Data Analytics for Discovery and Design of 2D Materials

Richard G. Hennig, University of Florida

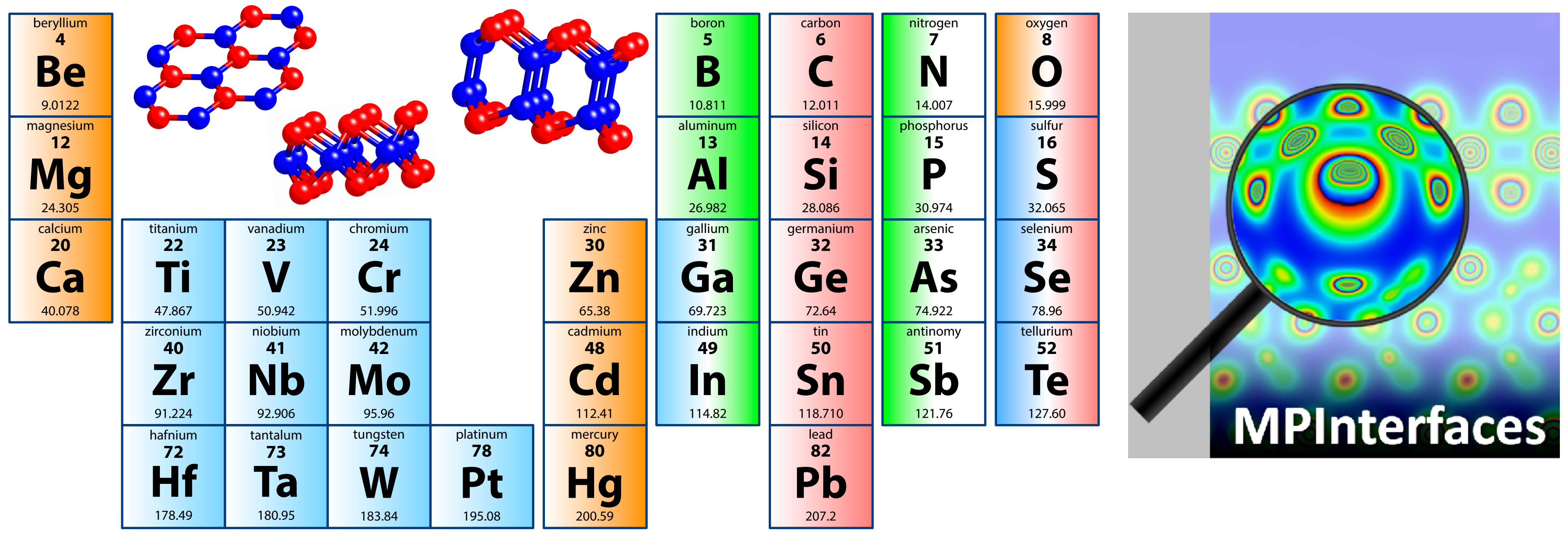
Search for 2D Materials

VASPsol

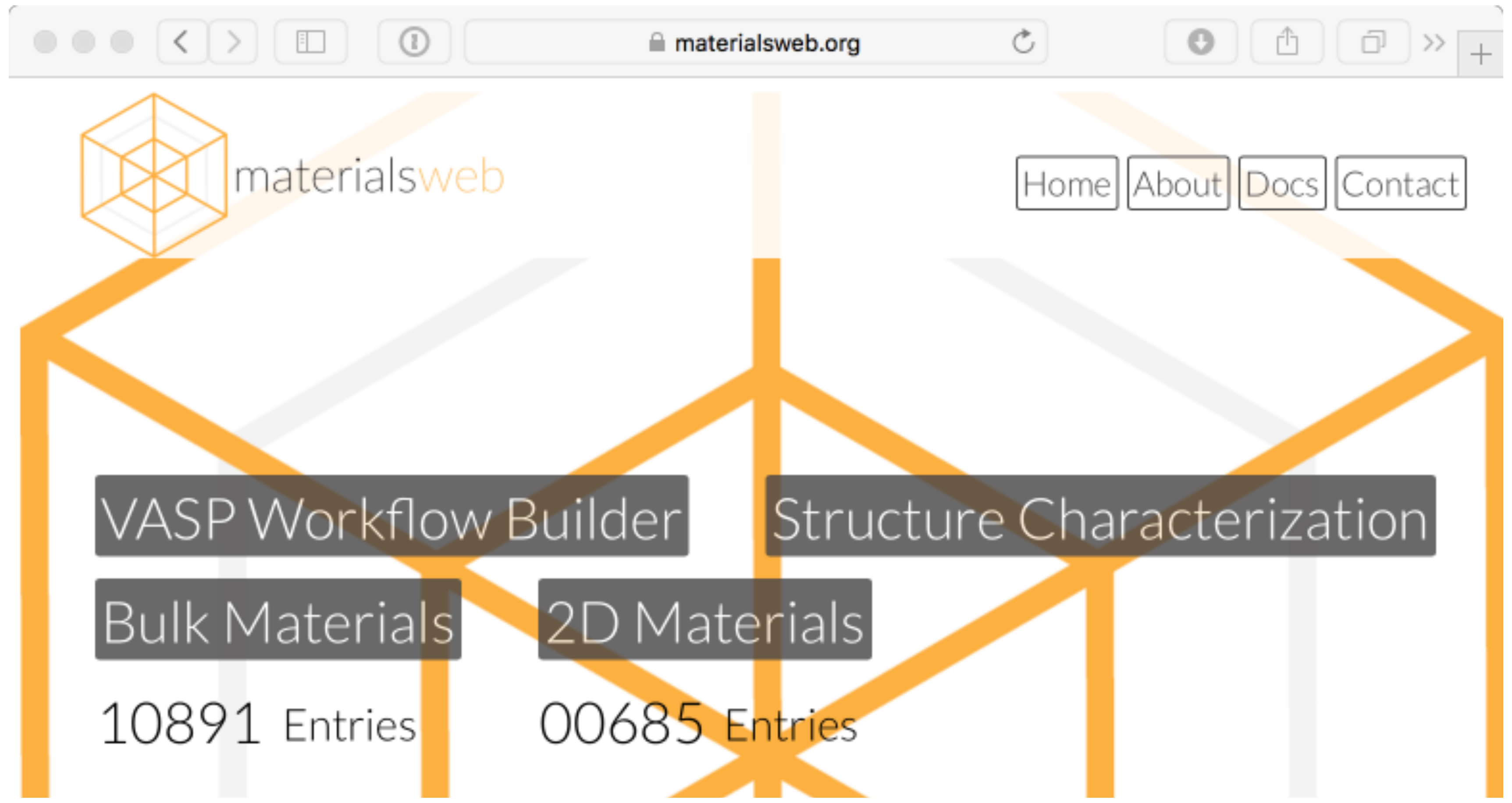
- Materials structure and microstructure
- Input from experiment required
- Need for new methods for non-equilibrium defects and processing
- Role of ML for dimensionality reduction

