

# NNCI Computation

Azad Naeemi

Georgia Institute of Technology

azad@gatech.edu



National Nanotechnology  
Coordinated Infrastructure



# Outline

## Objectives:

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

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

10 sites have reported collectively more than 65 commercial simulation tools and 40 internally developed simulation tools available for internal and/or external users (with and without fee).

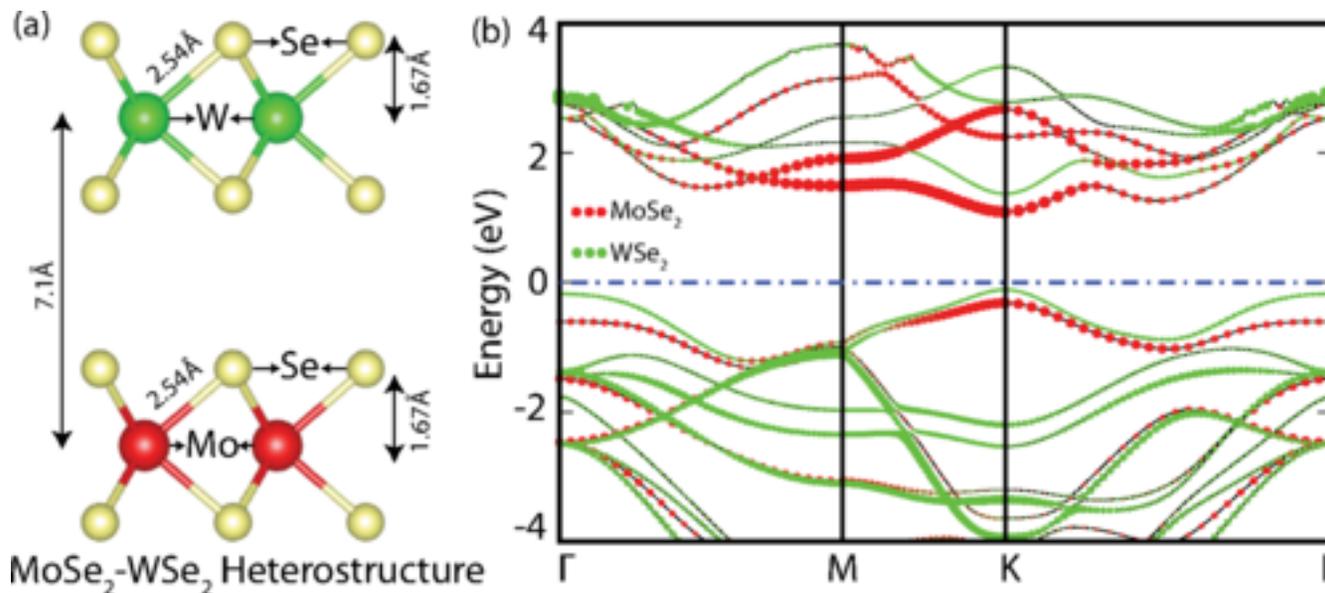
8 supercomputers or major computing clusters are available in various sites.

# Outline

- Modeling Efforts
  - 2D Materials
  - Thin Film Solar Cells
  - Spintronics
- Commercial Tools
  - Synopsys TCAD Sentaurus Tools
  - XperiDesk
- Breakout Session

# 2D Materials

- One of the most active areas of materials research.
- Heterostructures are often used for optical or electronic applications.
- The ways the bands align determines the suitability of a heterostructure.



