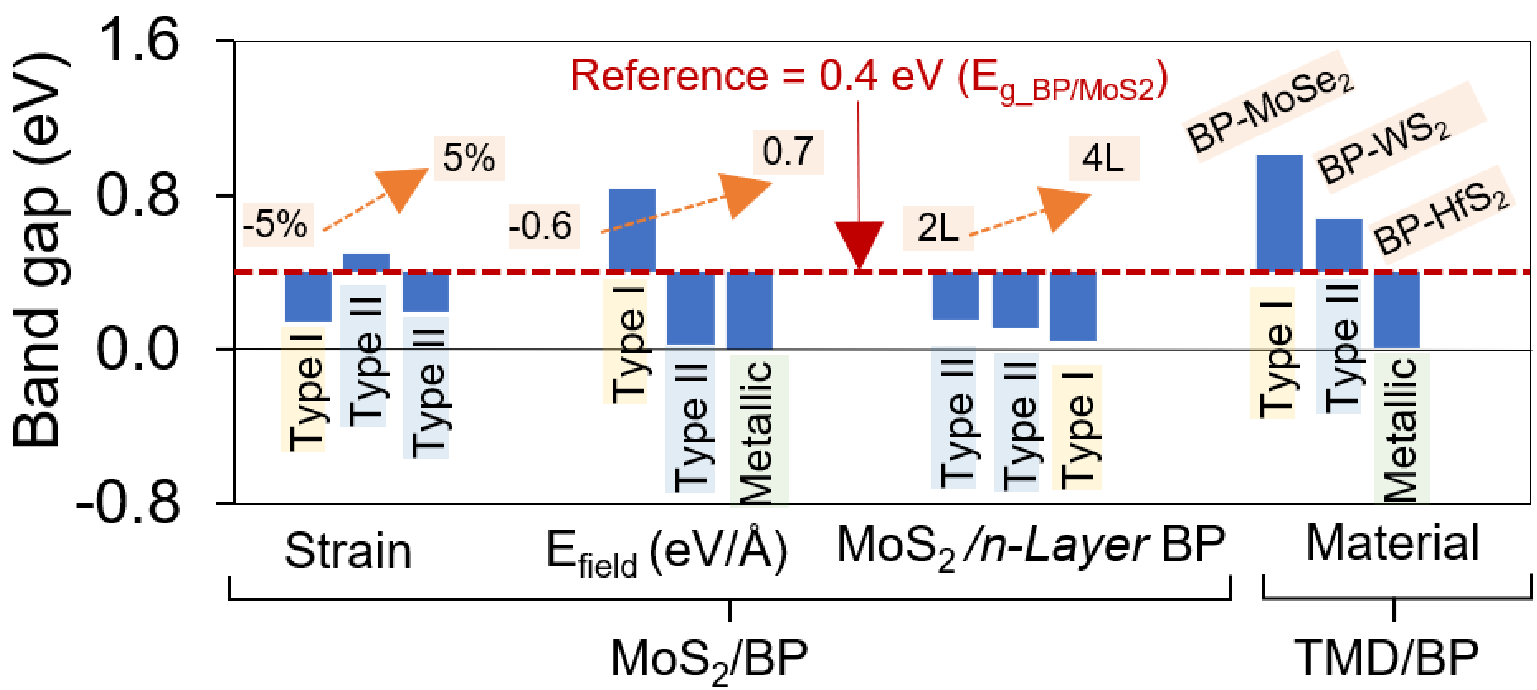
Type I: $E_{c,A} > E_{c,B}$, $E_{v,A} > E_{v,B}$; $E_g = E_{c,A} - E_{v,A}$

Type II: $E_{c,A} > E_{c,B}$, $E_{v,B} > E_{v,A}$; $E_g = E_{c,A} - E_{v,B}$

Type III $E_{c,A} > E_{c,B}$, $E_{v,B} > E_{v,A}$; $E_g = E_{c,A} - E_{v,B} < 0$

A more rigorous approach to addressing band *alignments* in 2D material heterostructures and a larger design space—addition of applied strain and electric fields.

