### NNCI Computation

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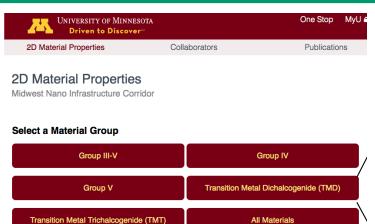
## Objectives

- 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.

### 2D Materials Database on MNIC Website



| period 1 | group 1<br>1.00794 220<br>H                            |  |  |  |  |   |  |   | _                                  | The  | e Per   | iodic   | Tab   | le                                    |
|----------|--|--|--|--|--|---|--|---|------------------------------------|--|---|---|---|---------------------------------------|
| 2        | Hydrogen<br>No<br>6.941 cose 3<br>Li<br>Uthium         | 2<br>9.012182<br>8855 1.57 4<br>Beylium<br>berylium                              | 1st ion  | atomic mass<br>able mass number<br>zation energy<br>in k2/mol<br>emical symbol | - 762.5  | e <sup>45</sup> .83 <u>2</u>                        | +6<br>+6<br>+5<br>+3<br>+2   | omic number<br>ectronegativi                        | ty alkali                          | i metals<br>ine metals<br>metals<br>ition metals | netalloi<br>nonmeti<br>halogen<br>noble ga          | als<br>s  | 13  | 12.01<br>108.5<br>Carbs               |
| 3        | 22.96976<br>66.8 0.88<br>Na<br>Sodium<br>Nei 2r        | 24.3050<br>7277 1.31<br>12<br>Magnesum<br>Nei 34                                 | 3  | name<br>configuration<br>4   | - [Ar] 30<br>5   | 6   | -2 m   | sidation state                                      | ectin                              | 10   | radioactive<br>masses in p                          | 12  | 20.90153<br>1773 1.01<br>Aluminium<br>Ne(30'30'               | 28.08<br>7845<br>Silco<br>78124       |
| 4        | 39.0583<br>19<br>K<br>Potasskum<br>(Ac)4e <sup>1</sup> | 40.078<br>5883 1.00 20<br>Caloum<br>(Attain                                      | 44.95591 21<br>Scandium<br>(A) 51 40                     | 47.867<br>585.8 1.54<br>Titanium<br>(4) 50' 40'                                | 50.9415<br>1239 135<br>Vanadum<br>(Ar)30*44 <sup>1</sup> | 51.9962 24<br>Chromium<br>(Actor 4e                 | 54.53804 25<br>7/23 1.55 25<br>Marganese<br>(41.56* 46*  | 55.845<br>N2.5 1.83 26<br>Fe<br>Ion<br>Io() 50* 60* | 58.93319 27<br>Cobat<br>Pr(35'44)  | 58.6934 28<br>Nickel<br>Mickel                   | Copper<br>(AC 54" 44"                               | 55.38<br>stat 4<br>2nc<br>period for test       | 60.723<br>104 141 31<br>Gallum<br>Pr/Det* 447 441             | 72.64<br>382.0<br>Germ<br>(He) 30*    |
