NNCI Computation

Azad Naeemi

Georgia Institute of Technology

azad@gatech.edu

National Nanotechnology Coordinated Infrastructure

Objectives

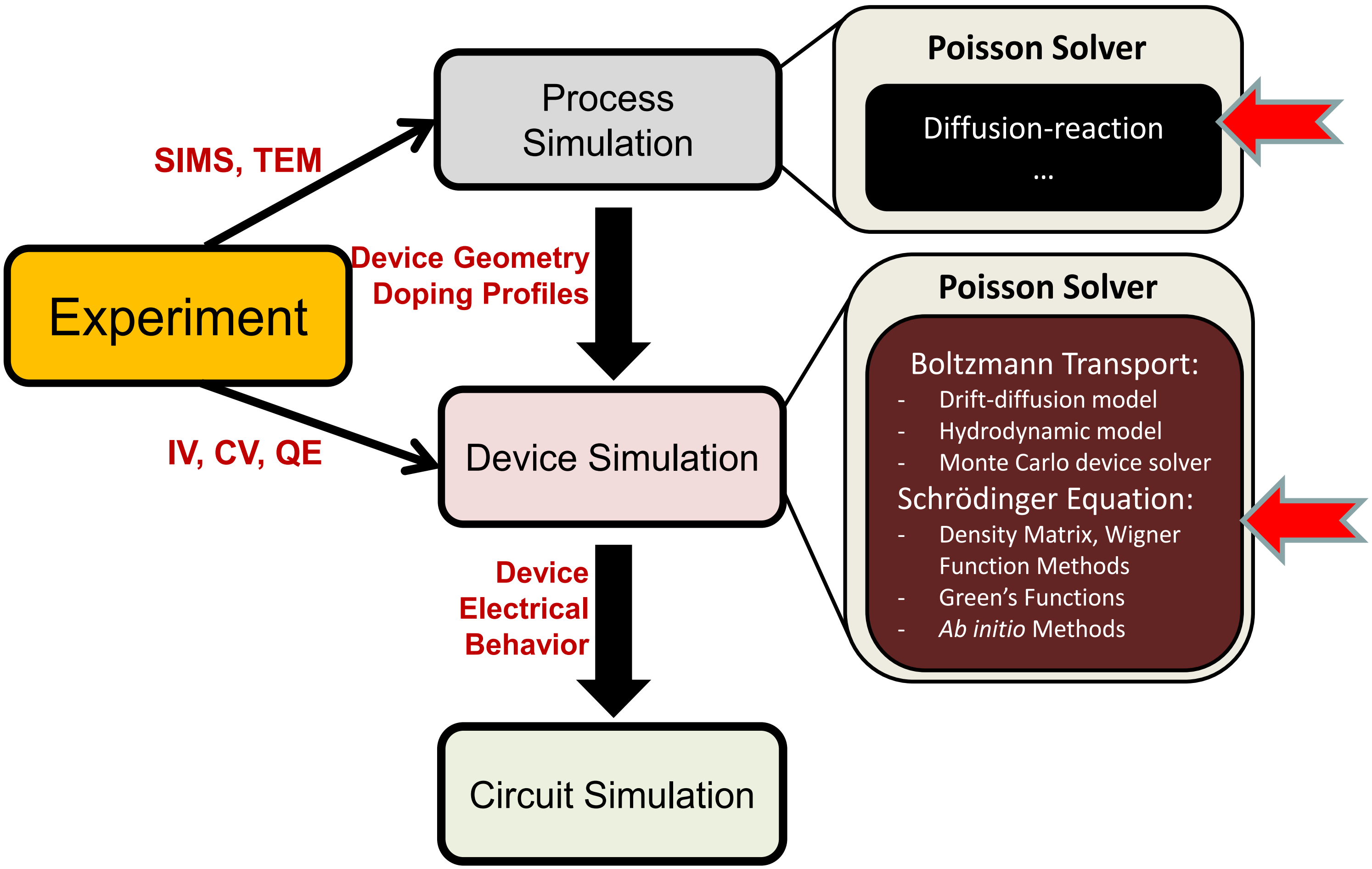
- To facilitate access to the modeling and simulation capabilities and expertise
- To identify the strategic areas for growth
- To promote and facilitate the development of the new capabilities.