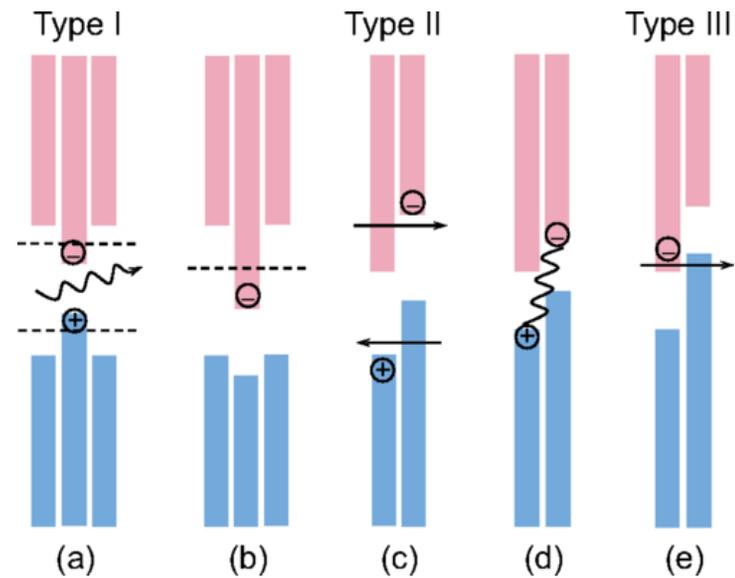
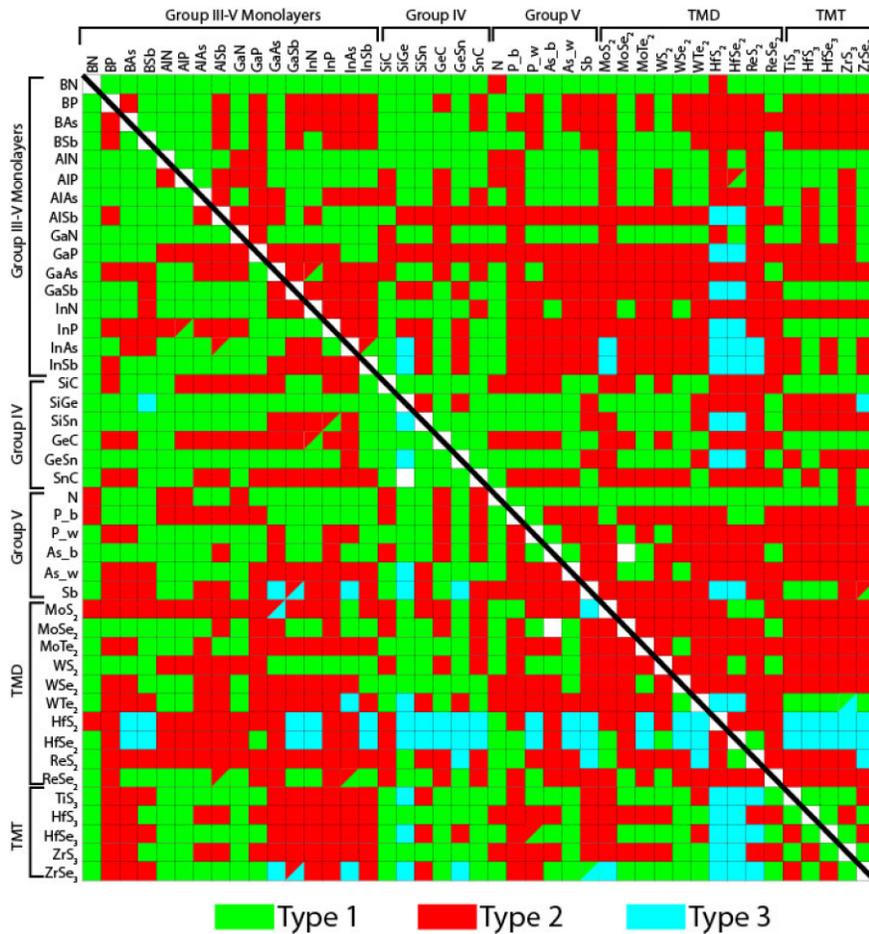
DFT input/output files available

<http://apps.minic.umn.edu/2D/v>

O. Ongun et al, Phys. Rev. B 94, 035125 (2016)  
Tony Low Group @ U Minnesota

# 2D Materials

- A periodic table of 2D heterostructures is developed.



DFT input/output files available

<http://apps.minic.umn.edu/2D/v>

O. Ongun et al, Phys. Rev. B 94, 035125 (2016)

Tony Low Group @ U Minnesota

# 2D Materials Data Base on MNIC Website


**UNIVERSITY OF MINNESOTA**  
 Driven to Discover™
 One Stop MyU

2D Material Properties
Collaborators
Publications

## 2D Material Properties

Midwest Nano Infrastructure Corridor

### Select a Material Group

Group III-V

Group IV

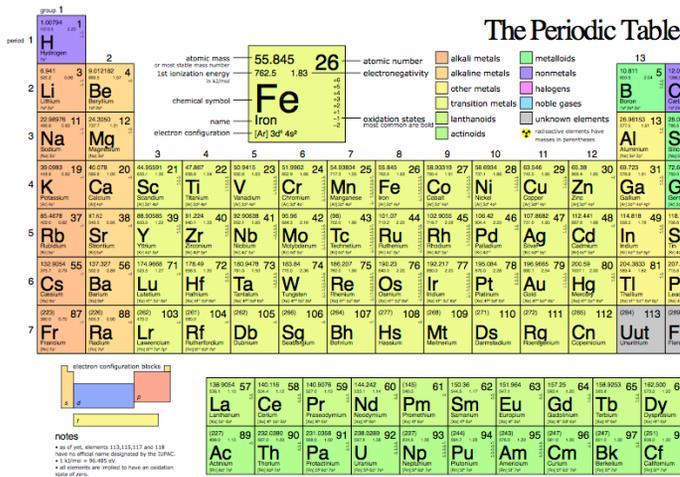
Group V

Transition Metal Dichalcogenide (TMD)

Transition Metal Trichalcogenide (TMT)

All Materials

### The Periodic Table



The periodic table shows elements color-coded by groups: alkali metals (orange), alkaline metals (yellow), other metals (green), transition metals (blue), lanthanoids (purple), actinoids (red), metalloids (light green), nonmetals (light blue), halogens (pink), noble gases (grey), and unknown elements (grey).