| 5        | 85.4678<br>colo colo 37<br>Rubidium<br>pojsv           | 87.62<br>5435<br>Shortium<br>Shortium  | 88.90585 39<br>Yitskam<br> 9 40'50'                      | 91,224 40<br>40.1 1.33 40<br>Zrconium<br>NO APT Sof                            | 82 90538 41<br>Nicolium<br>(0) 47 50                     | 95.95 2.16 42<br>Molybolenum                        | (98) 1.50 43   | 101.07<br>7:0.2 2.30<br>Ruthenium<br>10) 44' 54'    | 102.9055<br>7197 2.20 45<br>Rhodum | 106.42 46<br>Pd<br>Palladium<br>90145*           | 107.8682 47   | 112.441<br>67.3 1.00<br>Cadmium<br>(0).44".54"  | 114.818 49  | 118.7<br>7065<br>Th<br>(M) 47         |
| 6        | 132.9054 55<br>  | 137.327 56<br>Sct 9 5.60 56<br>Barium<br>(k) or                                  | 174.9668 71<br>523.5 1.27 71<br>Lutetum<br>(sq) 41 52 54 | 178.49<br>98.5 1.30 72<br>Hafniam<br>(No) 47 52 60*                            | 180.9478 73<br>7810 1.50<br>Tantalum<br>(Ke) 41" Sorter  | 183.84<br>7700 2.36<br>Tungsten<br>(X4) 411 501 501 | 186.207<br>761.0 1.50<br><b>Ree</b><br>Rhenkum<br>(xij 4" sr ee  | 190.23<br>600 2.30<br>76<br>Osmium<br>(k) 4" 57 64" | 192.217 77                         | 195.084 78<br>Pt 228<br>Platinum<br>(x) 4" of to | 196.9685 79<br>801 2.54<br>Gold<br>(54) 41" 54" 65" | 80.59<br>Nort 2.00<br>Meacoby<br>(N) 4" 54" 64" | 204.3833 81<br>5934 152 81<br>Thallum<br>(ks) 41" 53" 64" 65" | 207.2<br>754<br>Pl<br>Lead<br>(Ne) 4P |
| 7        | (223) 0.70 87<br>Francium<br>(34(7))                   | (226) 5.00 88<br>Radum<br>Pictor   | (2662) 103<br>(25.0<br>Lawnencium<br>(567.52-52)         | (261) 104<br>100.0<br>Rf<br>Rutherfordium<br>Physics Set Set                   | (262) 105<br>Dibnum                                      | (200) 106<br>Seatorgium                             | (284) 107<br>Bh<br>Botnium   | (277) 108<br>Hassium                                | (268) 109<br>Mt<br>Metherium       | <sup>(271)</sup> 110<br>DS<br>Darmstadium        | (272) 111<br>Rg<br>Roentgenium                      | (285) 112<br>Copernicium                        | (284) 113<br>Uut<br>Ununtrium                                 | (280)<br>Flaro                        |
|          | s d  | tron configurati   | p  | 138.900<br>Sali 1<br>Lanthar   | Ce   |   |  |   | hium Samari                        | n Eu   | G   |   | D   | alum                                  |
|          | <ul> <li>1 k3/mol</li> </ul>                           | elements 113,115,<br>Icial name designat<br>= 96,485 eV.<br>Its are implied to h | ed by the SUPAC.   | (227)<br>Actinue<br>(Per Ger Tr  | 89 232.03<br>ar a<br>Thorius                             | 10 90 231.03  | 58 91 208.00<br>3 91 007.00<br>3 91 007.00<br>1.50 91 00<br>1.50 000 | 100 92 (237)<br>1.56 92 (01.5<br>NR                 | 93 (244)<br>54.7<br>PLUD           | 94 (243)   |   | n <sup>36</sup> (247)<br>Berkek                 | 97 (25.1)<br>50.0<br>Cf                                       | 98                                    |