An inventory of available modeling and simulation resources and expertise is being complied. The directory is hosted by nanoHub.org.

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

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

Modeling and Simulation @ NCI-SW



Year 2019:
Diffusion-Reaction Modeling of Metastabilities in CdTe Solar Cells

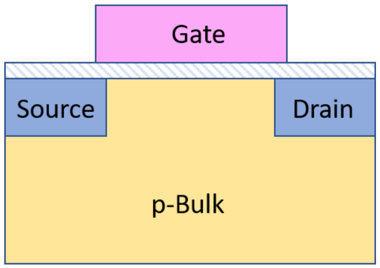
Year 2020:
Full-Band Device Simulator for Modeling 4H SiC Power Electronic Devices (VDMOS)

Dragica Vasileska, ASU (NCI-SW)

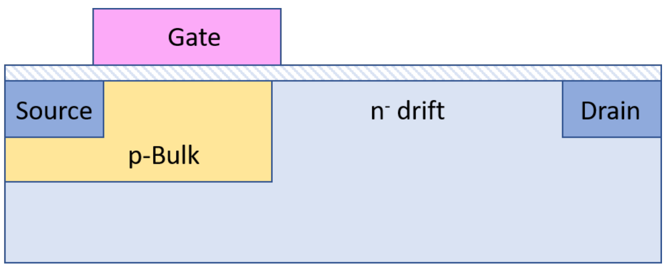
National Nanotechnology Coordinated Infrastructure

Device Simulation

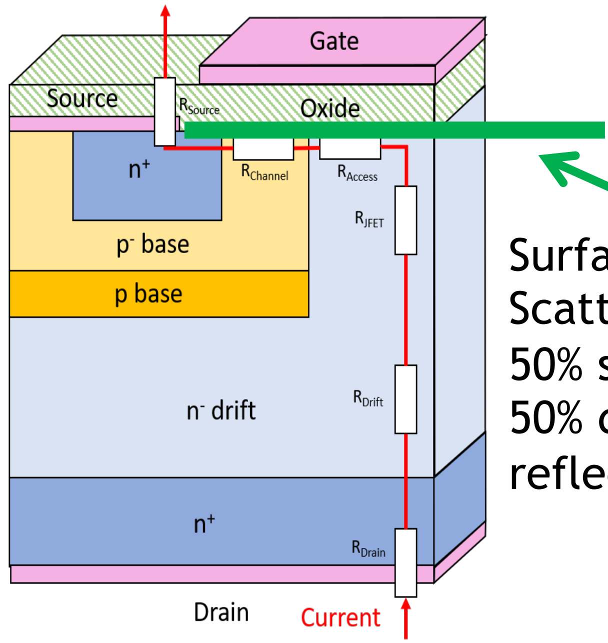
Conventional MOSFET



LDMOS: Lateral Double-Diffused MOSFET



VDMOS: Vertical Double-Diffused MOSFET



Surface Roughness Scattering:
50% specular
50% diffusive
reflection assumed

An in-house full-band Monte Carlo (FBEMC) device simulation tool is developed and validated.

National Nanotechnology Coordinated Infrastructure

$N_1 > N_2$

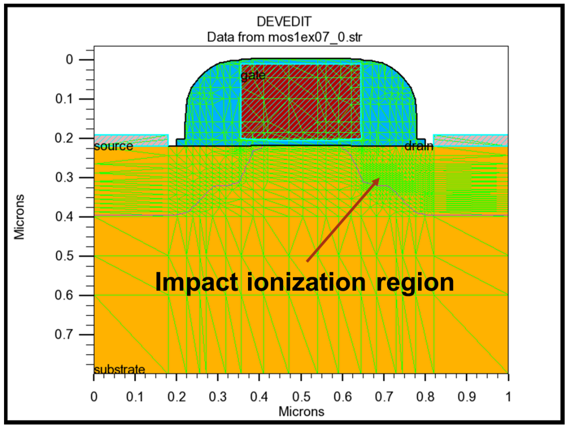
Dragica Vasileska, ASU (NCI-SW)

