NNCI Computation

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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.

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

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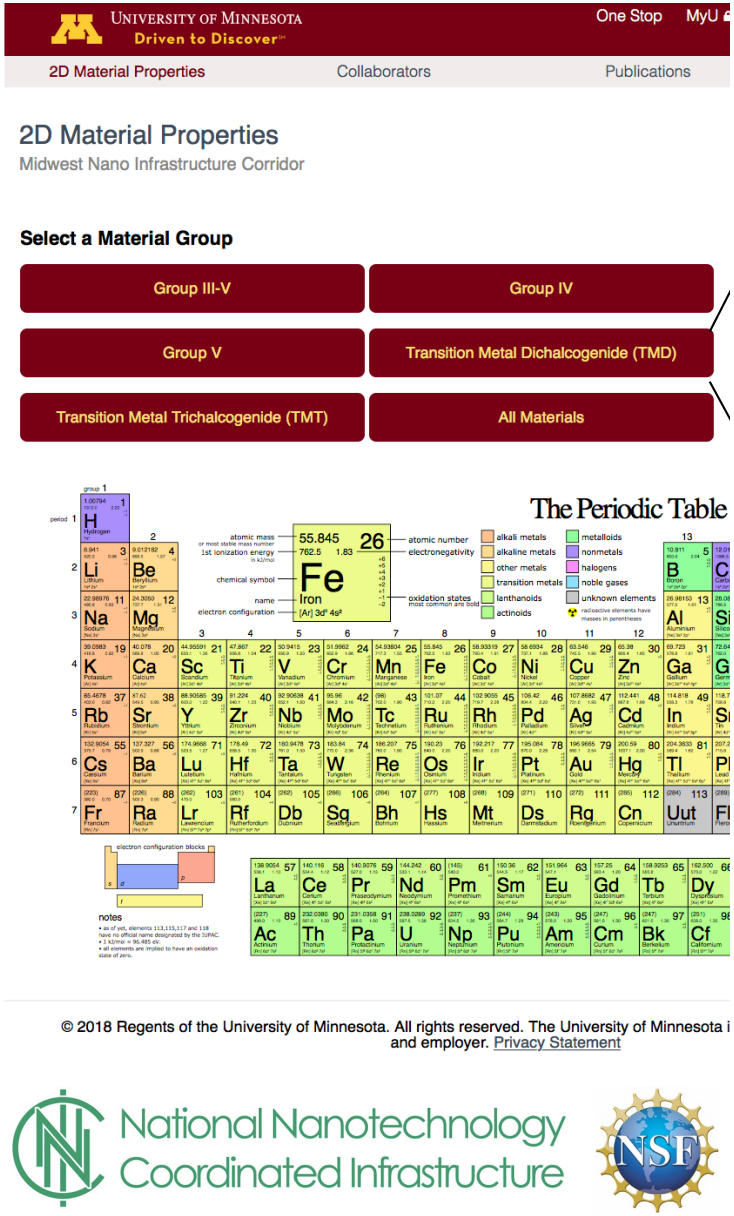
NSF