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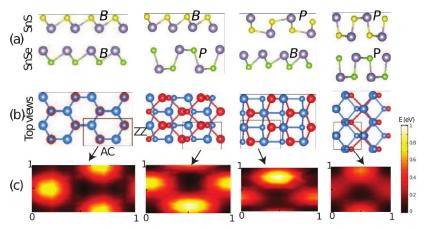




|                               | WSe2  |  |  |  |  |  |  |  |
|-------------------------------|---|--|--|--|--|--|--|--|
| Property                      | Property Description/Value  |  |  |  |  |  |  |  |
|                               | Bulk  | Monolayer  |  |  |  |  |  |  |
| Lattice constant (a)          | 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]<br>1.25 eV (calculation) [2]                                      |  |  |  |  |  |  |
| Coordination geometry         | Trigonal prismatic (W <sup>IV</sup> ),<br>Pyramidal (Se <sup>-2</sup> ) [3, 4, 7] | Trigonal prismatic (W <sup>IV</sup> ),<br>Pyramidal (Se <sup>-2</sup> ) [3, 4,7]             |  |  |  |  |  |  |
| Crystal structure             | hP6, space group P6 <sub>3</sub> /mmc, No<br>194 [3,7]                            | hP6, space group P6 <sub>3</sub> /mmc,<br>No 194 [3, 7]                                      |  |  |  |  |  |  |
| Appearance                    | Grey to black solid [3, 7]  |  |  |  |  |  |  |  |
| Group                         | Transition Metal<br>Dichalcogenide [7]  | Transition Metal<br>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 (ɛ1)=-22,<br>Imaginary part (ɛ2)=-10 (at<br>1.7 eV incident photon<br>energy) [10] |  |  |  |  |  |  |
| Effective masses              |   | $m_e = 0.53 m_o, m_h = 0.52 m_o$<br>[11]   |  |  |  |  |  |  |
| Effective Bohr radius         |   |  |  |  |  |  |  |  |
| Thermal expansion coefficient |   | 11.08×10 <sup>-6</sup> /°C [12]  |  |  |  |  |  |  |
| Bulk Modulus (B)              |   |  |  |  |  |  |  |  |
| Refractive Index              |   | 5.68 [13]  |  |  |  |  |  |  |
|                               | Carrier mobility in WSe <sub>2</sub>  |  |  |  |  |  |  |  |
| Thicknesses                   | BN/SiO <sub>2</sub> /Si substrate   | SiO <sub>2</sub> /Si Substrate   |  |  |  |  |  |  |
| 8 nm                          |   | ~350 cm <sup>2</sup> /V.Sec (hole) [14]  |  |  |  |  |  |  |
| Monolayer                     | ~31 cm <sup>2</sup> /V.Sec [15]   |  |  |  |  |  |  |  |
| Bulk                          |   |  |  |  |  |  |  |  |