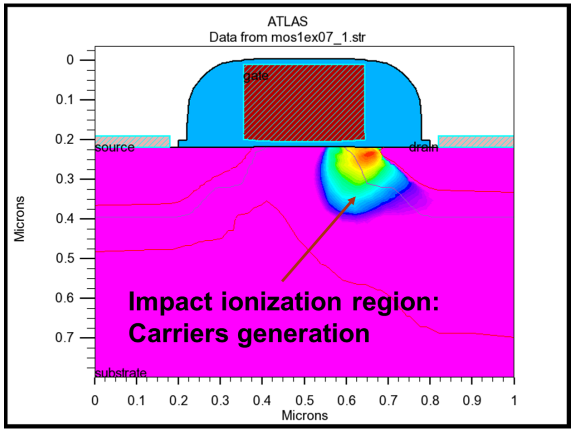
Device and Process Simulation Course

Developed ONLINE Graduate Level Semiconductor Device and Process Modeling Class (primarily focused on Silvaco device/process modeling).

27 students are currently taking the class at ASU from all over United States.

- The form of the input file statements is:
  <STATEMENT> <PARAMETER> = <VALUE>
  The parameter can be: real, integer, character and logical.
- The order in which the ATLAS commands occur is the following:
  - ***A) Structure specification:*** MESH, REGION, ELECTRODE, DOPING
  - ***B) Material models specification:*** MATERIAL, MODELS, CONTACT, INTERFACE
  - ***C) Numerical method selection:*** METHOD
  - ***D) Solution specification:*** LOG, SOLVE, LOAD, SAVE
  - ***E) Results analysis:*** EXTRACT, TONYPLOT
- The input file can be created using the DeckBuild Command Menu:
  Commands/Command Menu





Dragica Vasileska, ASU (NCI-SW)

National Nanotechnology Coordinated Infrastructure

Contributions to nanoHUB.org

Developed Bound States Calculation Lab:

www.nanohub.org/tools/bsclab

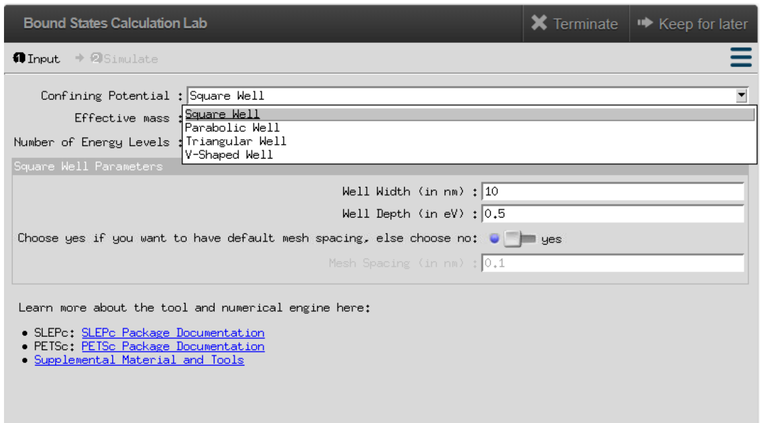
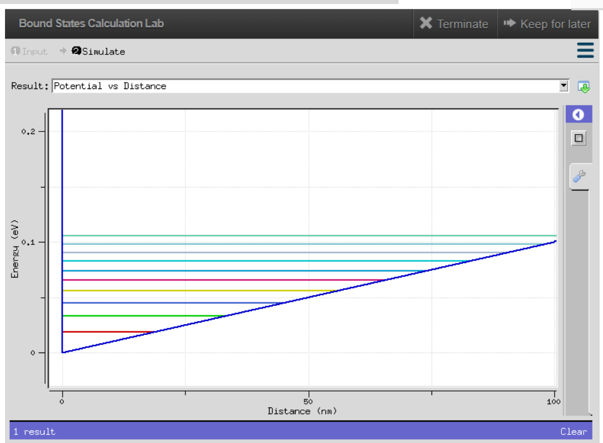
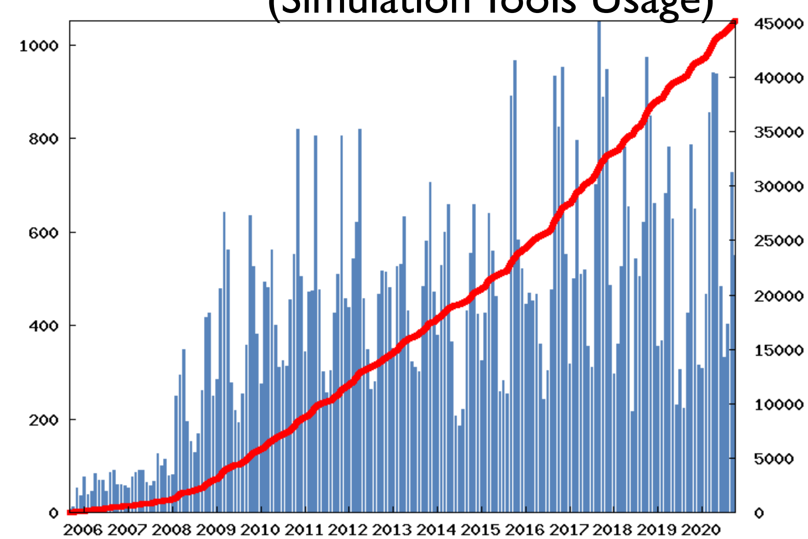