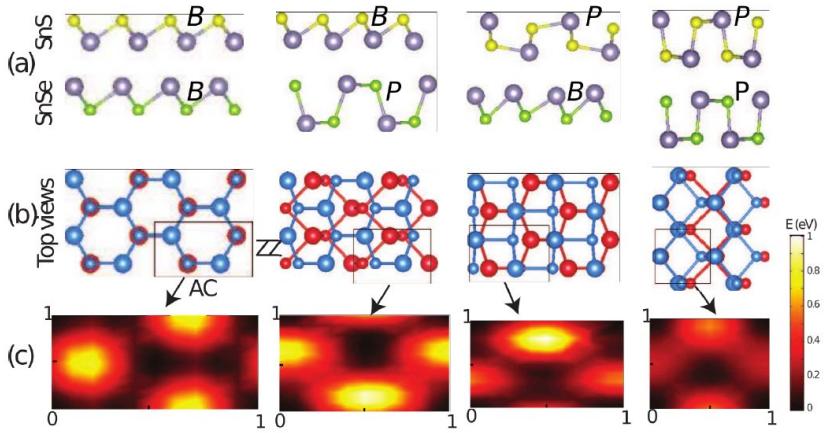
2D Materials Database on MNIC Website



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	----------	----------

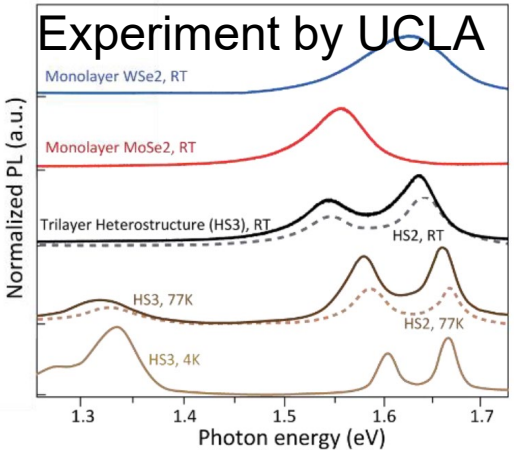
New Capabilities

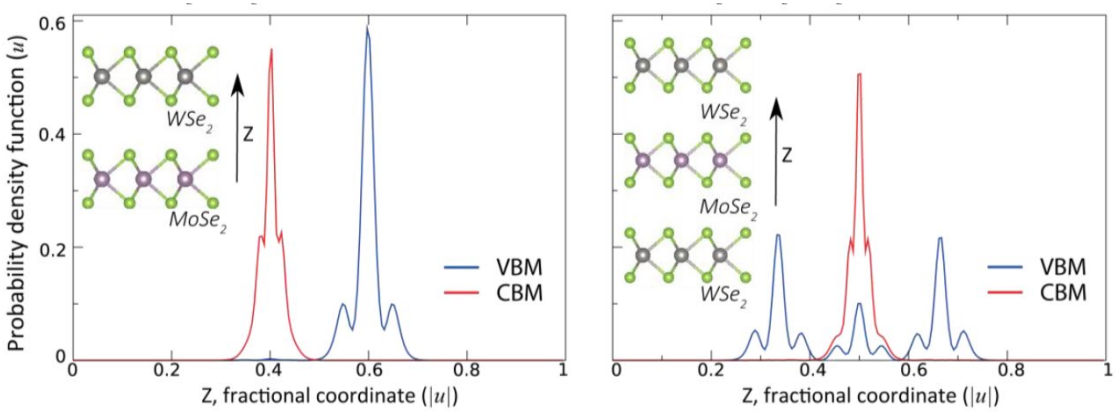
Mechanically stable tin-monochalcogenides heterostructure