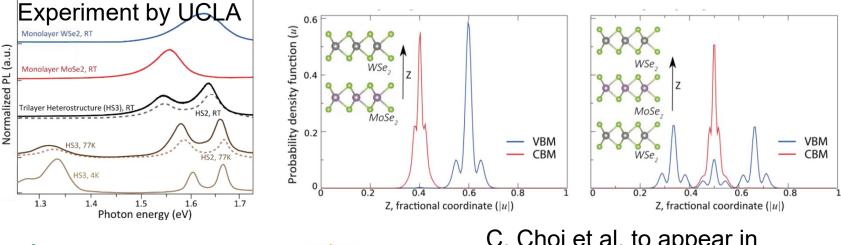
### New Capabilities

### Mechanically stable tin-monochalcogenides heterostructure



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

### 2D materials heterostructures engineering for optoelectronics

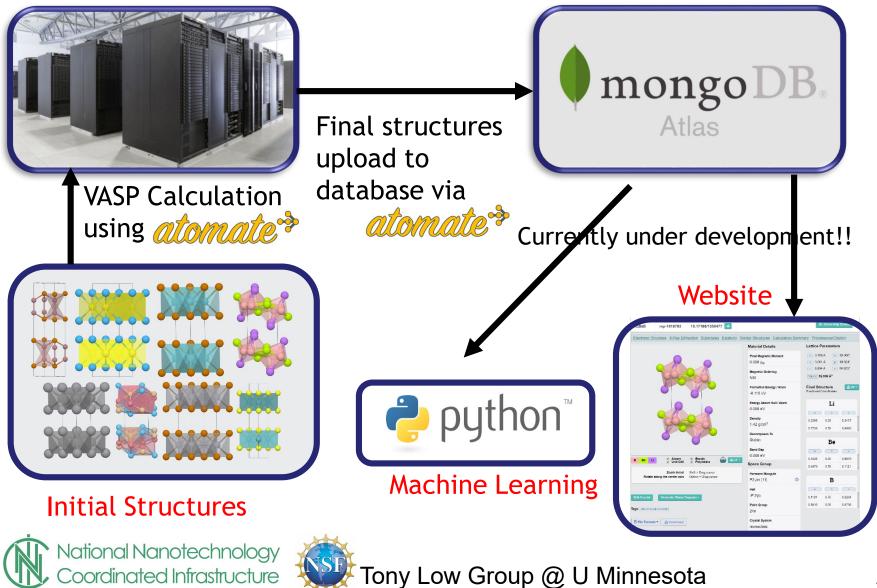


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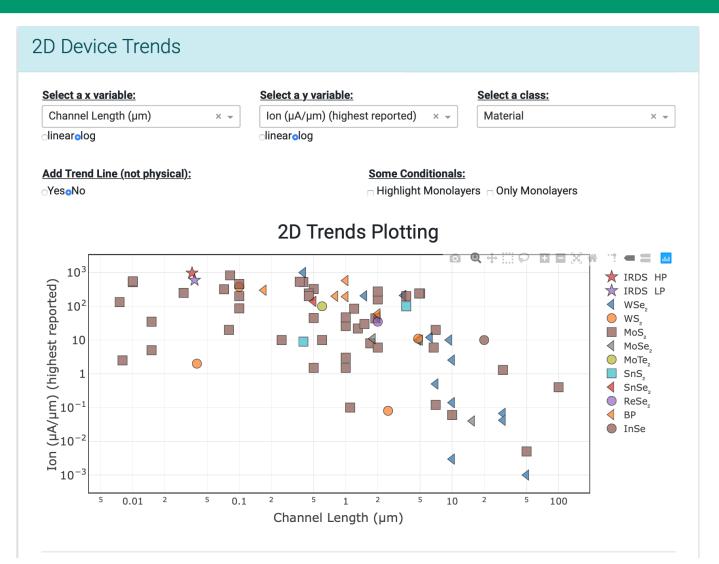


## C. Choi et al, to appear in Nature 2D Materials (2018)

### What is Next



### 2D Materials @Stanford



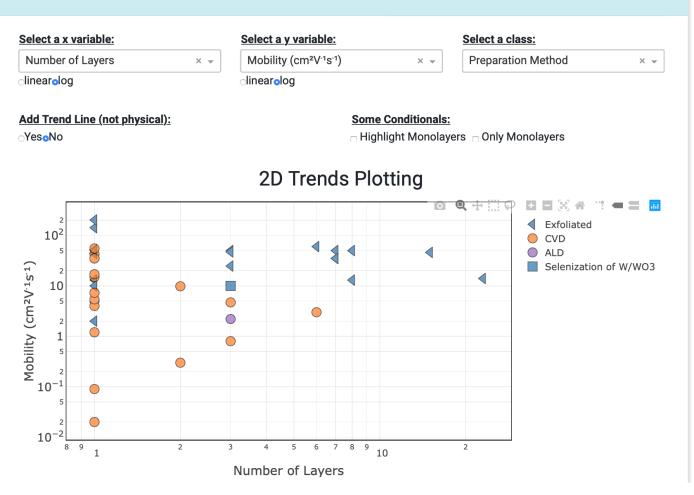
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Eric Pop, Stanford, http://2d.stanford.edu/2D\_Trends