Table 1: Overview	
Item	**Value**
Contributions:	378
Rank by Contributions:	3 / 2375
First Contribution:	09 Mar 2005
Last Contribution:	19 Mar 2020
Citations on Contributions:	181
Usage in Courses/Classrooms:	7,516 users served in 480 courses from 47 institutions

235 users/6 months
(*since April 2020*)



Dragica Vasileska's Impact Graph on nanoHUB.org
(Simulation Tools Usage)



National Nanotechnology Coordinated Infrastructure

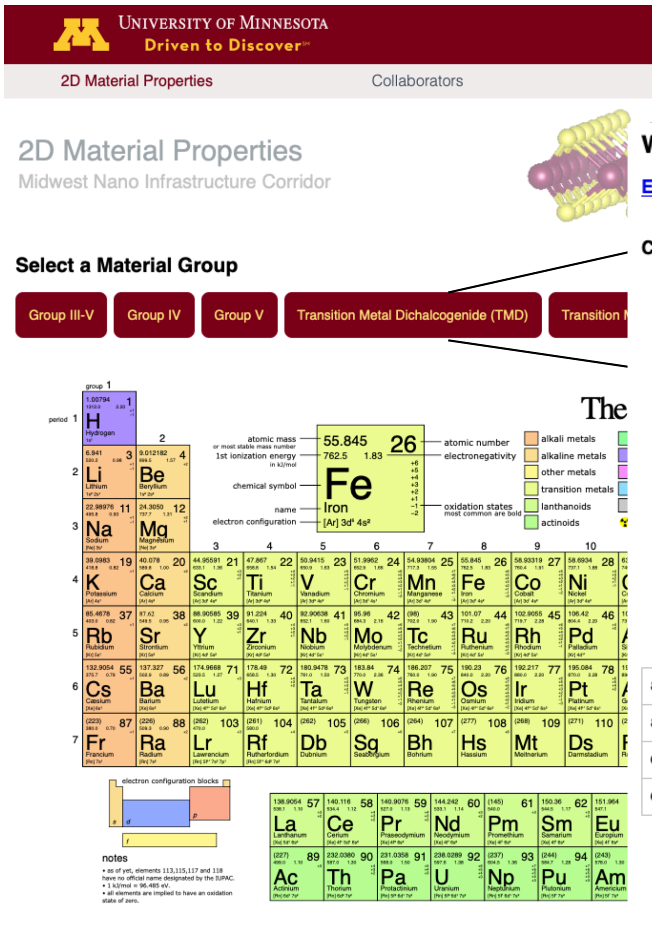
NSF

CNF Computing Capabilities

Resources available remotely during COVID-19

- Nanoscale simulation computing cluster
  Runs Scientific Linux 7 w OpenHPC & Slurm; Bring Your Own License!
- Pseudopotential Virtual Vault
  Online web database of over 1100 pseudopotential or Projected Augment Wave Method (PAW) files
- Remote access to software tools via "CNF Thin" Hotdesking service
  CAD (BEAMER, L-Edit, Java GDS, AutoDesk); Simulation (Coventor, Cadence, PROLITH, Layout LAB, TRACER); Image/Data Analysis (ProSEM, NanoScope Analysis, WinFLX)
- Virtual CAD Room
  Remote access to a virtual CNF CAD Rm Windows desktop w CNF SW
- AWS Conversion Cloud
  Large memory or CPU or long running CAD conversion jobs

2D Materials Database on MNIC Website



WSe$_2$		
Property	**Description/Value**	
	Bulk	**Monolayer**
Lattice constant (a)	3.28 Å [1]	3.32 Å [2]
Molar mass	341.76 g/mol [3, 4]	341.76 g/mol [3, 4]
Band gap type	Indirect [5]	Direct [5]
Band gap energy	1.2 eV (experimental) [6]	1.65 eV (experimental) [5] 1.25 eV (calculation) [2]