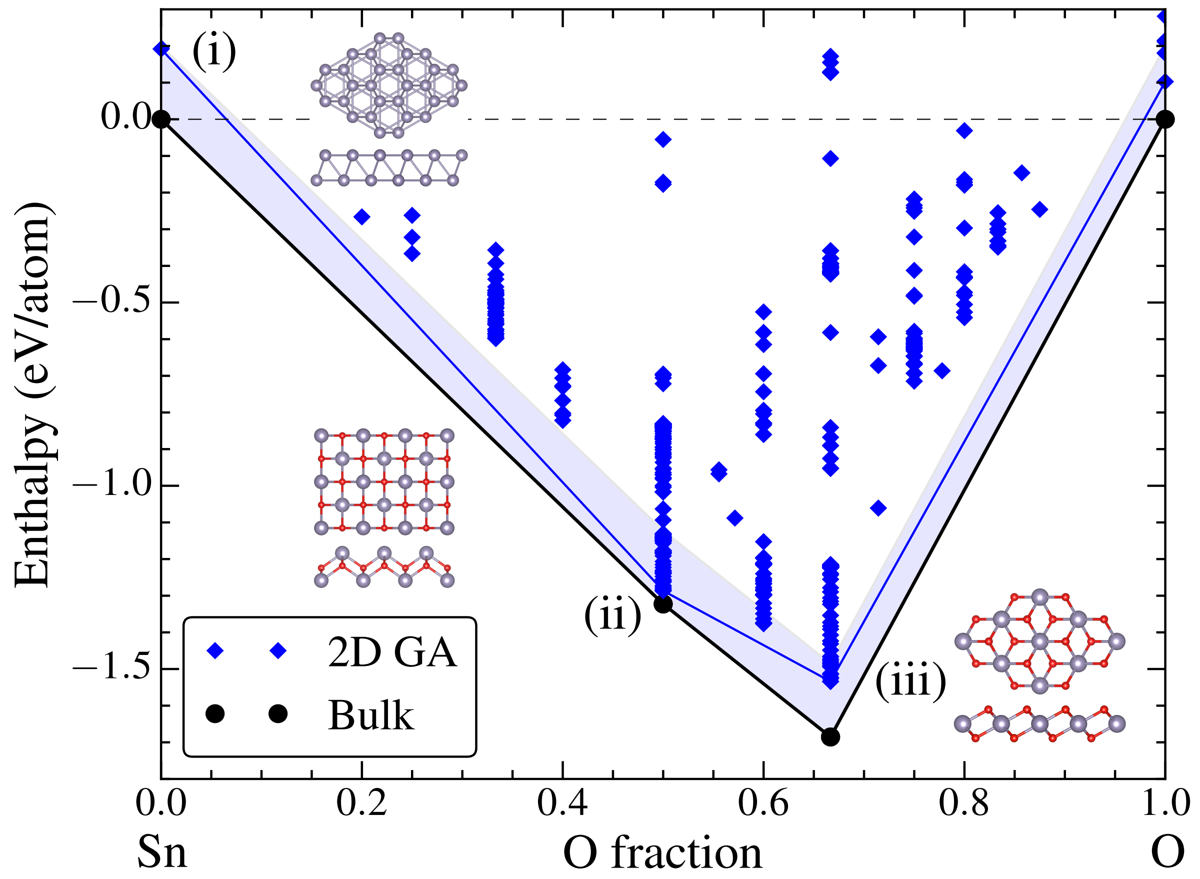
VASPSol - Ab initio methods for solid/liquid interfaces