### 2D Materials @Stanford

#### 2D Device Trends





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





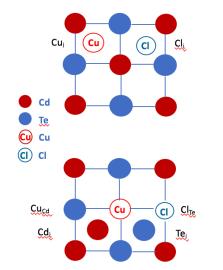




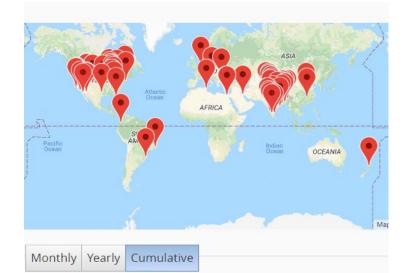
### CdTe Solar Cells @ ASU

### Physical Model: Point Defects

- Intrinsic Defects in CdTe:
  - Cd<sub>i</sub>(0/2+), V<sub>cd</sub>(0/2-), Te<sub>i</sub>, Cd<sub>Te</sub> ...
- Extrinsic Defects in CdTe:
  - <u>Cu Defects</u>
     Cu<sub>i</sub>(0/+), <u>Cu<sub>cd</sub>(0/-), Cd<sub>i</sub>-Cu<sub>cd</sub>(0/+)</u>...
  - <u>Cl Defects</u> <u>Cl<sub>i</sub>(0/±)</u>, <u>Cl<sub>Te</sub>(0/+)</u>, <u>Cl<sub>Te</sub>-V<sub>Cd</sub>(0/-)</u>...
  - <u>Cu-Cl Complexes</u>
     <u>Cl<sub>Te</sub>-Cu<sub>Cd</sub>(0), Cl<sub>i</sub>-Cu<sub>Cd</sub>...
    </u>



Dragica Vasileska, ASU (NCI-SW)



Available on nanoHUB and used globally.





# Limitations of PREDICTS Unified Solver

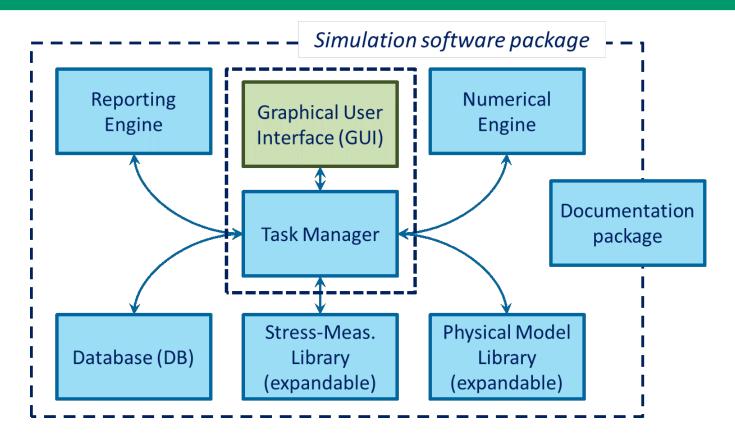
- Difficulties in extending the solver to incorporate new defect chemistry for CI, As dopants.
  - > Not user-friendly incorporation of DFT parameters.
  - Difficult to identify the root causes of issues.
- Numerical Algorithm instabilities with As defect chemistry for 0D reactions.
  - Mainly because of chain reactions.
- CI 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 <u>http://pvrdfasp.com/</u>

The Python based community version is available online at <u>https://gitlab.com/abdul529</u> <u>/pycdts</u> Can be installed with python as \$ pip install pycdts





### **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

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- 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 Xeons

u/cluster

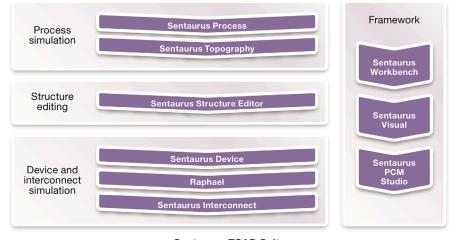
### **CNF Local Computing Capabilities**

- 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: <u>Simulation</u>: Coventor; PROLITH; Layout LAB; TRACER <u>CAD</u>: BEAMER; Autodesk; L-Edit; LinkCAD; Java GDS <u>Mindel Potata Anolicies</u>: <u>Excenteriore</u> NanoScope Analysis; <u>Winel V</u>

### **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.







- 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.