Coordination geometry	Trigonal prismatic (W^{IV}), Pyramidal (Se^{-2}) [3, 4, 7]	Trigonal prismatic (W^{IV}), Pyramidal (Se^{-2}) [3, 4,7]
Crystal structure	hP6, space group $P6_3/mmc$, No 194 [3,7]	hP6, space group $P6_3/mmc$, No 194 [3, 7]
Appearance	Grey to black solid [3, 7]	---------------
Group	Transition Metal Dichalcogenide [7]	Transition Metal Dichalcogenide [7]
Spin-orbit splitting	---------------	0.47 eV [2]
Poisson's ratio	--------------	0.19 [2]
Cohesive energy per unit cell	------------------	15.45 eV [2]
Charge transfer of W atom	0.96 e [2]	0.96 e [2]
In-plane stiffness	------------	115.52 N/m [2]
Density	9.32 g/cm^3 [3]	9.32 g/cm^3 [3]
Melting point	1500 °C [8]	------------------
Exciton binding energy	---------------	0.79 eV [9]
W-Se bond length	---------------	2.55 Å [2]
Dielectric constant (ε)	---------------	Real part (ε1)=~22, Imaginary part (ε2)=~10 (at 1.7 eV incident photon energy) [10]
Effective masses	--------------	m_e= 0.53 m_o, m_h= 0.52 m_o [11]
Effective Bohr radius	--------------	-------------------
Thermal expansion coefficient		11.08×10^{-6} /^{o}C [12]
Bulk Modulus (B)		----------------
Refractive Index	-------------------	5.68 [13]
Carrier mobility in WSe$_2$		
Thicknesses	**BN/SiO$_2$/Si substrate**	**SiO$_2$/Si Substrate**
8 nm	---------------------	~350 cm^2/V.Sec (hole) [14]
Monolayer	~31 cm^2/V.Sec [15]	---------------------
Bulk	--------------------	---------------------