Key properties for Iron (Fe) are highlighted: atomic mass 55.845, atomic number 26, chemical symbol Fe, name Iron, and electron configuration [Ar] 3d<sup>6</sup> 4s<sup>2</sup>.

© 2018 Regents of the University of Minnesota. All rights reserved. The University of Minnesota is an equal opportunity institution. Privacy Statement

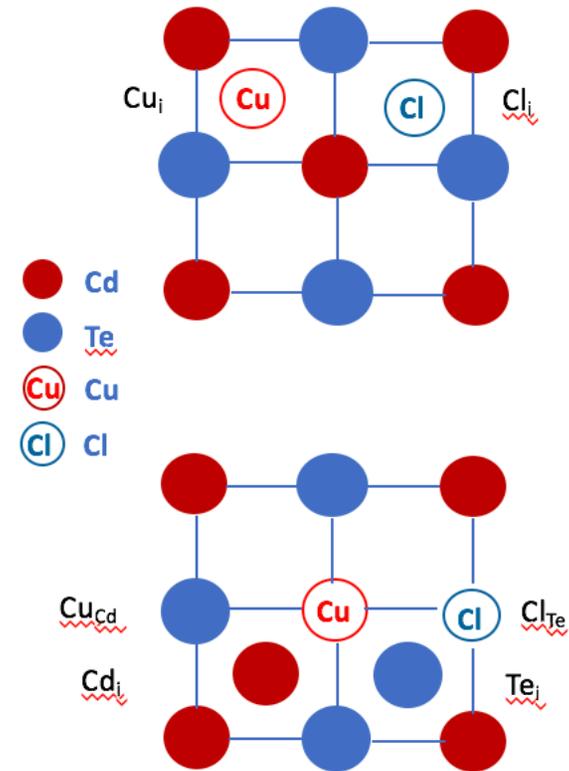


Property	WSe <sub>2</sub>	
	Bulk	Monolayer
Lattice constant (a)	3.28 Å [1]	3.32 Å [2]
Molar mass	341.76 g/mol [3, 4]	341.76 g/mol [3, 4]
Band gap type	Indirect [5]	Direct [5]
Band gap energy	1.2 eV (experimental) [6]	1.65 eV (experimental) [5] 1.25 eV (calculation) [2]
Coordination geometry	Trigonal prismatic (W <sup>IV</sup> ), Pyramidal (Se <sup>-2</sup> ) [3, 4, 7]	Trigonal prismatic (W <sup>IV</sup> ), Pyramidal (Se <sup>-2</sup> ) [3, 4, 7]
Crystal structure	hP6, space group P6 <sub>3</sub> /mmc, No 194 [3,7]	hP6, space group P6 <sub>3</sub> /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 <sup>3</sup> [3]	9.32 g/cm <sup>3</sup> [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 (ε <sub>1</sub> )=-22, Imaginary part (ε <sub>2</sub> )=-10 (at 1.7 eV incident photon energy) [10]
Effective masses	-----	m <sub>e</sub> = 0.53 m <sub>0</sub> , m <sub>h</sub> = 0.52 m <sub>0</sub> [11]
Effective Bohr radius	-----	-----
Thermal expansion coefficient	-----	11.08×10 <sup>-6</sup> /°C [12]
Bulk Modulus (B)	-----	-----
Refractive Index	-----	5.68 [13]
<b>Carrier mobility in WSe<sub>2</sub></b>		
<b>Thicknesses</b>	<b>BN/SiO<sub>2</sub>/Si substrate</b>	<b>SiO<sub>2</sub>/Si Substrate</b>
8 nm	-----	~ 350 cm <sup>2</sup> /V.Sec (hole) [14]
Monolayer	~ 31 cm <sup>2</sup> /V.Sec [15]	-----
Bulk	-----	-----