O. Ongun et al, Phys. Rev. Mat., 051003 (2018)

2D materials heterostructures engineering for optoelectronics





C. Choi et al, to appear in Nature 2D Materials (2018)

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What is Next

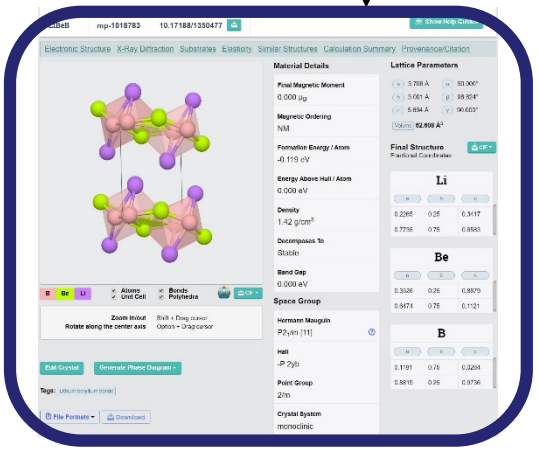
VASP Calculation using atomate

Final structures upload to database via atomate

mongoDB Atlas

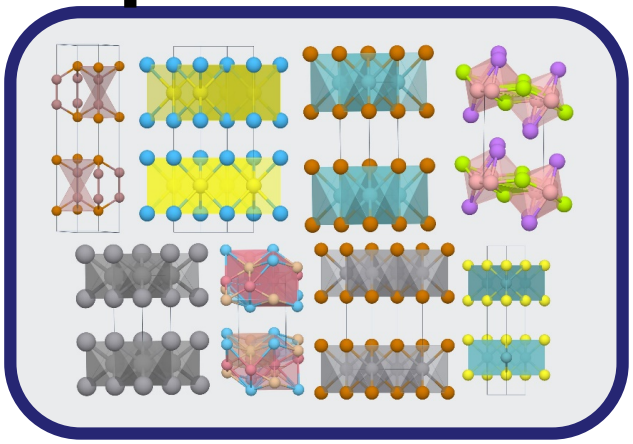
Currently under development!!

Website



python™

Machine Learning



Initial Structures

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Tony Low Group @ U Minnesota

2D Materials @Stanford

2D Device Trends

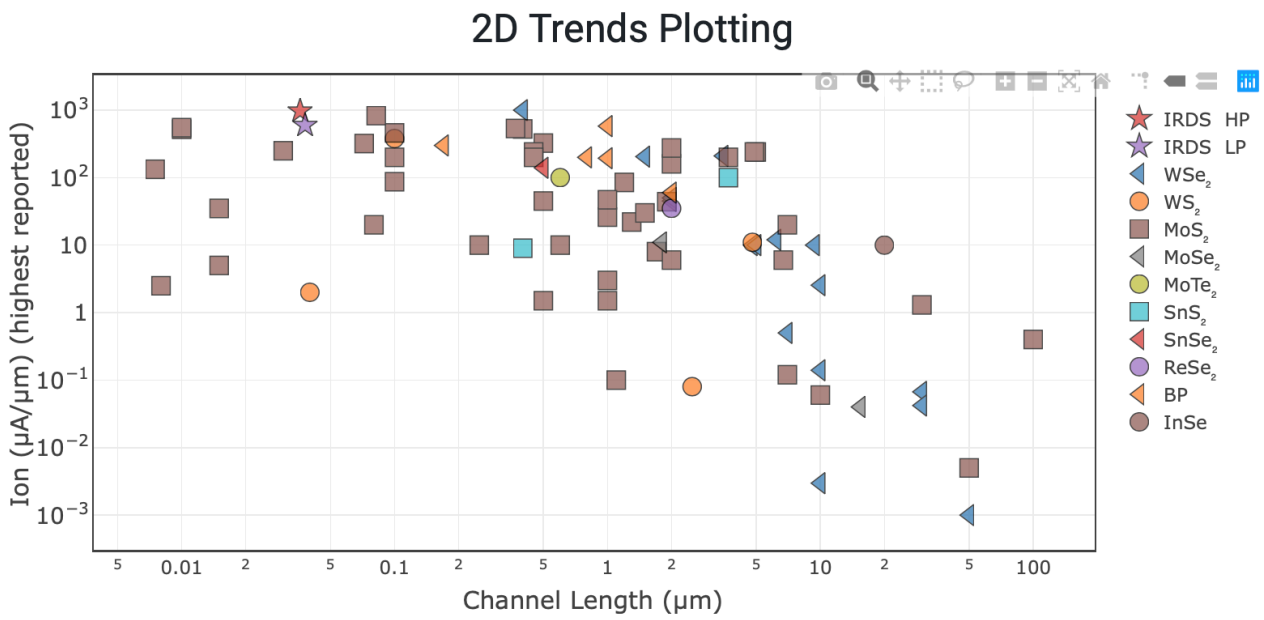
Select a x variable: Channel Length (μm) — linear log

Select a y variable: Ion (μA/μm) (highest reported) — linear log

Select a class: Material

Add Trend Line (not physical): Yes No

Some Conditionals: Highlight Monolayers, Only Monolayers



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Eric Pop, Stanford, http://2d.stanford.edu/2D_Trends