MPInterfaces - High throughput framework for 2D materials



Data available at http://materialsweb.org

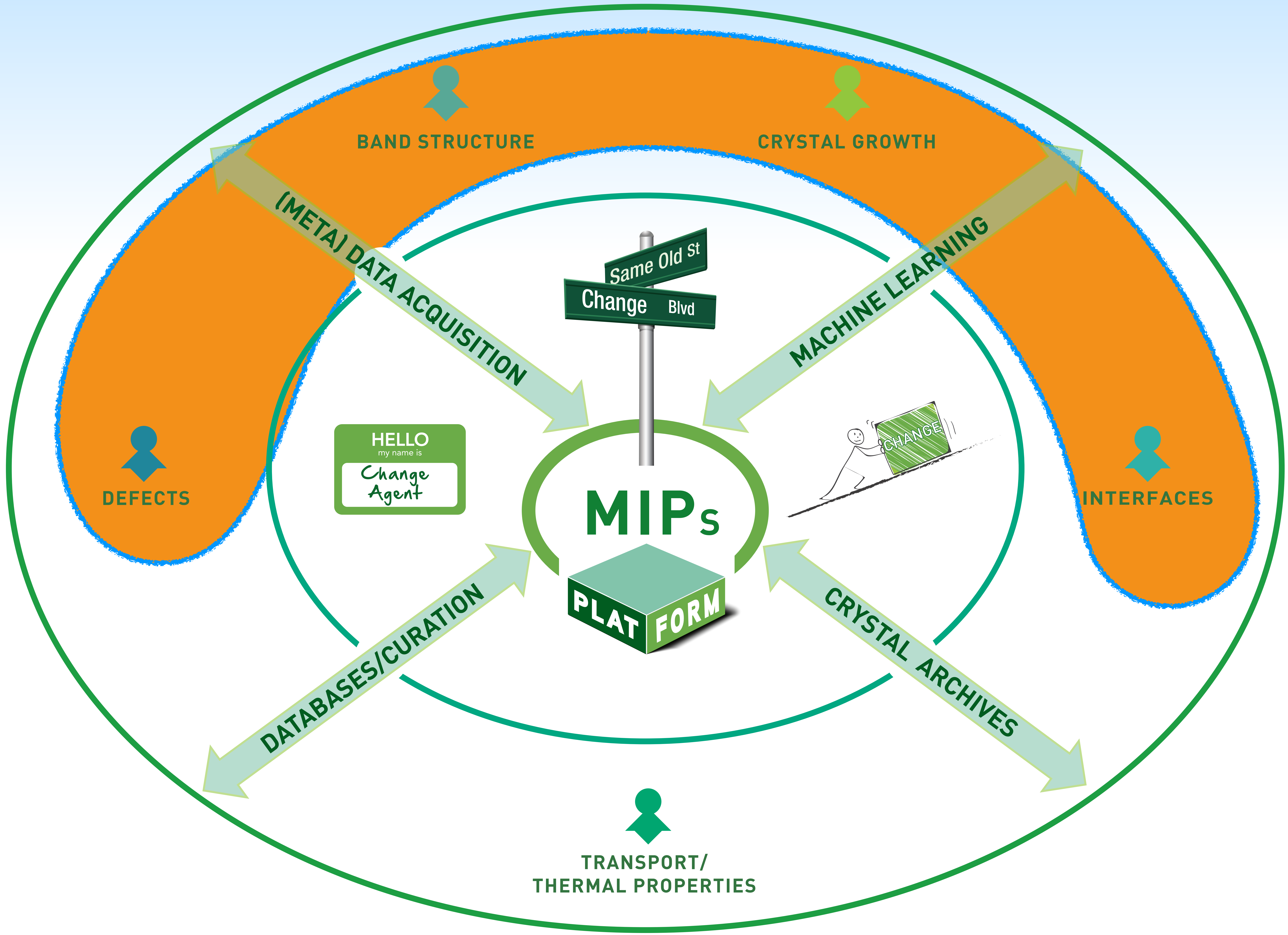




GASP - Genetic algorithm and machine learning for structure predictions

Powered by MPInterfaces & materialsweb

Open source available at https://github.com/henniggroup



BAND STRUCTURE
CRYSTAL GROWTH
DEFECTS
INTERFACES
TRANSPORT/
THERMAL PROPERTIES
(META) DATA ACQUISITION
MACHINE LEARNING
DATABASES/CURATION
CRYSTAL ARCHIVES
Same Old St
Change Blvd
HELLO
my name is
Change Agent
CHANGE
MIPs
PLATFORM

Acknowledgment

- MPInterfaces and novel 2D materials: K. Mathew, A. Singh, M. Ashton, J. Paul, D. Gluhovic, H. Zhuang, J. Gabriel, M. Blonsky, M. Johannes, R. Ramanathan, R. Duan, Z. Ziyu, F. Tavazza, S. Sinnott, D. Stewart
- GASP genetic algorithm and machine learning: B. Revard, W. Tipton, A. Yesupenko, S. Honrao, S. Xie, A. M. Tan, B. Antonio
- Financial support by NSF, DOE, NIST
- Computational resources: HiPerGator@UF, NSF XSEDE, and Google Cloud Platform

NSF NIST

Center for BRIGHT BEAMS
A National Science Foundation Science & Technology Center

Office of Basic Energy Sciences • Serving the Present, Shaping the Future •

XSEDE

HiPerGator 2.0
The University of Florida Supercomputer

Google Cloud Platform

Powered by
MPInterfaces & materialsweb

rhennig@ufl.edu
http://hennig.mse.ufl.edu

Data Analytics and Materials Informatics

Data Analytics

- <u>Discovery</u>, <u>interpretation</u>, and <u>communication</u> of meaningful patterns in data and applying those patterns towards effective decision making

Materials Informatics

- Applies the principles of informatics to materials science and engineering to better understand the use, selection, development, and discovery of materials

Types of data

- Computational and experimental structures, properties, processing
- Detailed meta data to enable retrieval and machine-learning of patterns

Data analytics needs

- Identify promising candidate materials
- Enable close comparison between ab-initio theory and measurements

Source: Wikipedia.org

Goal: Generate relevant data for materials discovery and design.

Part I: Hierarchy of Materials Structures

Materials Hierarchy - Structure Classification

Long-range order present? Measured by sharp diffraction peaks.

Yes → Crystal

No → Glass

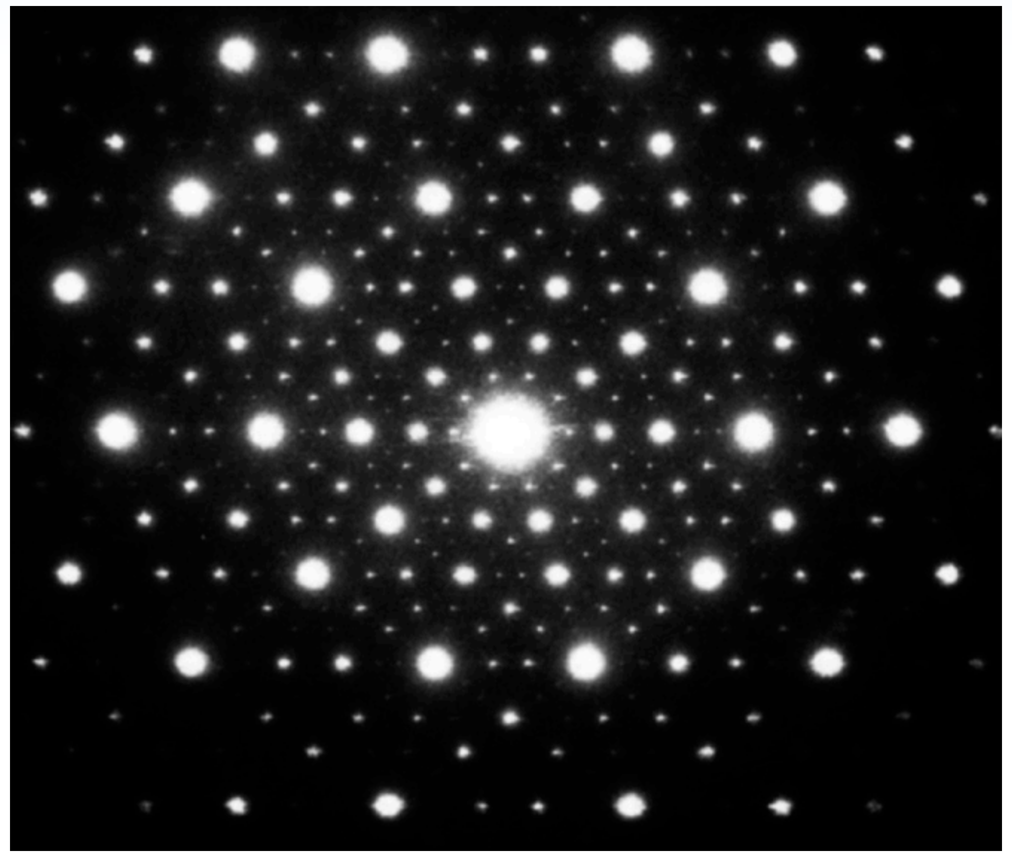
$$\mathbf{k} = \sum_{i=1}^{n} h_i \mathbf{a}_\mathbf{i}^*$$