# CdTe Solar Cells

## Physical Model: Point Defects

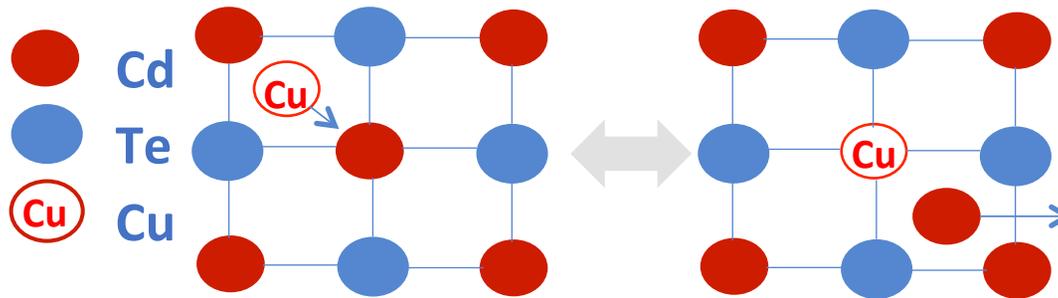
- **Intrinsic Defects in CdTe:**
  - $\text{Cd}_i(0/2+)$ ,  $\text{V}_{\text{Cd}}(0/2-)$ ,  $\text{Te}_i$ ,  $\text{Cd}_{\text{Te}}$  ...
- **Extrinsic Defects in CdTe:**
  - Cu Defects  
 $\text{Cu}_i(0/+)$ ,  $\text{Cu}_{\text{Cd}}(0/-)$ ,  $\text{Cd}_i\text{-Cu}_{\text{Cd}}(0/+)$  ...
  - Cl Defects  
 $\text{Cl}_i(0/\pm)$ ,  $\text{Cl}_{\text{Te}}(0/+)$ ,  $\text{Cl}_{\text{Te}}\text{-V}_{\text{Cd}}(0/-)$  ...
  - Cu-Cl Complexes  
 $\text{Cl}_{\text{Te}}\text{-Cu}_{\text{Cd}}(0)$ ,  $\text{Cl}_i\text{-Cu}_{\text{Cd}}$ ...



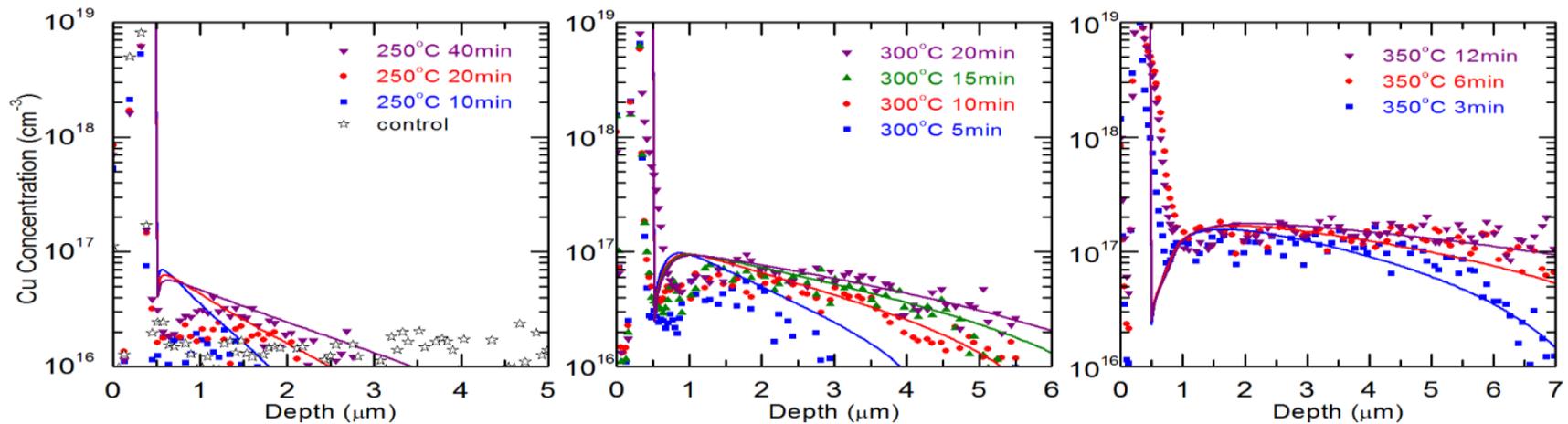
Dragica Vasileska, ASU (NCI-SW)

# Simulation Results

$\text{Cu}_i$  &  $\text{Cu}_{\text{Cd}}$  defect system investigated.