Altering Band Alignment in BP/TMD Heterostructures



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

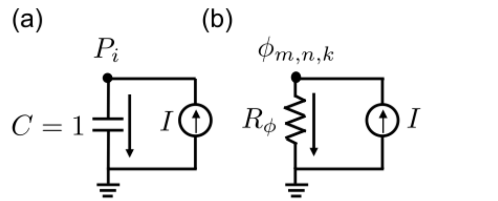
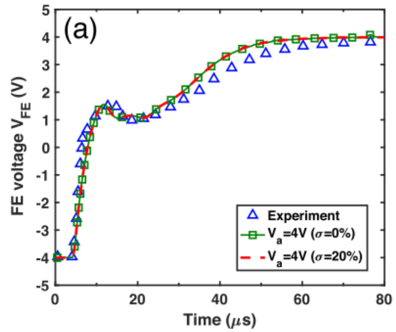
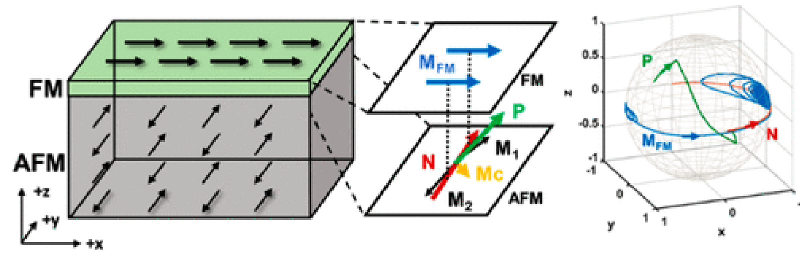


Fig. 1. SPICE equivalent circuit diagrams of (a) TDGL equation, whe
$i = 1, 2, 3$. (b) Poisson's equation.



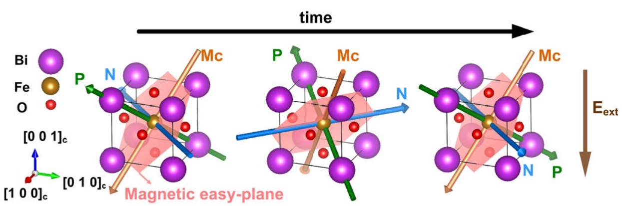
Physics-Based Circuit Models for Phase-Field FE Simulations

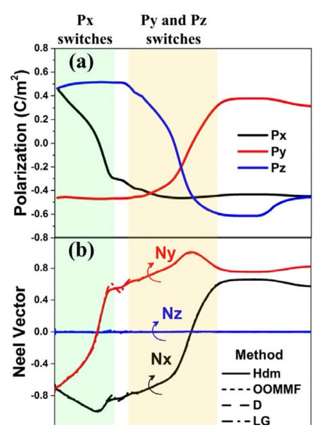
IEEE-Trans. Electron Devices, 2020



Dynamic Response of BFO/CoFe Heterostructure

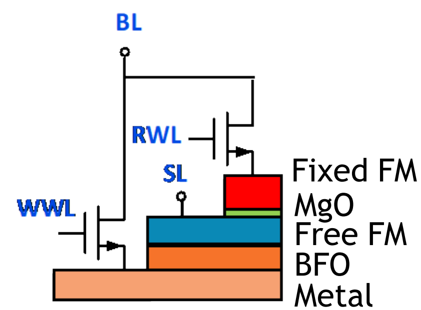
Nano Letters, 2020





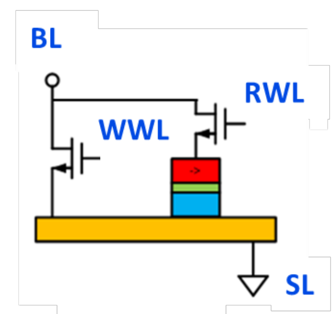
Magnetization Dynamics of a Single-Domain BiFeO3 Nanoisland