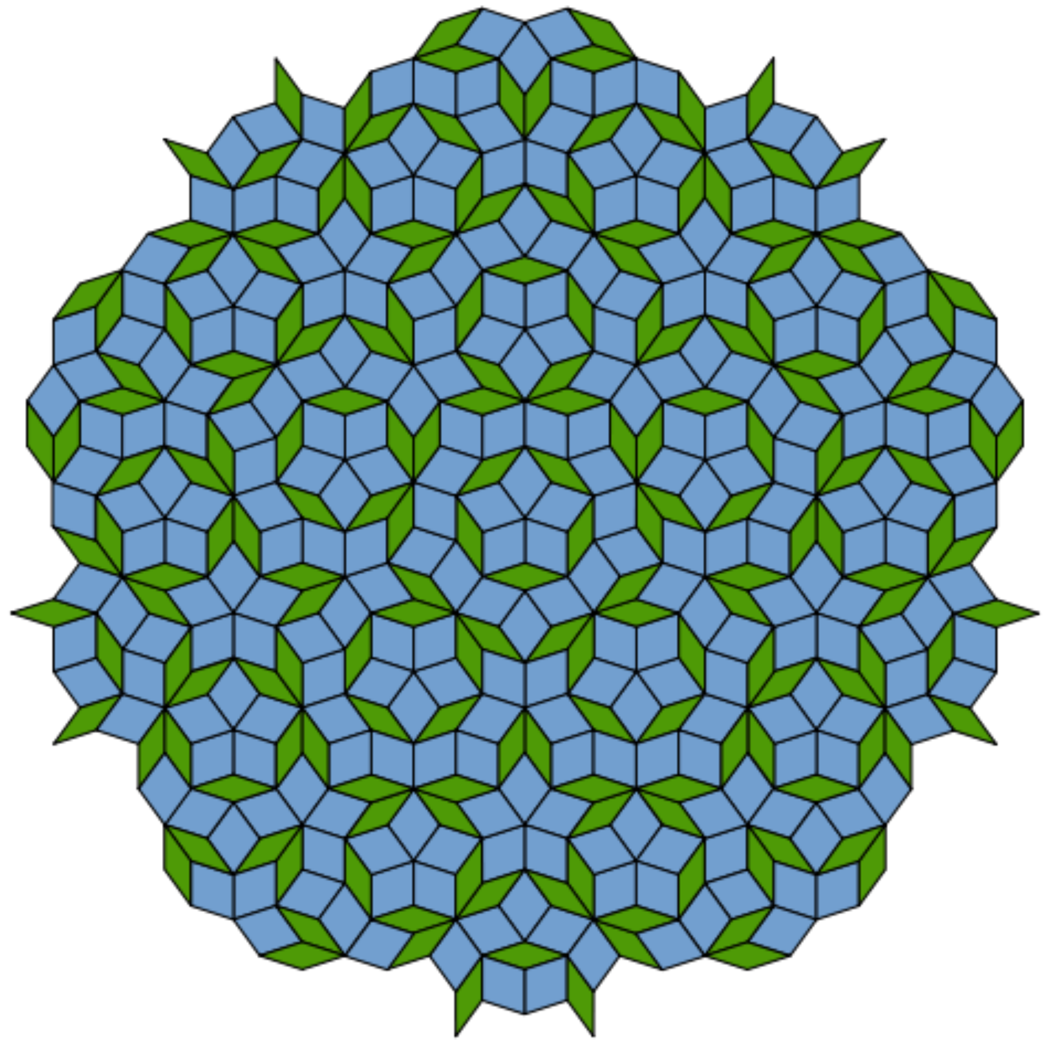
Crystal:

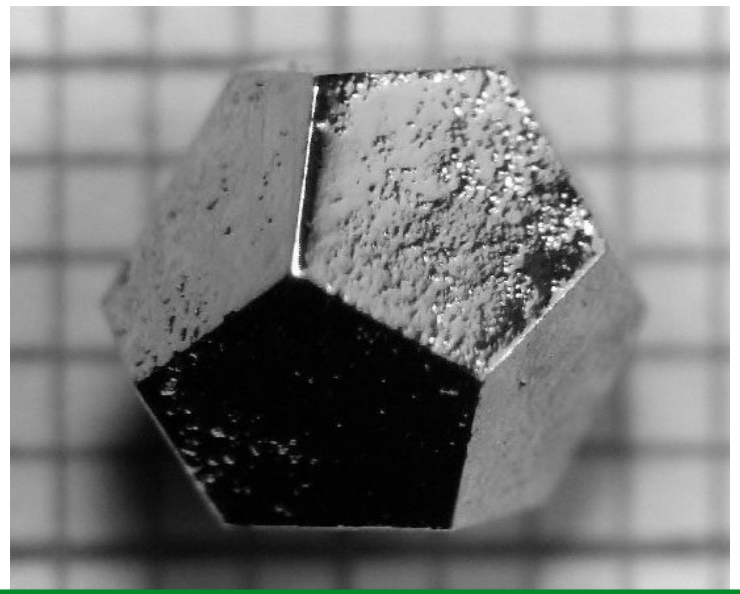
- *n=d* → Periodic crystal
- *n>d* → Aperiodic crystal

