NNCI Computation

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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 complied. 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.

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Outline

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

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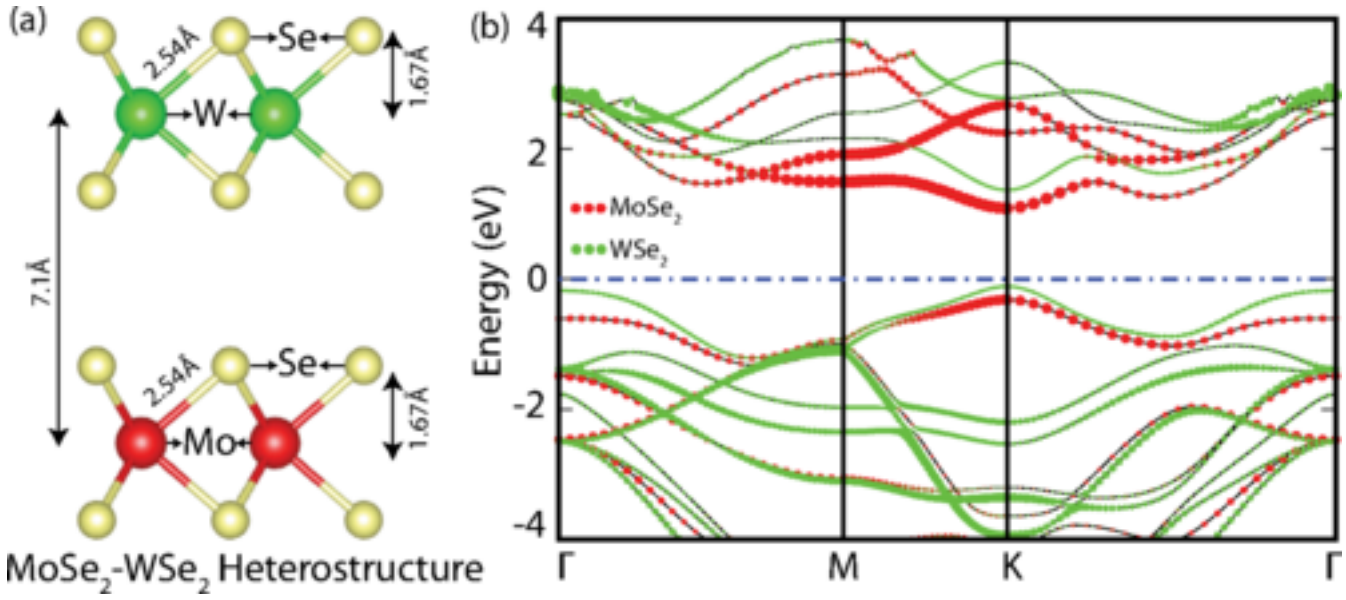
2D Materials

- 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.