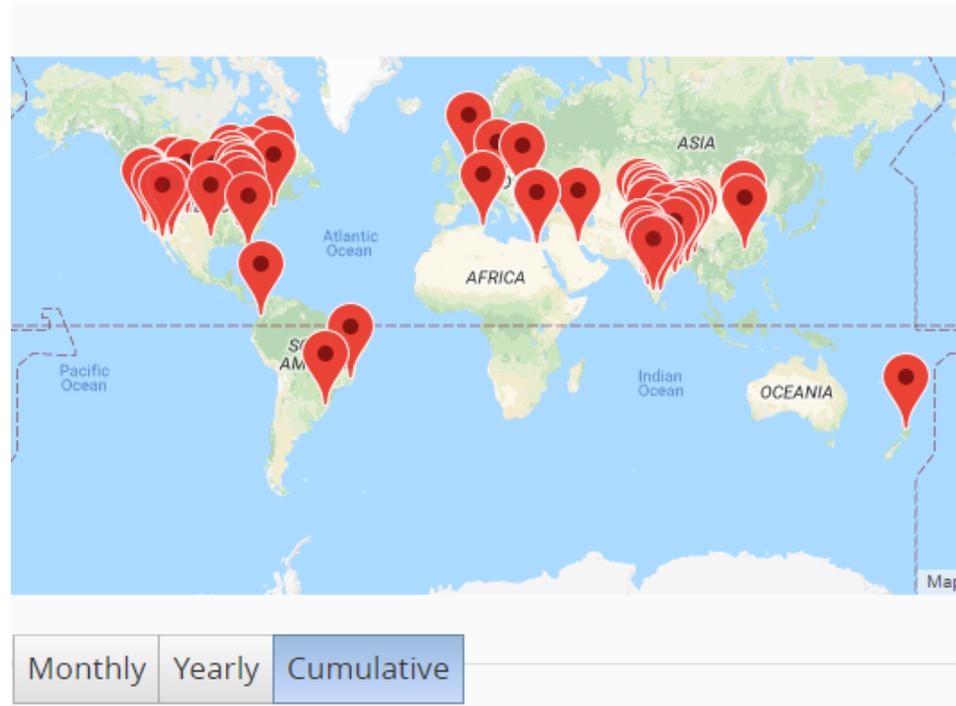
Good matching with experiments:



# 1D and 2D Simulation Tools on nanoHUB

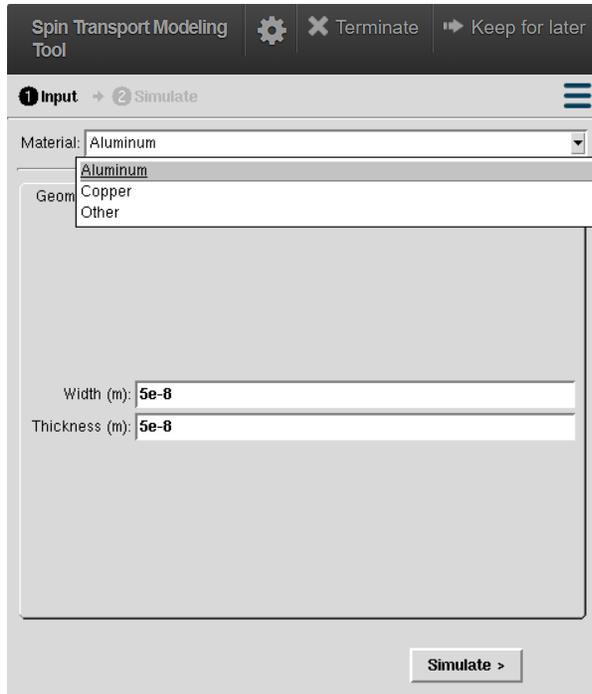
Tools created by  
Vasileska's Group  
and related to  
Process Modeling