Aperiodic crystal – Forbidden rotations:

- Yes → Quasicrystal
- No → Incommensurate crystal





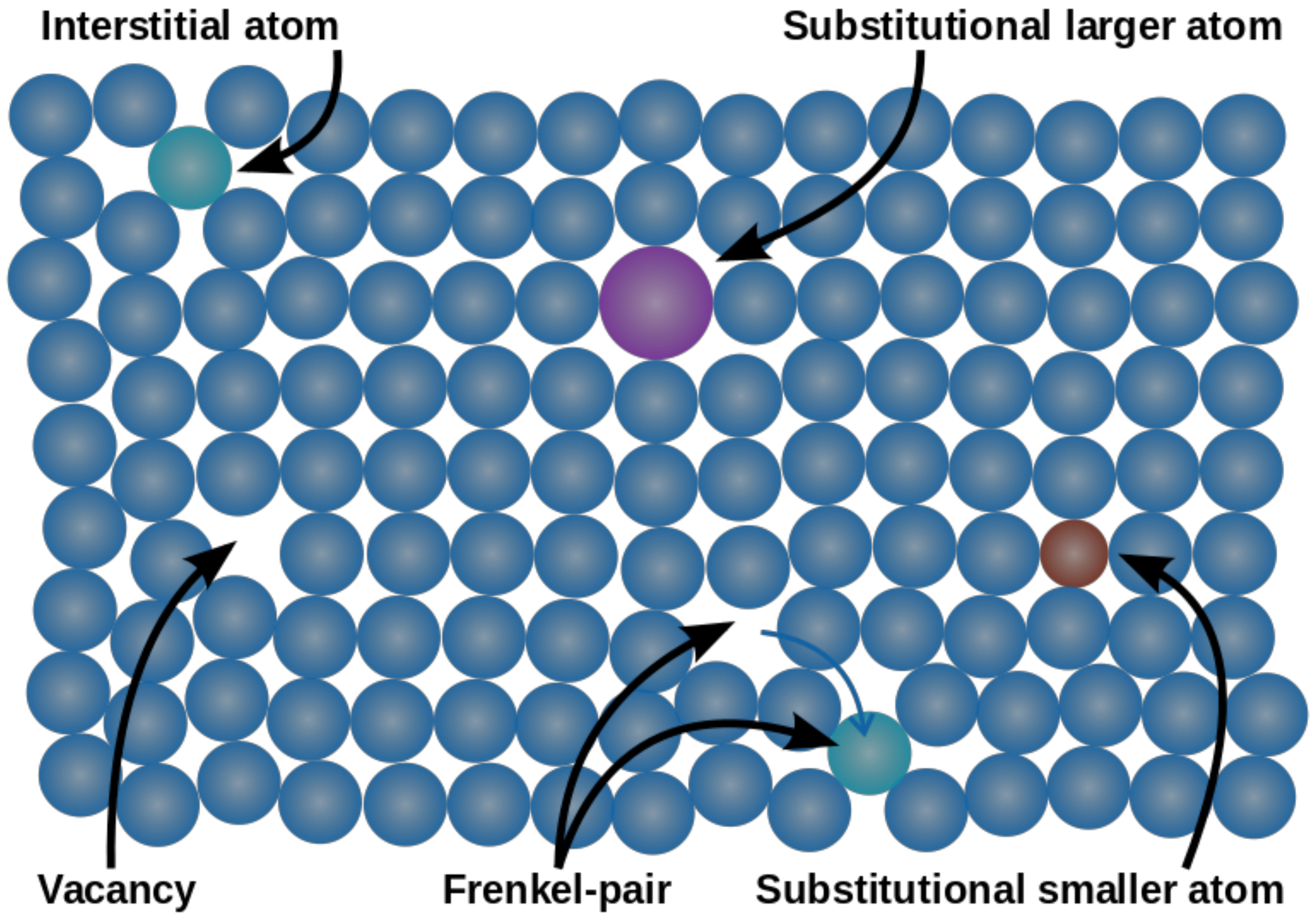


- Lack of translational symmetry complicates methods
- Concepts of unit cell(s), tilings, lattice sites
- Complication due to partial occupancy of lattice sites

Structures lacking periodicity require new computational methods.

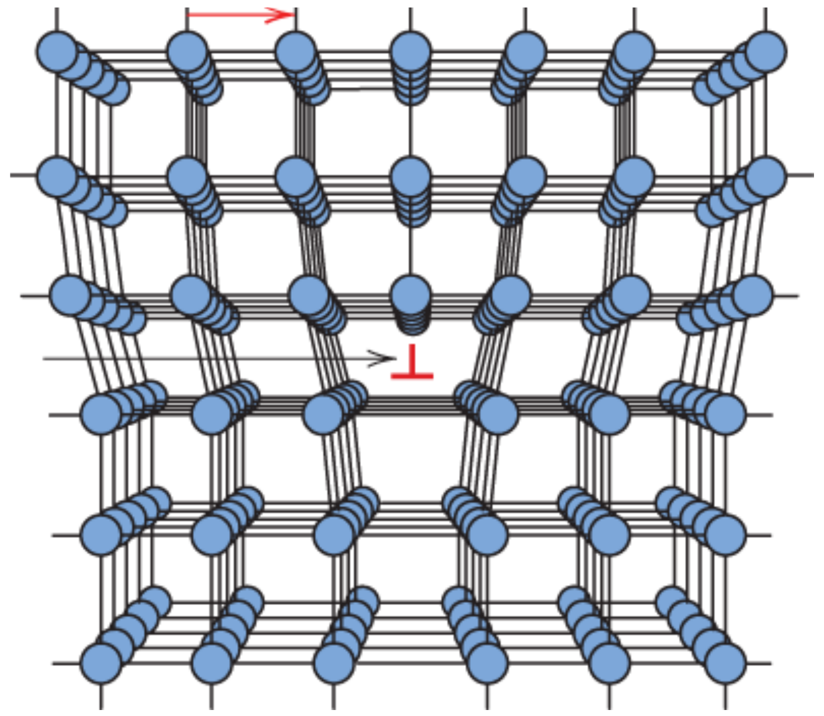
Materials Hierarchy - Defects by Dimensionality