$MoSe_2$-WSe_2 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

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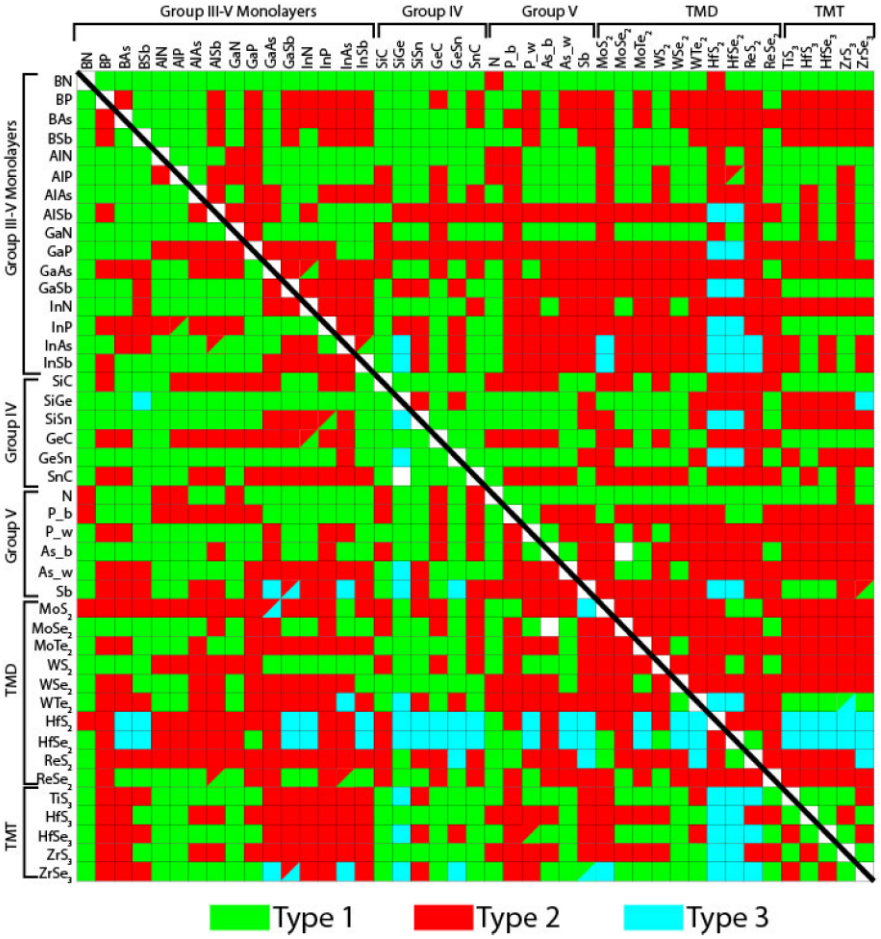
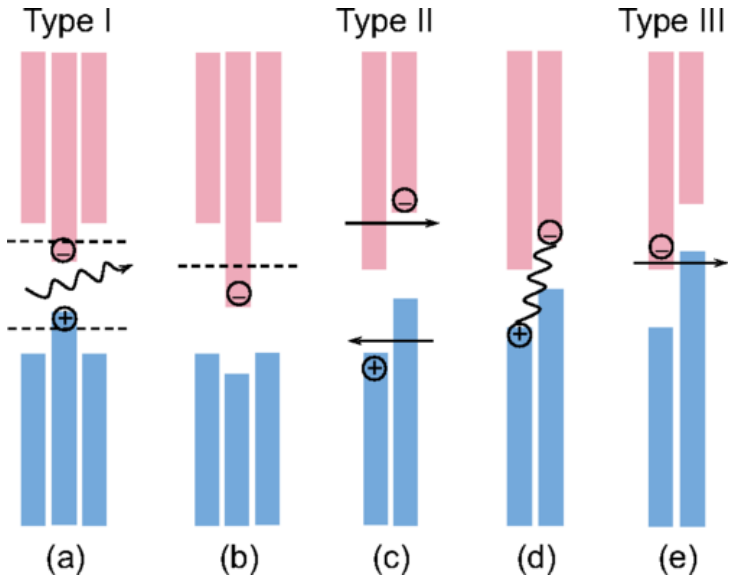
2D Materials

- A periodic table of 2D heterostructures is developed.





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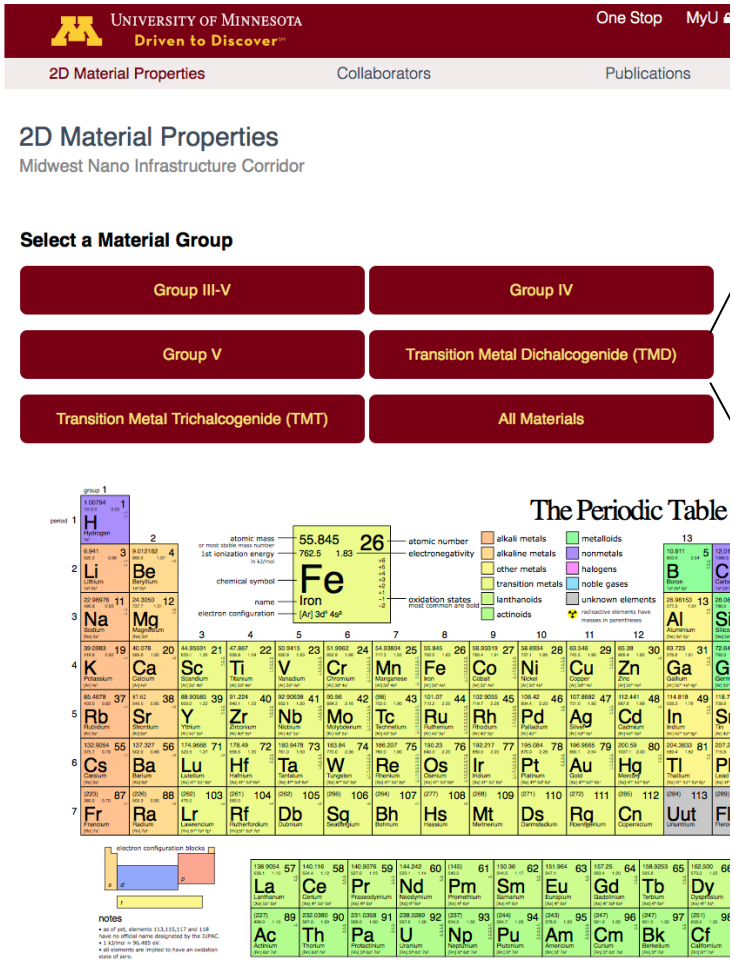
2D Materials Data Base on MNIC Website