2D Materials @Stanford

2D Device Trends

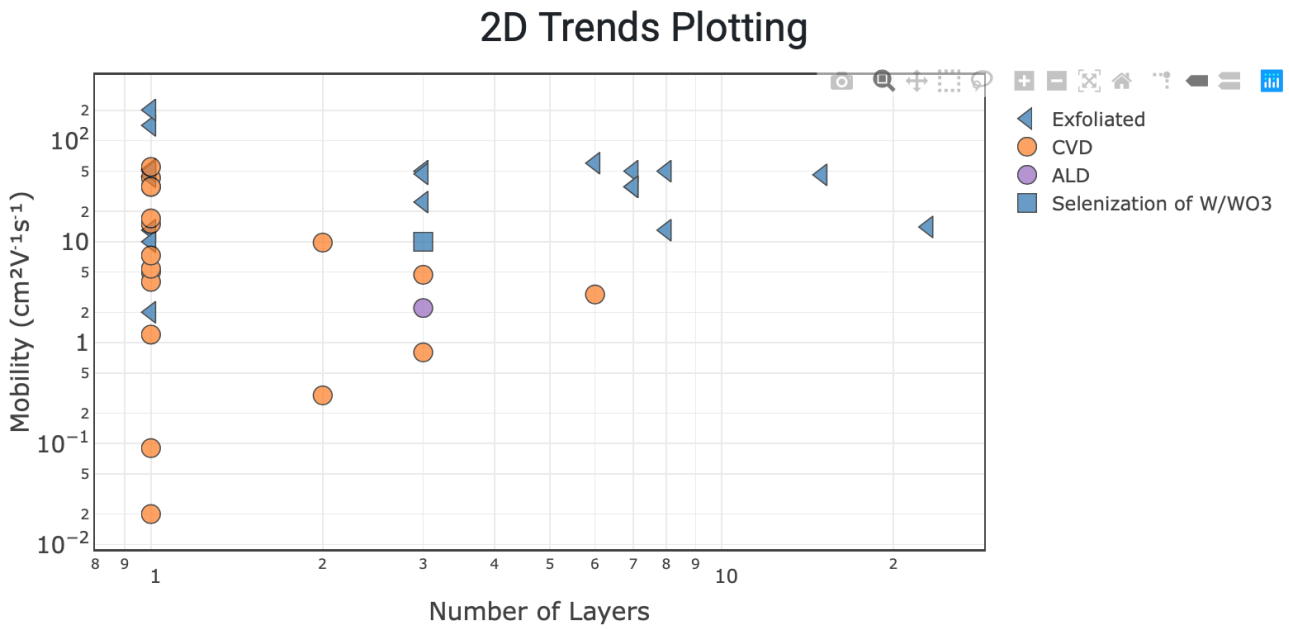
Select a x variable: Number of Layers (linear / log)

Select a y variable: Mobility ($cm^2V^{-1}s^{-1}$) (linear / log)

Select a class: Preparation Method

Add Trend Line (not physical): Yes / No

Some Conditionals: Highlight Monolayers, Only Monolayers



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Eric Pop, Stanford, http://2d.stanford.edu/2D_Trends

Pseudopotential Virtual Vault @ Cornel

- Database of over 1100 pseudopotential or PAW files.
- Available for Abinit, Quantum Espresso, Qbox, and Siesta.
- Search by periodic table element
- Search for pseudopotentials with specific properties
- http://nninc.cnf.cornell.edu

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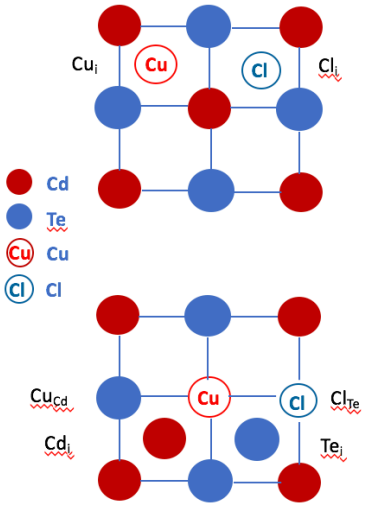
CNF Cornell NanoScale Science and Technology Facility