IEEE-Trans. Magnetism, 2020



Magnetoelectric MRAM

IEEE-JXCDC, 2020



Spin Orbit Torque MRAM

IEDM 2020

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NSF

Funded by Intel Co. and SRC

SPICE Subcircuits for FE Simulations on nanoHUB

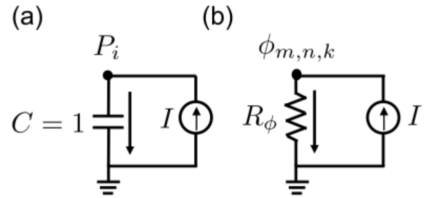
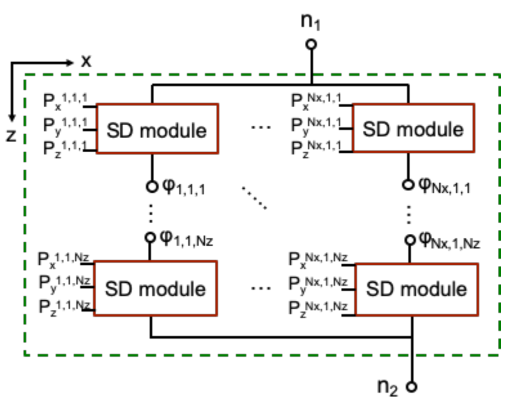
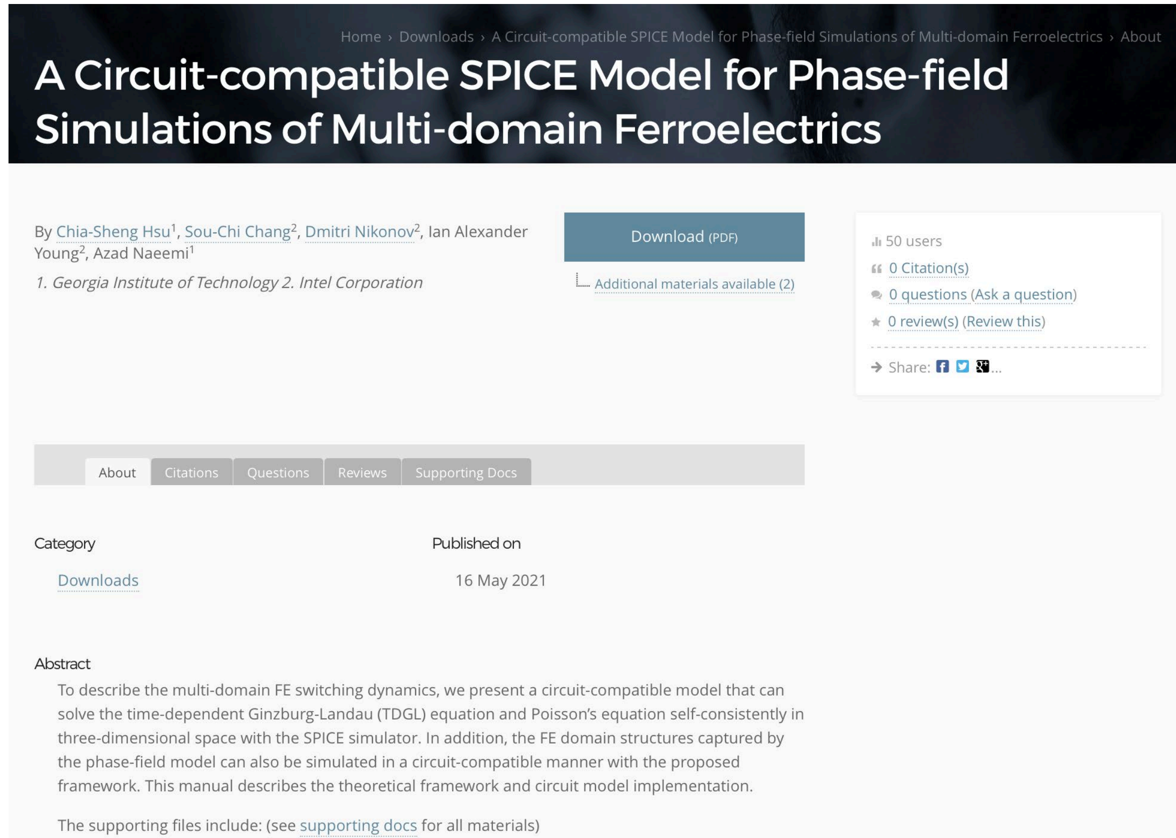