Property	WSe_2	
	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} /°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	----------	----------

CdTe Solar Cells

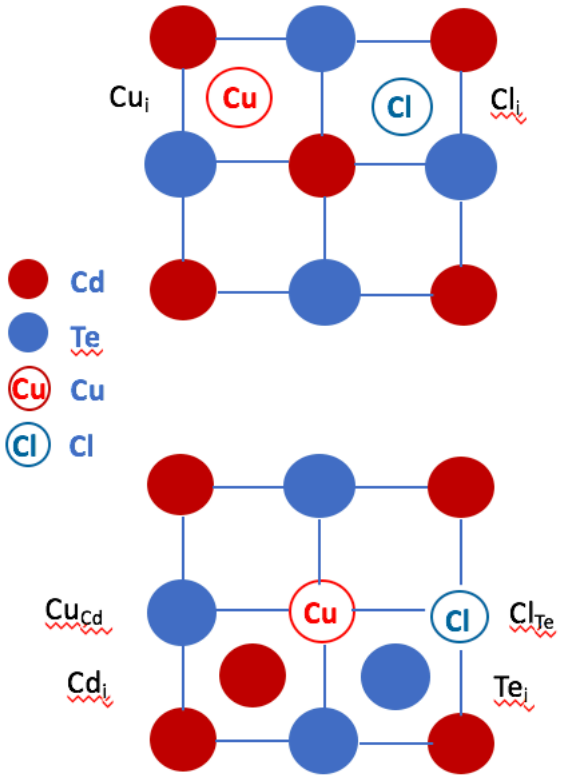
Physical Model: Point Defects

- **Intrinsic Defects** in CdTe:
  - **Cd_i(0/2+), V_{Cd}(0/2-),** Te_i, Cd_{Te} …
- **Extrinsic Defects** in CdTe:
  - Cu Defects

    Cu_i(0/+), Cu_{Cd}(0/-), Cd_i-Cu_{Cd}(0/+) …
  - Cl Defects

    Cl_i(0/±), Cl_{Te}(0/+), Cl_{Te}-V_{Cd}(0/-) …
  - Cu-Cl Complexes

    Cl_{Te}-Cu_{Cd}(0), Cl_i-Cu_{Cd}…



Dragica Vasileska, ASU (NCI-SW)

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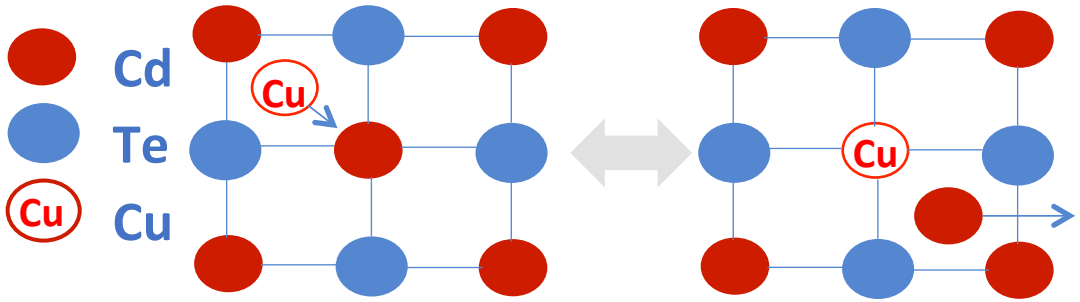
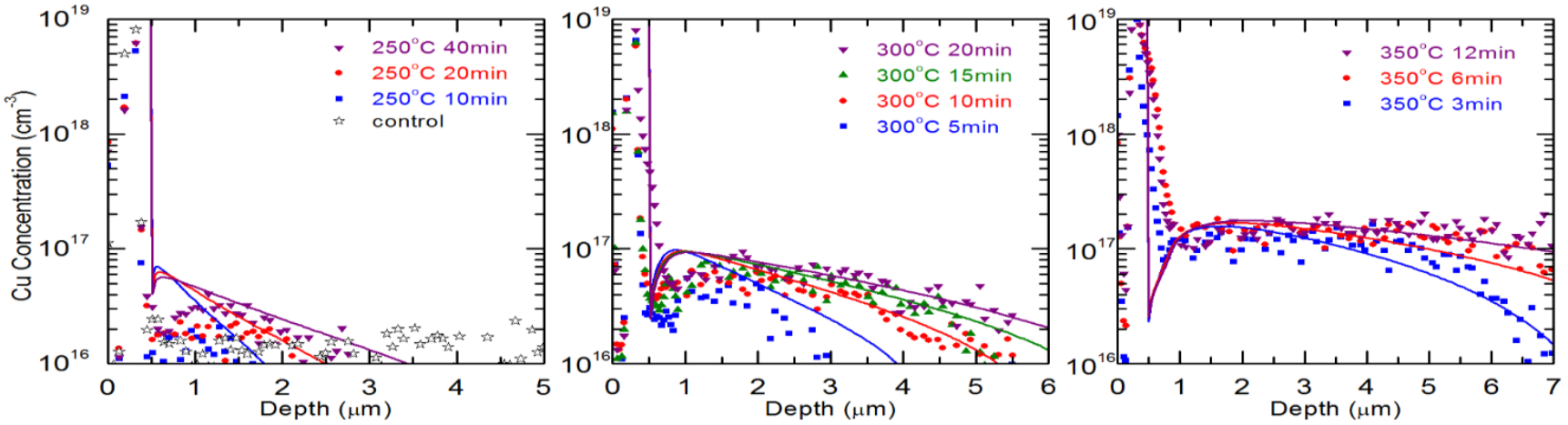
Simulation Results