CdTe Solar Cells @ ASU

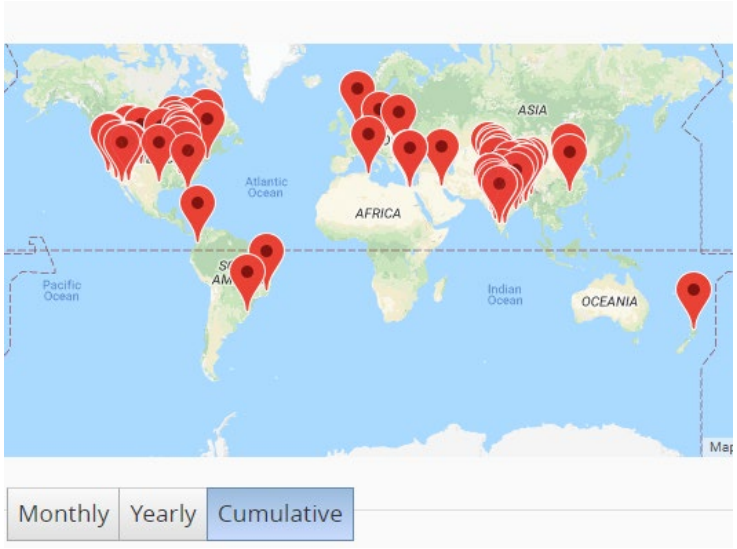
Physical Model: Point Defects

- **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)

Available on nanoHUB and used globally.



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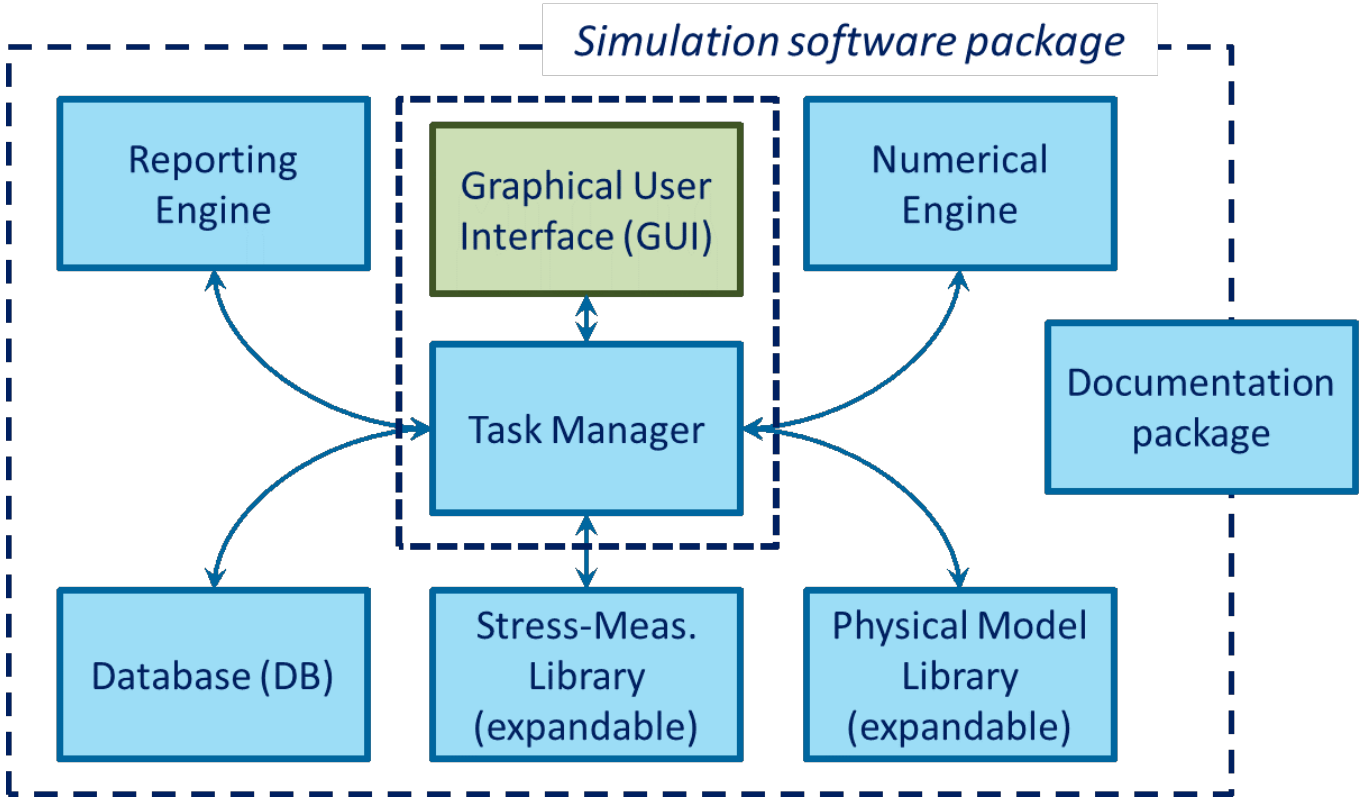
Limitations of PREDICTS Unified Solver