- **Cu in CdTe Lab:**  
1D: 59 Users  
2D: 78 Users

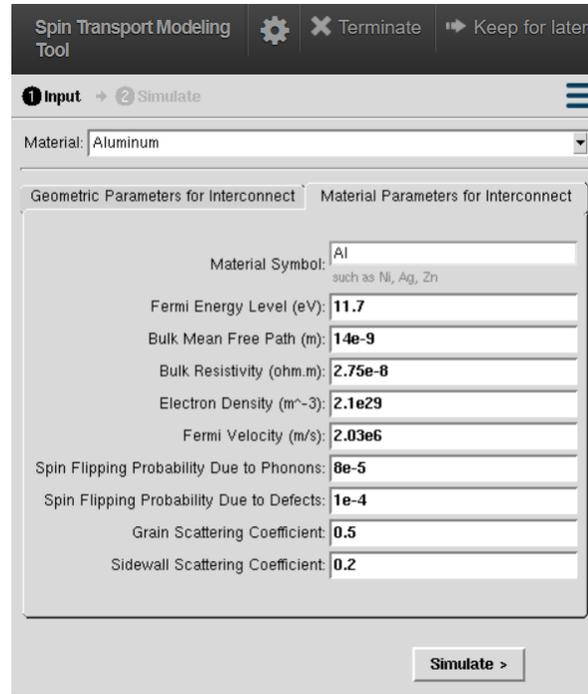


# Spintronic Transport Modeling Tool

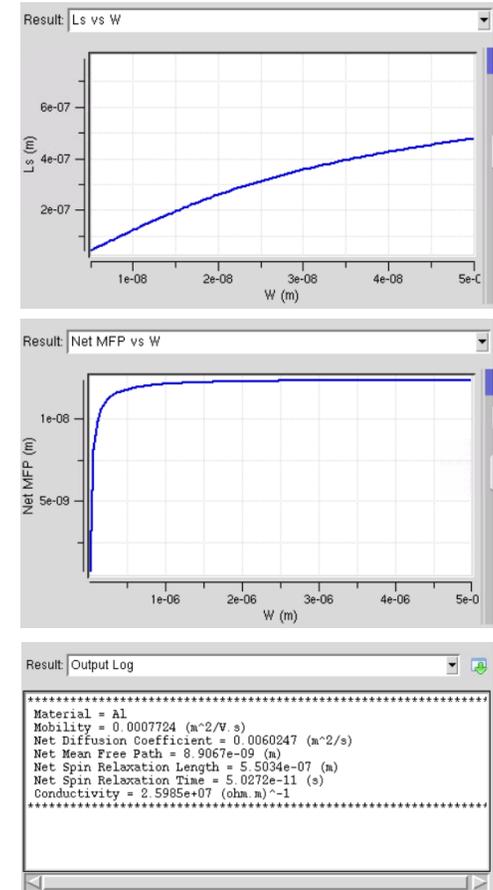
[nanohub.org/tools/spintransport/](http://nanohub.org/tools/spintransport/)



- Choose right material for your interconnect



- Use predetermined material parameters **OR** use your own



- Obtain electron-spin transport physics-based simulation results

# SPICE Subcircuit Netlist Generator for Spintronic Nonmagnetic Metallic Channel

[nanohub.org/tools/spincircuit/](http://nanohub.org/tools/spincircuit/)

SPICE Subcircuit Generator for Spintronic Nonmagnetic Metallic Channel Components

1 Interconnect Parameters → 2 Circuit Description Parameters → 3 Simulate

Material: Copper

Material Symbol: Cu  
such as Ni, Ag, Zn

Fermi Energy Level (eV): 7

Bulk Mean Free Path (m): 40e-9

Bulk Resistivity (ohm.m): 1.7e-8

Electron Density (m^-3): 8.5e28

Fermi Velocity (m/s): 1.57e6

Spin Flipping Probability Due to Phonons: 2e-3

Spin Flipping Probability Due to Defects: 7e-4

Grain Scattering Coefficient: 0.5

Sidewall Scattering Coefficient: 0.2

Circuit Description Parameters >

- Choose right material for your interconnect

SPICE Subcircuit Generator for Spintronic Nonmagnetic Metallic Channel Components

1 Interconnect Parameters → 2 Circuit Description Parameters → 3 Simulate

Number of segments: 10

< Interconnect Parameters Simulate >

The diagram shows a channel divided into segments  $cell_1, cell_2, \dots, cell_N$ . It includes current variables  $I_c(x), I_{s,x}(x), I_{s,y}(x), I_{s,z}(x)$  and their values at the end of the channel  $x+L$ . Below the main diagram, a detailed circuit model for a segment is shown, featuring resistors, capacitors, and current sources representing spin and charge transport.