Cu_i & Cu_{Cd} defect system investigated.



Good matching with experiments:



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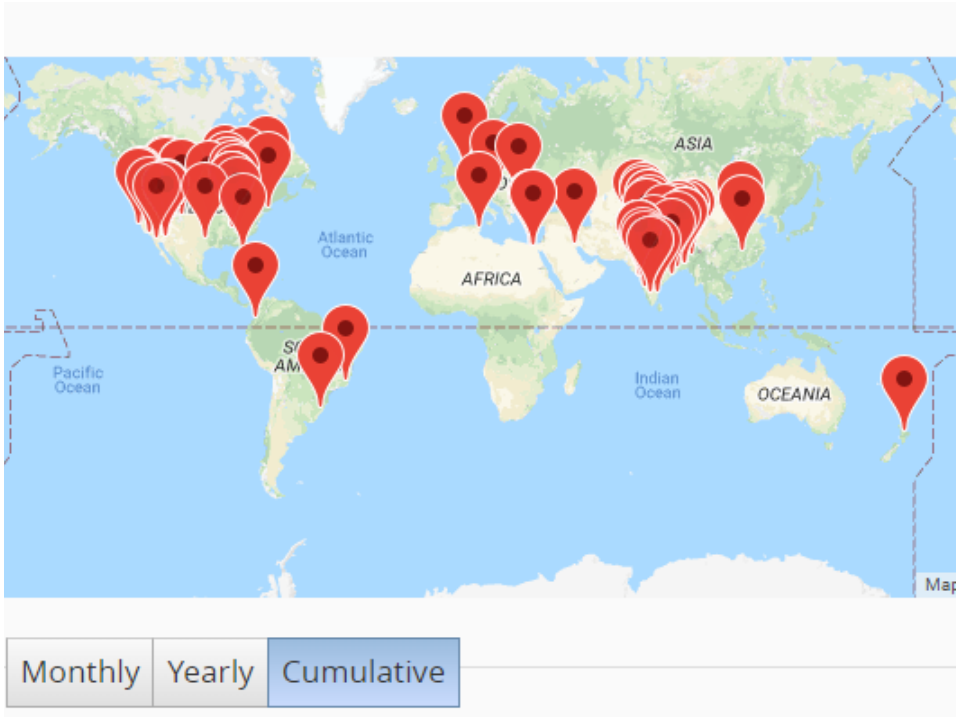
D. Guo, T. Fang, A. Moore, D. Brinkman, R. Akis, D. Krasikov I. Sankin, C. Ringhofer, and D. Vasileska, IEEE JPV (in press)