Includes more than 45 2D n

National Nanotechnology Coordinated Infrastructure

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

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

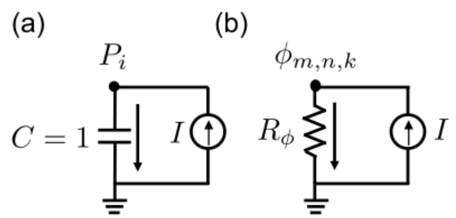
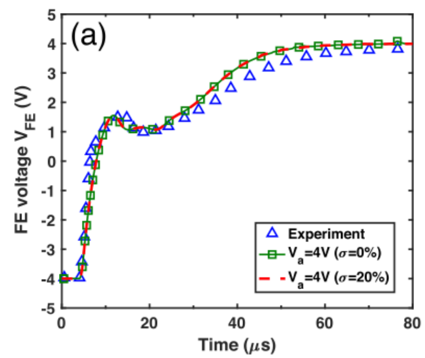
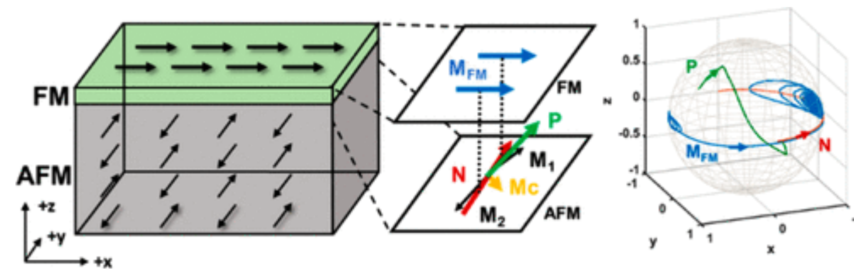


Fig. 1. SPICE equivalent circuit diagrams of (a) TDGL equation, whe $i = 1, 2, 3$. (b) Poisson's equation.



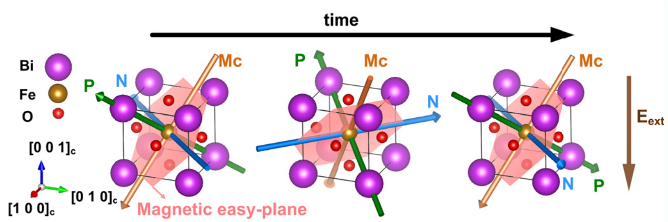
Physics-Based Circuit Models for Phase-Field FE Simulations

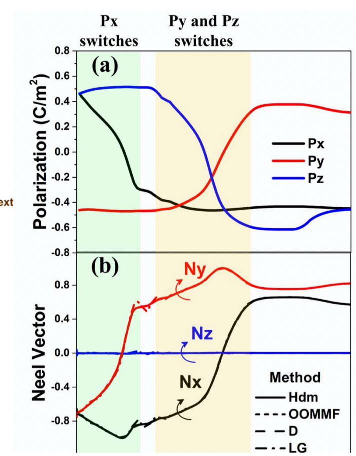
IEEE-Trans. Electron Devices, 2020



Dynamic Response of BFO/CoFe Heterostructure

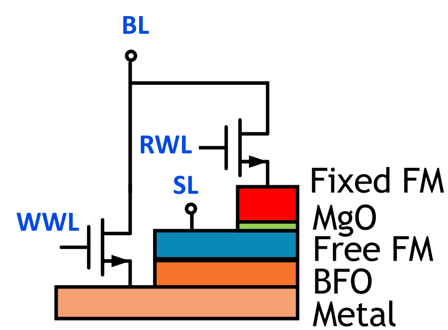
To appear in Nano Letters





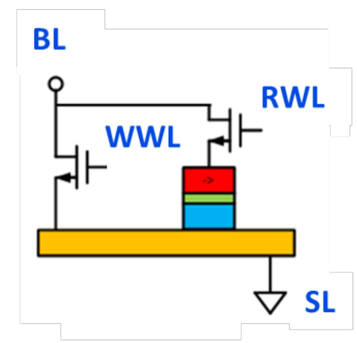
Magnetization Dynamics of a Single-Domain BiFeO3 Nanoisland

IEEE-Trans. Magnetism, 2020



Magnetoelectric MRAM

IEEE-JXCDC, 2020



Spin Orbit Torque MRAM

To appear in IEDM 2020

National Nanotechnology Coordinated Infrastructure

NSF

Funded by Intel Co. and SRC

Looking Ahead (Years 6-10)

- 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