- Use developed compact circuit model for spintronic transport

```
Result: interconnect.sbckt
*Channel Subcircuit
.subckt interconnect
+ vc0 vxL vx0 vxL vy0 vyL vz0 vzL
+ vc_gnd vx_gnd vy_gnd vz_gnd
*****
*Drift-Diffusion Channel Circuit Model
pcell11 vc0 vx1 vx1 vy1 vy1 vz1 vz1 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell12 vc1 vx2 vx2 vy2 vy2 vz2 vz2 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell13 vc2 vx3 vx3 vy3 vy3 vz3 vz3 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell14 vc3 vx4 vx4 vy4 vy4 vz4 vz4 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell15 vc4 vx5 vx5 vy5 vy5 vz5 vz5 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell16 vc5 vx6 vx6 vy6 vy6 vz6 vz6 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell17 vc6 vx7 vx7 vy7 vy7 vz7 vz7 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell18 vc7 vx8 vx8 vy8 vy8 vz8 vz8 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell19 vc8 vx9 vx9 vy9 vy9 vz9 vz9 vc_gnd vx_gnd vy_gnd vz_gnd cell
pcell110 vc9 vx10 vx10 vy10 vy10 vz10 vz10 vc_gnd vx_gnd vy_gnd vz_gnd cell
*****
.ends interconnect
```

```
Result: cell.sbckt
*Single Cell Subcircuit
.subckt cell
+ vc+ vx- vx+ vx- vy- vy+ vz- vz+
+ vc_gnd vx_gnd vy_gnd vz_gnd
*****
*Parameters
*Spin Transport Parameters
.param mu=0.0016096
.param D=0.0075113
*****
*Spin Circuit Parameters
.param Relec=0.68439
.param Gelec=1.2949e-18
.param Rspin=0.68439
.param Cspin=5.4711e-13
.param Gspin=0.069804
*****
*Drift-Diffusion Segment Circuit Model
*Charge Current
R_c1 vc+ vc- t 'Relec'
V_c1 vc+ t vc- DC 0
R_c2 vc- vc+ t 'Relec'
V_c2 vc- t vc+ DC 0
C_c vc vc_gnd 'Gelec'
*Spin_x Current
R_x1 vx+ vx- 'Rspin'
E_x1 vx+ vx- I=(mu/D)*I(V_c1)*(V(vx)-V(vy_gnd))
R_x2 vx vx- 'Rspin'
E_x2 vx vx- I=(mu/D)*I(V_c2)*(V(vx)-V(vx_gnd))
C_x vx vx_gnd 'Cspin'
R_x vx vx_gnd '1/Gspin'
*Spin_y Current
R_y1 vy+ vy- 'Rspin'
E_y1 vy+ vy- I=(mu/D)*I(V_c1)*(V(vy)-V(vy_gnd))
R_y2 vy vy- 'Rspin'
E_y2 vy vy- I=(mu/D)*I(V_c2)*(V(vy)-V(vy_gnd))
C_y vy vy_gnd 'Cspin'
R_y vy vy_gnd '1/Gspin'
*Spin_z Current
R_z1 vz+ vz- 'Rspin'
E_z1 vz+ vz- I=(mu/D)*I(V_c1)*(V(vz)-V(vz_gnd))
R_z2 vz vz- 'Rspin'
E_z2 vz vz- I=(mu/D)*I(V_c2)*(V(vz)-V(vz_gnd))
C_z vz vz_gnd 'Cspin'
R_z vz vz_gnd '1/Gspin'
*****
.ends cell
```

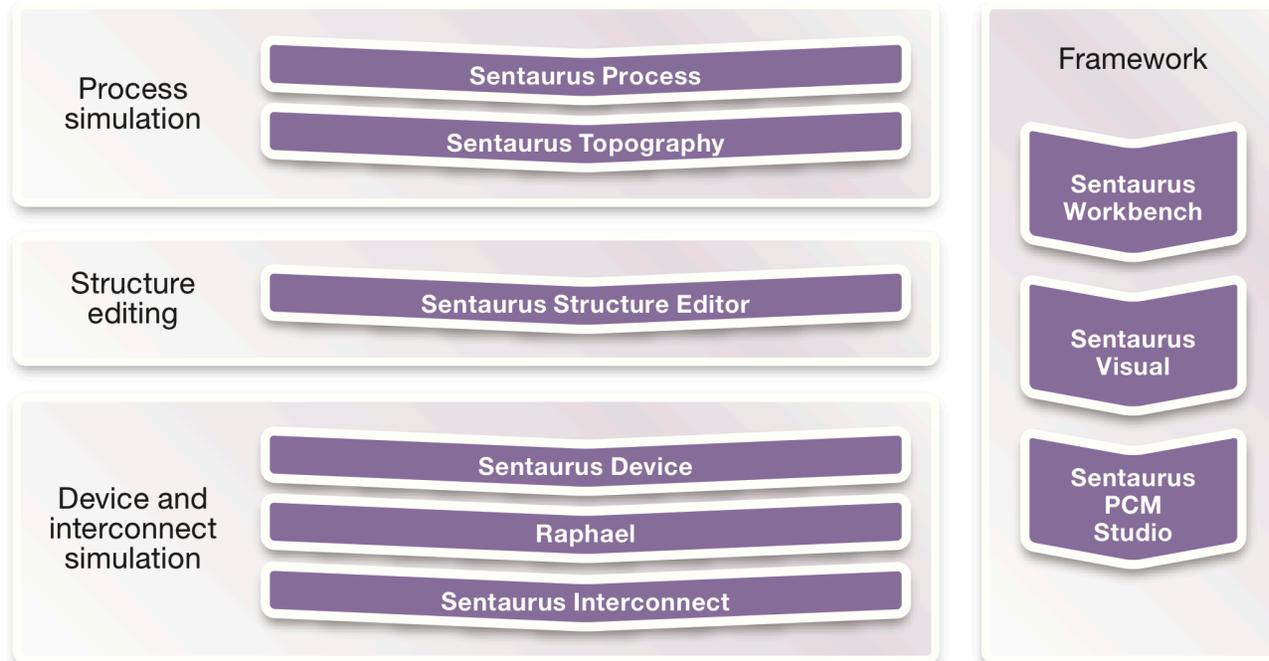
- Obtain SPICE subcircuit netlist describing spin & electron transport in channel