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*



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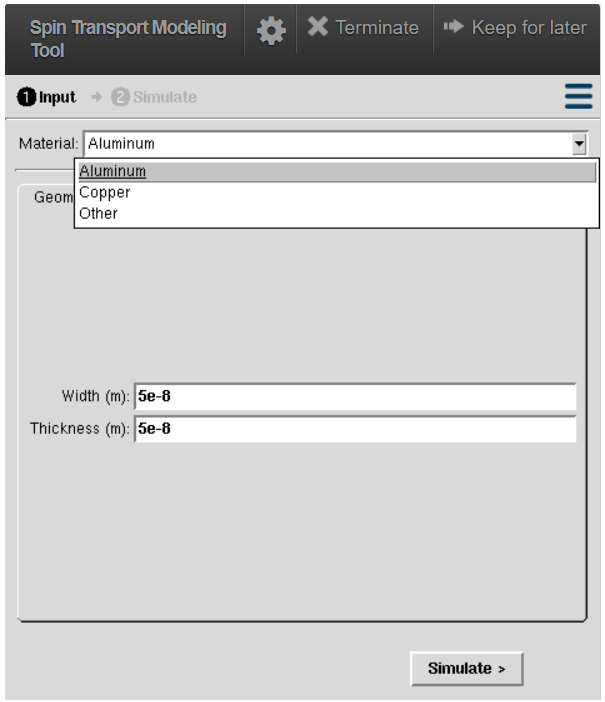
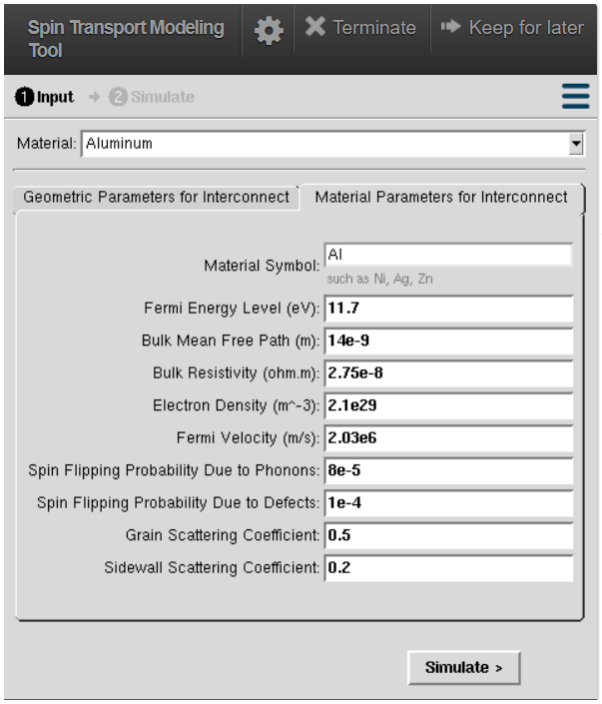
Spintronic Transport Modeling Tool