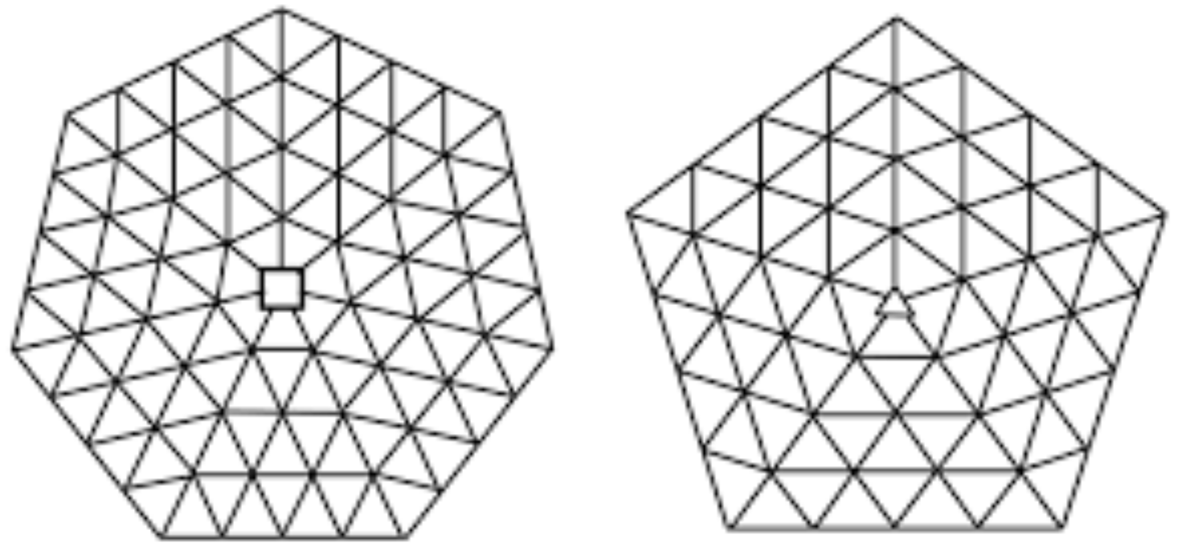
0D - Point defects
present in thermodynamic equilibrium



1D - Line defects
present in thermodynamic equilibrium

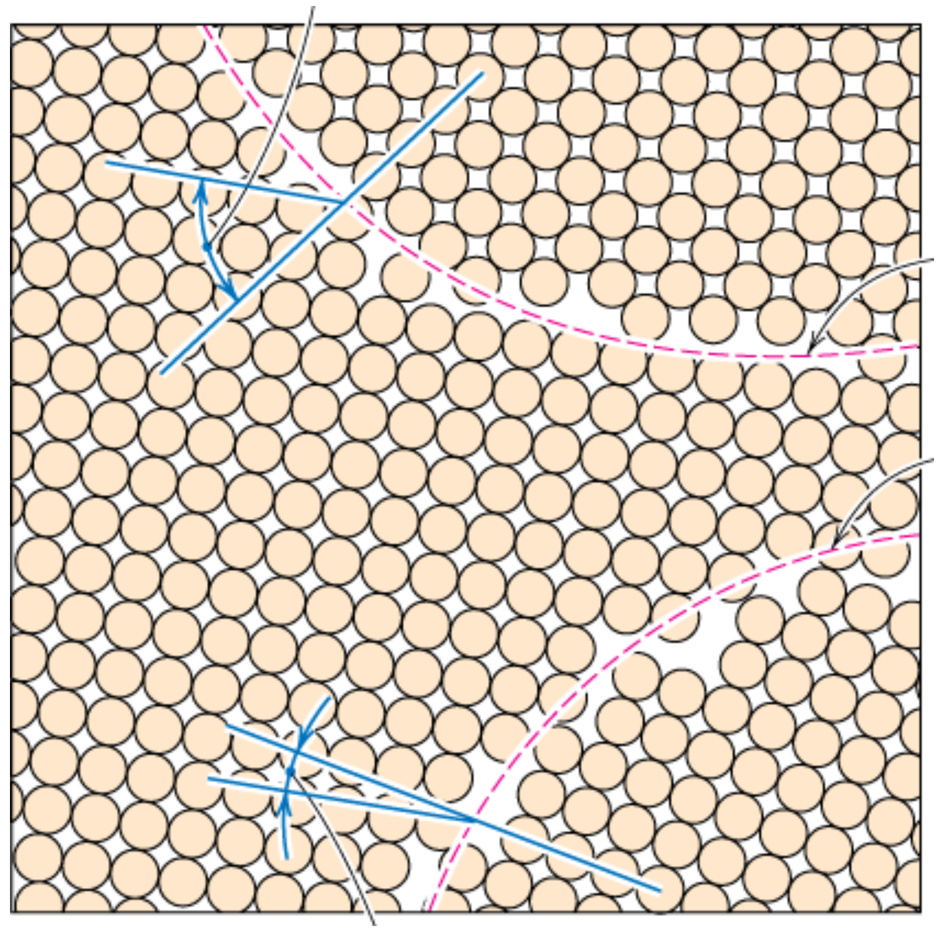
Dislocations





Disclinations

2D - Area defects
Stacking faults, twin, grain,
and interface boundaries, surfaces