Fig. 1. SPICE equivalent circuit diagrams of (a) TDGL equation, where $i = 1, 2, 3$. (b) Poisson's equation.



Physics-Based Circuit Models for Phase-Field FE Simulations

IEEE-Trans. Electron Devices, 2020



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A Circuit-compatible SPICE Model for Phase-field Simulations of Multi-domain Ferroelectrics

By Chia-Sheng Hsu[1], Sou-Chi Chang[2], Dmitri Nikonov[2], Ian Alexander Young[2], Azad Naeemi[1]

1. Georgia Institute of Technology 2. Intel Corporation

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Published on: 16 May 2021

Abstract

To describe the multi-domain FE switching dynamics, we present a circuit-compatible model that can solve the time-dependent Ginzburg-Landau (TDGL) equation and Poisson's equation self-consistently in three-dimensional space with the SPICE simulator. In addition, the FE domain structures captured by the phase-field model can also be simulated in a circuit-compatible manner with the proposed framework. This manual describes the theoretical framework and circuit model implementation.

The supporting files include: (see supporting docs for all materials)

https://nanohub.org/resources/35041

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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.NET

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https://www.youtube.com/watch?v=GXOzi5J01eU

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NNCI Seminar Series

June 23, 2021 | 4PM - 5PM EDT

Computation Talk: A Case Study of Essential Physics and Technology Challenges as Revealed Trough 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

https://www.youtube.com/watch?v=9dqwETsA0x0

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Upcoming NNCI Computation Webinar

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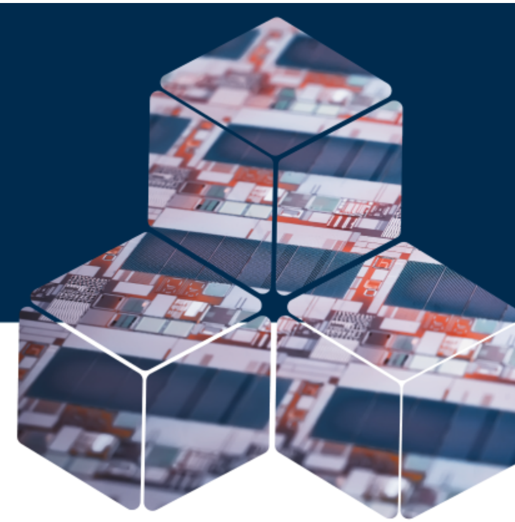
NNCI Computation Webinar

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

Abstract: Today, nearly every aspect of an integrated circuit is designed using electronic design automation (EDA) software. Technology computer aided design (TCAD) tools are used for modeling front-end-of-line manufacturing, including the fabrication (Process TCAD) and electrical characterization (Device TCAD) of individual transistors. These tools have been utilized over the last six decades to help realize Moore's law scaling – the driver behind the exponential increase in transistor density – alleviating the high cost of expensive fabrication experiments. The development of each logic node has, in turn, driven the development of the TCAD tools to account for new fabrication and manufacturing techniques.

In this talk, I will discuss how Process TCAD has evolved to keep up with technology evolution and how new drivers in electronics applications, such as 5G, IoT, and autonomous vehicles are driving the next generation process TCAD tools.

Access the Event @ | https://tinyurl.com/NNCIcompTCAD

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