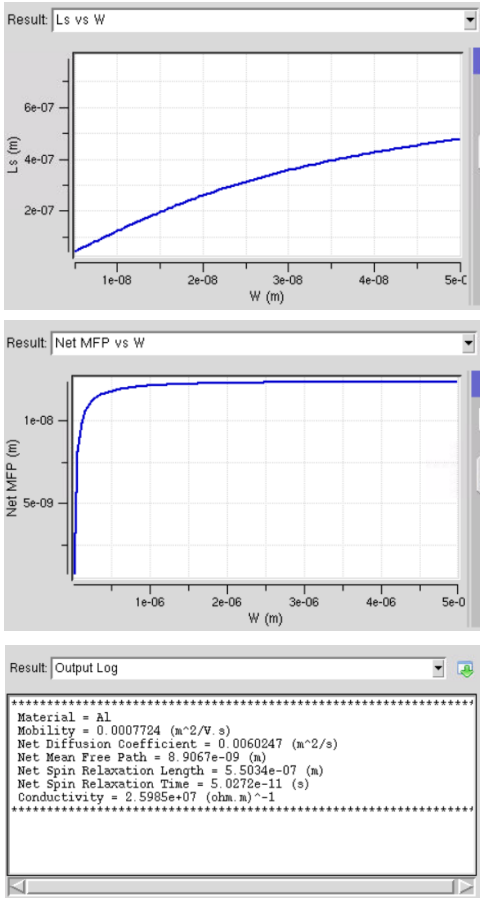
nanohub.org/tools/spintransport/



- Choose right material for your interconnect



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



- Obtain electron-spin transport physics-based simulation results

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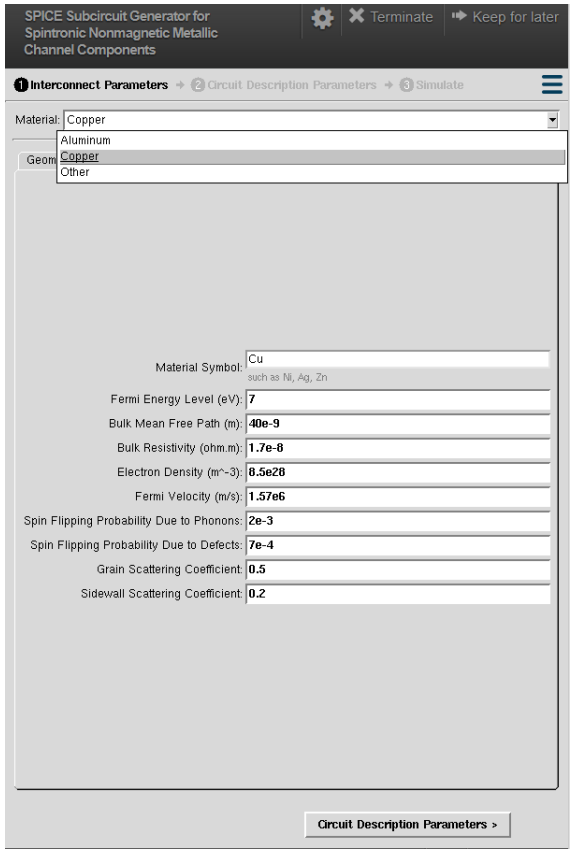
SPICE Subcircuit Netlist Generator for Spintronic Nonmagnetic Metallic Channel

nanohub.org/tools/spincircuit/



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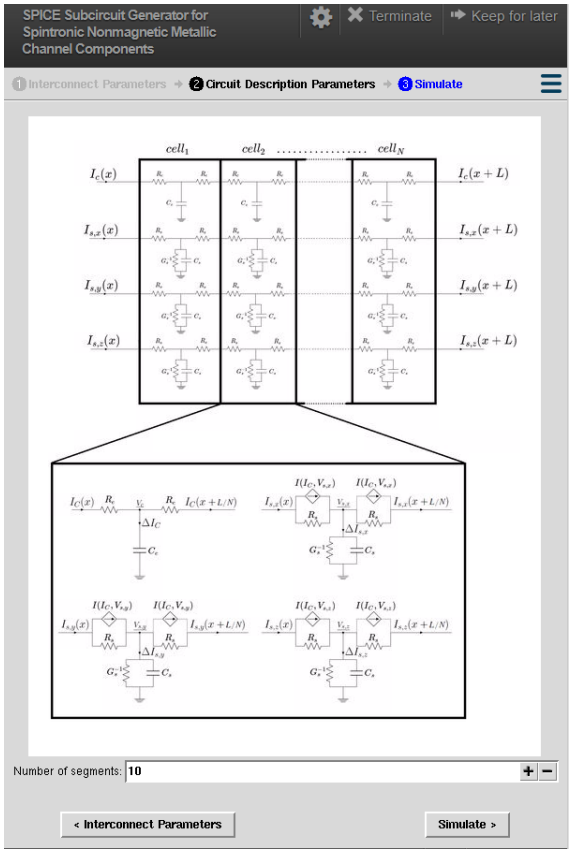
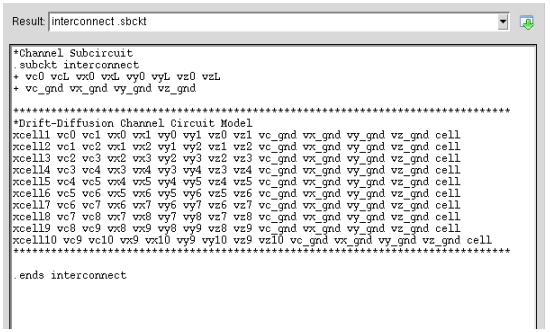
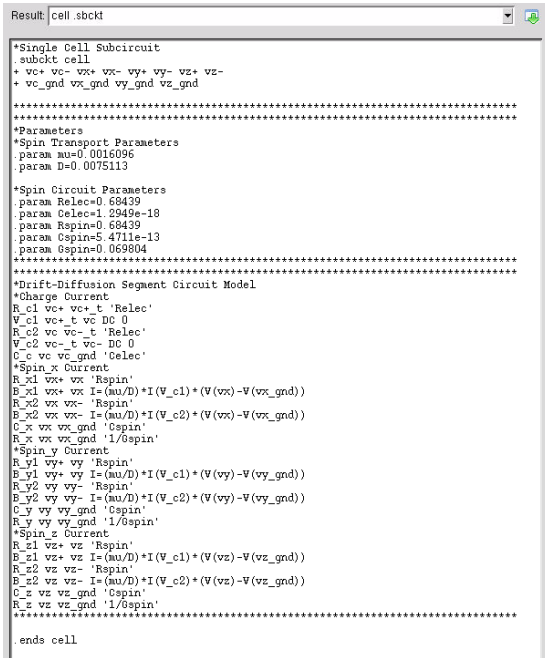