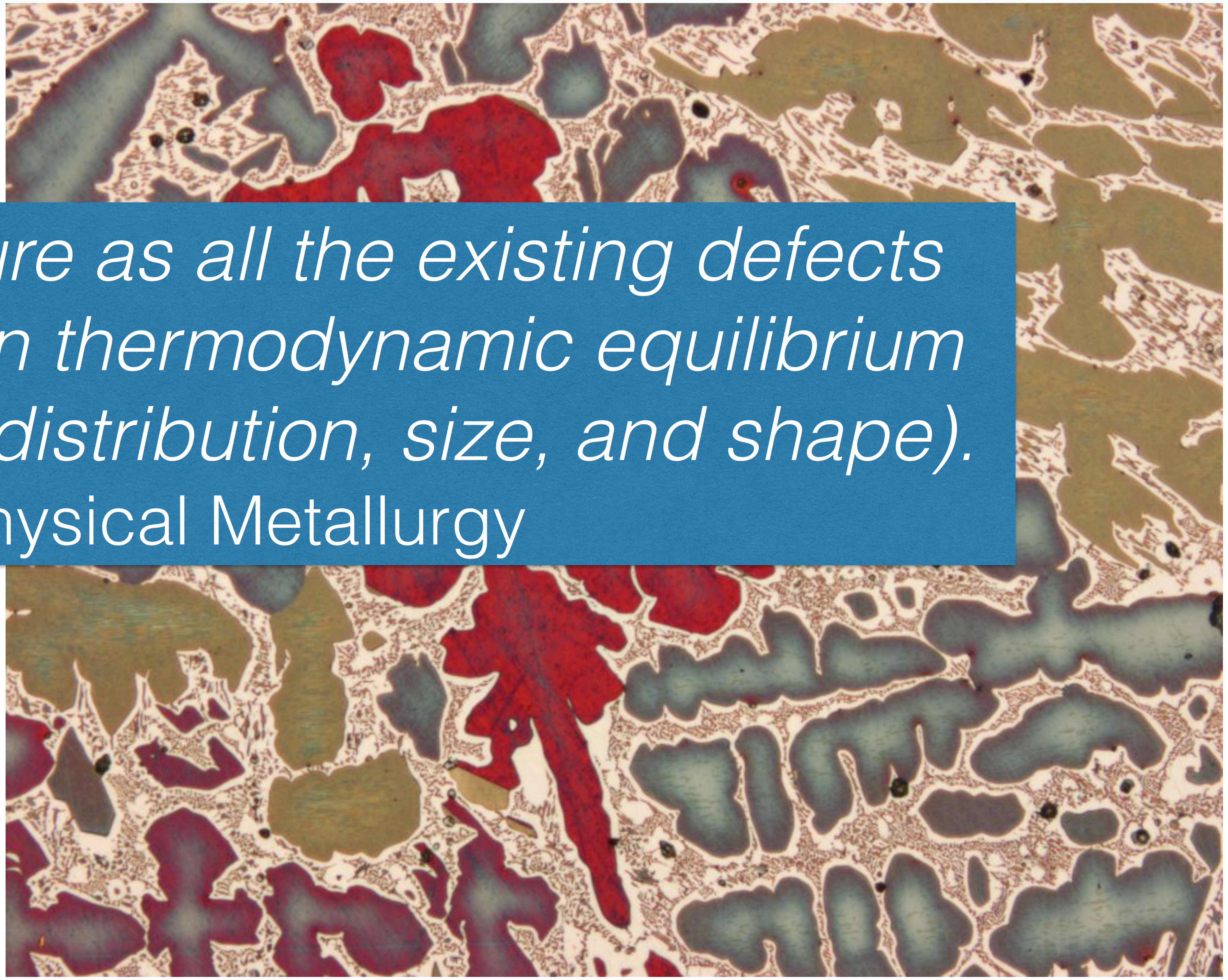


3D - Volume defects
Precipitates, voids, inclusions

High-throughput methods for 1D to 3D defects needed

Materials Hierarchy - Microstructure

- Combination of crystal/amorphous structure, point defects, and microstructure
- Microstructure is processing dependent
- Modelling of processing requires **dimensionality reductions**
  ⇒ Oppo
- Issue is **objectiv**
- Overcome by merging Physics and AI?
- Incorporate knowledge of possible phases and defects requires multiscale approaches
- Opportunity to develop and use defect databases