# Outline

- Modeling Efforts
  - 2D Materials
  - Thin Film Solar Cells
  - Spintronics
- Commercial Tools
  - Synopsys TCAD Sentaurus Tools
  - XperiDesk
- Breakout Session

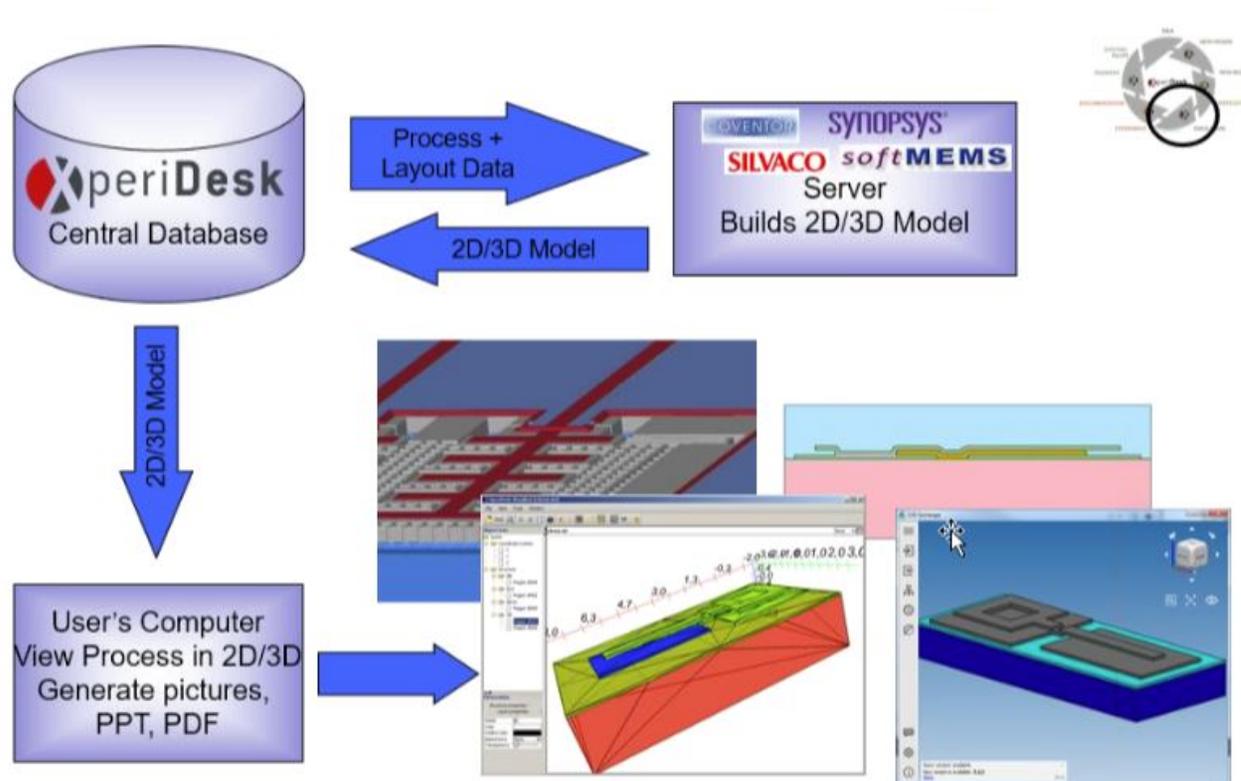
# Synopsys TCAD Sentaurus Tools



Sentaurus TCAD Suite

Synopsys offers quarterly 3-day “Basic Training Workshops on TCAD Sentaurus Tools” at their Mountain View, CA, headquarters.

# XperiDesk



A knowledge capture repository for process flows which can generate 3D renderings of devices to be fabricated.

Results can be fed directly into Sentaurus, Silvaco, SoftMEMS and Coventor.

# Breakout Session

- How can NNCI Computation be most useful for the NNCI community?
- What can we do in the short term and what should be long term goals?
- How can we grow the existing computational resources?
- How can we make it easier to access computational resources?