- Use developed compact circuit model for spintronic transport





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

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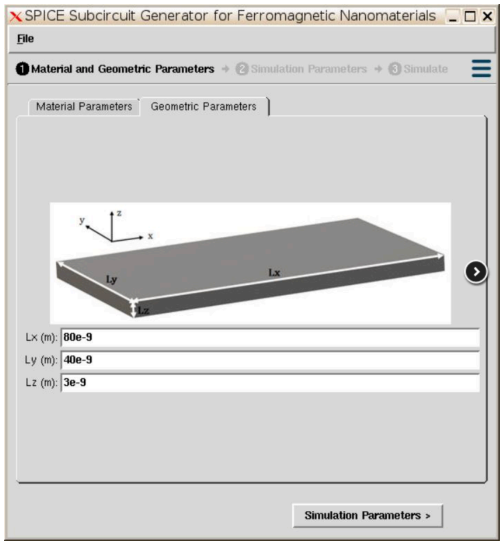
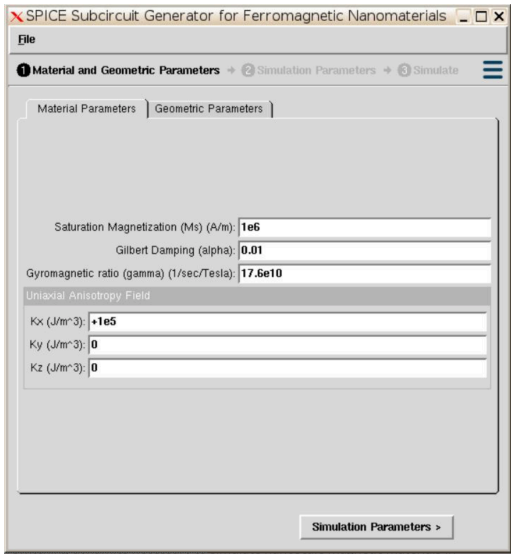
SPICE SubCircuit Generator for Ferromagnetic Nanomaterials





Since Feb. 2018, more than 40 users and 80 simulation runs.

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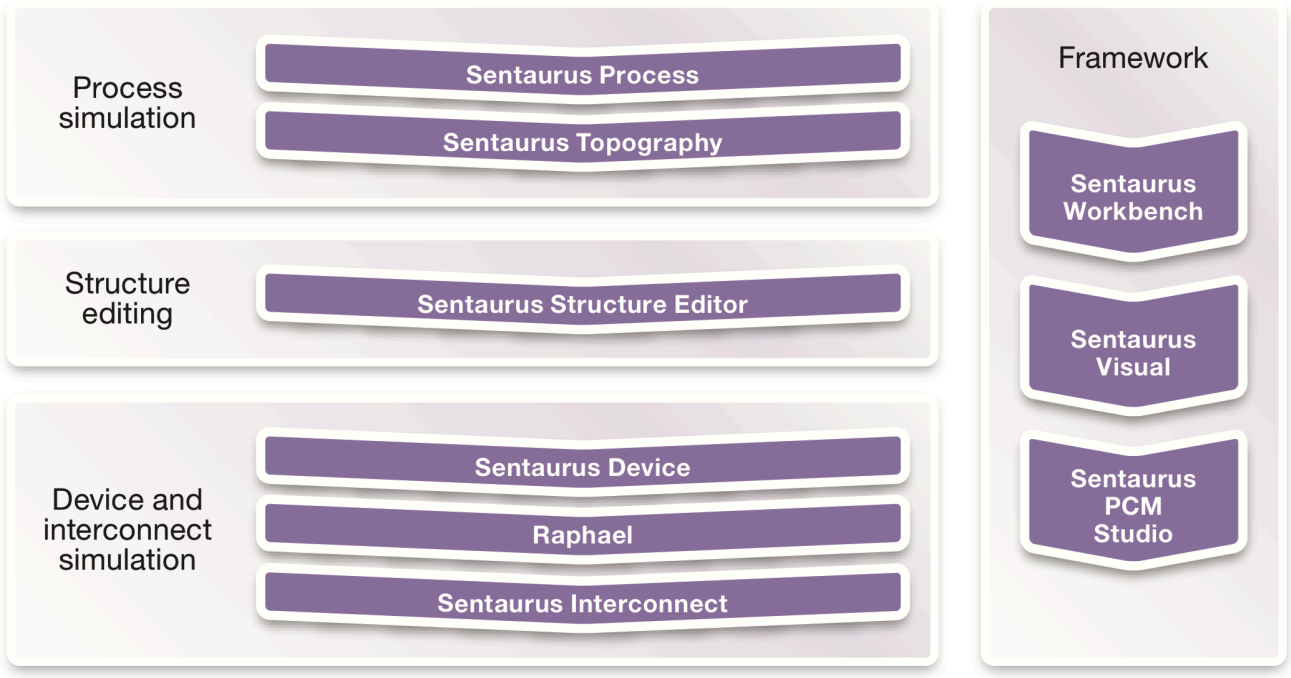
Synopsys TCAD Sentaurus Tools