- Difficulties in extending the solver to incorporate new defect chemistry for Cl, As dopants.
  - Not user-friendly incorporation of DFT parameters.
  - Difficult to identify the root causes of issues.
- Numerical Algorithm instabilities with As defect chemistry for 0D reactions.
  - Mainly because of chain reactions.
- Cl diffusion and segregation at grain boundaries (GB) was not clear with the modeling assumptions.

From Da Guo, PhD Dissertation, Arizona State University 2017.

Next Generation: The PVRD-FASP Solver



Modules for the PVRD-FASP Solver. (FASP:= First Solar, ASU, SJSU, Purdue)

Abdul R Shaik, et al., "PVRD-FASP: A Unified Solver for Modeling Carrier and Defect Transport in Photovoltaic Devices", IEEE J. Photovoltaics, 2019 online

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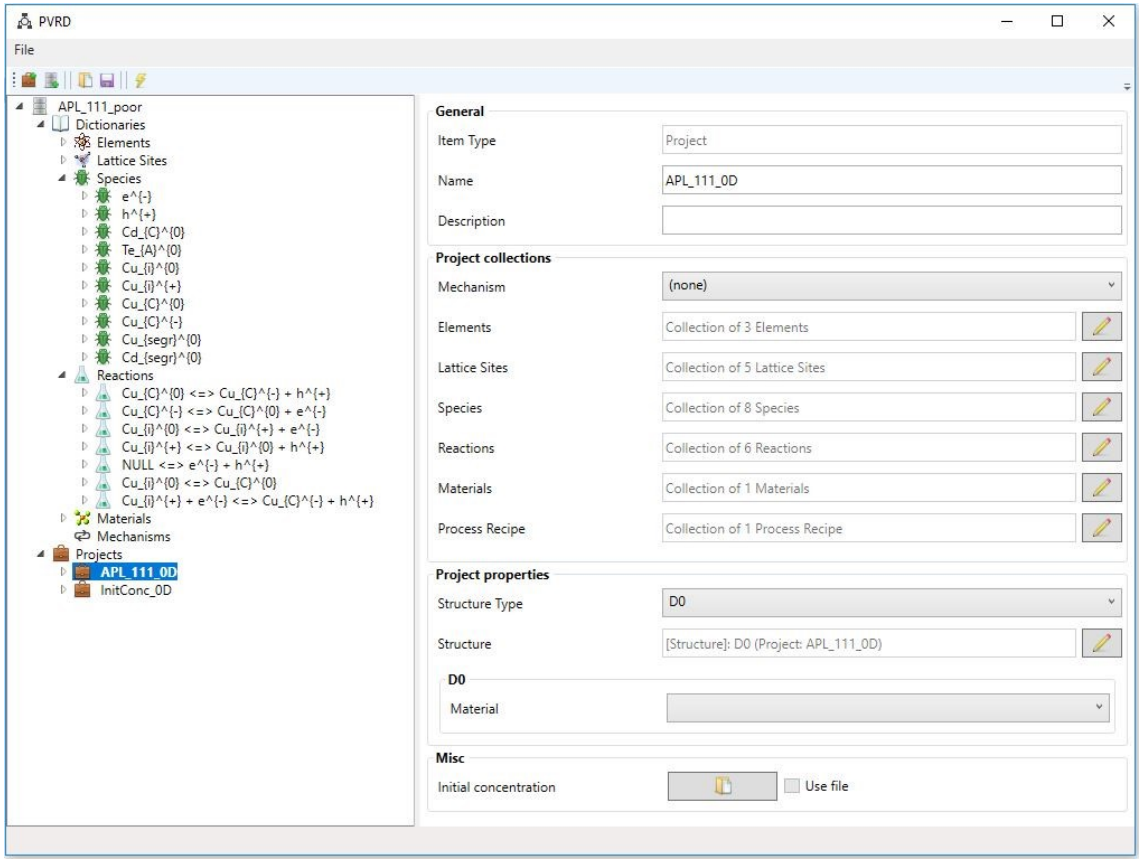
PVRD-FASP Graphical User Interface



The Tool and the documentation is publicly available online at http://pvrdfasp.com/

The Python based community version is available online at https://gitlab.com/abdul529/pycdts

Can be installed with python as

$ pip install pycdts

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CNF Nanoscale Simulation Cluster

- Users can make use of modeling software tailored for nanoscale systems, devices, & processes.
- Model with existing codes, develop and test new codes, or bring your own license for commercial software!
- Scientific Linux 7, SLURM, and OpenHPC
- New head node with 9TB of shared disk space
- 2 new compute nodes ea. w. 256GB RAM, 2 Intel Gold 6136
- 18 legacy nodes ea. with 24GB/32GB of R
  Xeons
- [illegible]

Available to both Local and Remote Users

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http://computing.cnf.cornell.edu/cluster

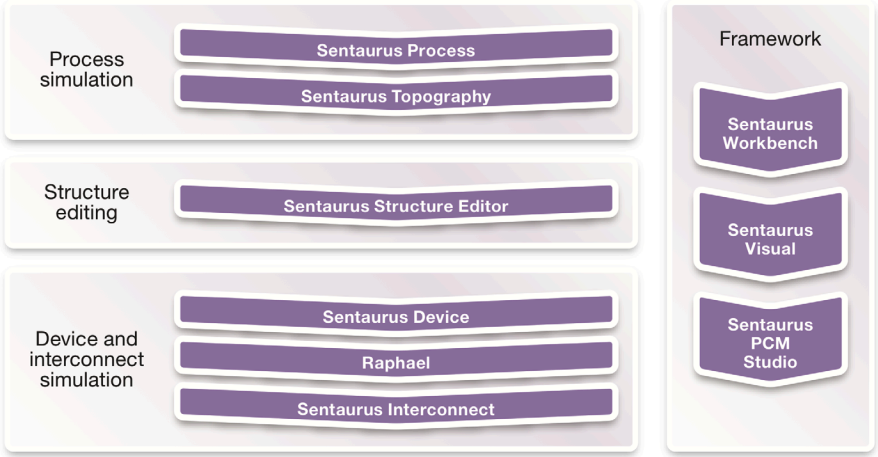
CNF Local Computing Capabilities

- Goal: support of users performing research at the CNF
- Windows workstations for CAD in computing lab and individual tool labs
- CNF Thin linux-based hotdesking… take your login session with you!
- Linux conversion computers and AWS cloud for simulations and conversion of files from GDS to tool native file formats
- Available software:
  Simulation: Coventor; PROLITH; Layout LAB; TRACER
  CAD: BEAMER; Autodesk; L-Edit; LinkCAD; Java GDS
  Image/Data Analysis: ProSEM; NanoScope Analysis; WinFLX

Commercial Tools

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

Tuition is waived for students, staff, and faculty affiliated with all NNCI sites even if their school does not have a license.



Sentaurus TCAD Suite

The typical license fee of some of the major simulation tools have been collected and shared with site directors.

Had some discussions with Coventor about a discounted license fee.

Summary

- New and updated databases and simulation tools have been released.
- Several major updates are forthcoming.
- Cornel Computing cluster came back on line last year.
- NNCI can potentially better negotiate with vendors.