Sentaurus TCAD Suite

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

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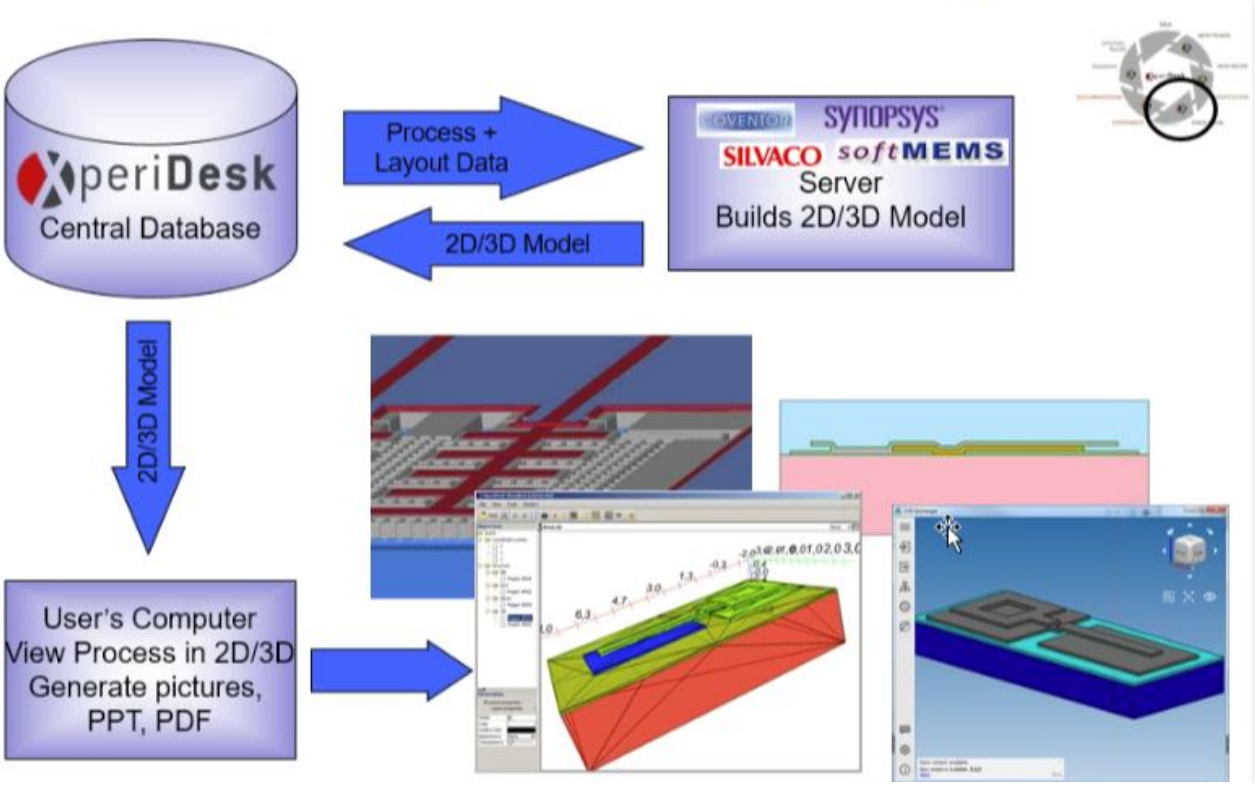
XperiDesk



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.

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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?