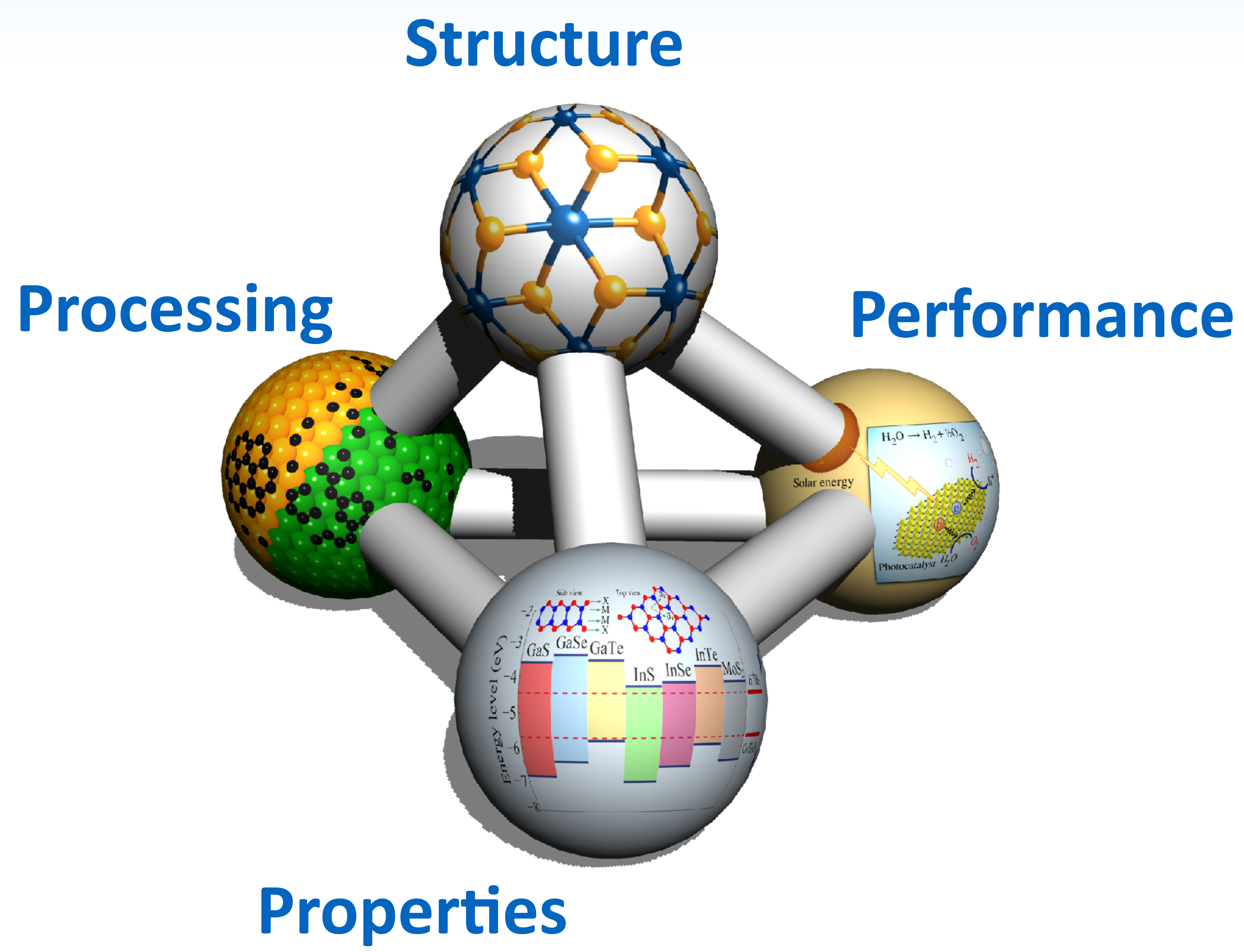
We thus define microstructure as all the existing defects in a material, which are not in thermodynamic equilibrium (according to type, number, distribution, size, and shape).
Peter Haasen, Physical Metallurgy

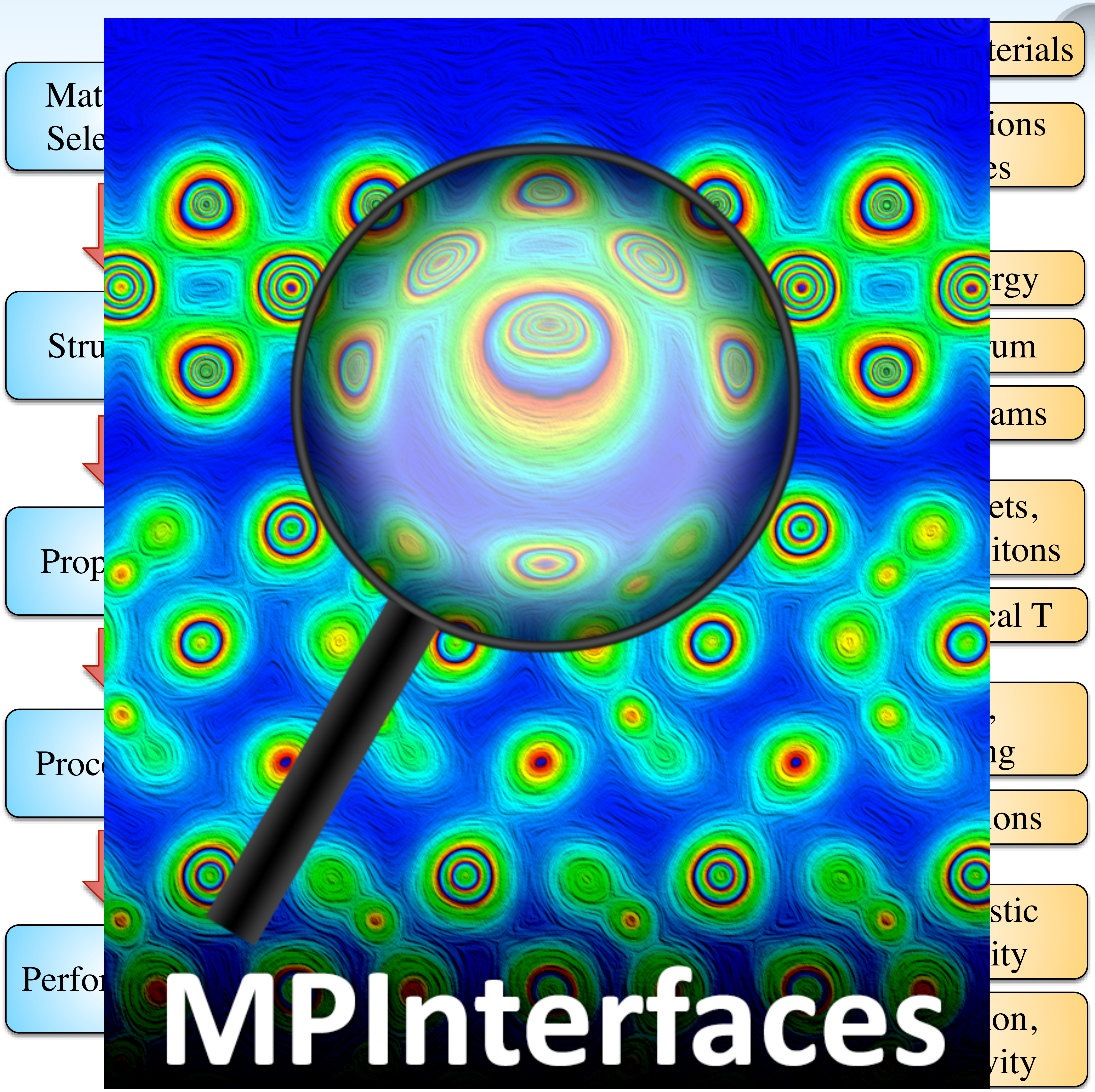
How to predict microstructures from phases, defects, and processing?

Part II: Materials Informatics for 2D Materials Structures

rhennig@ufl.edu
http://hennig.mse.ufl.edu

Materials Informatics of 2D Materials



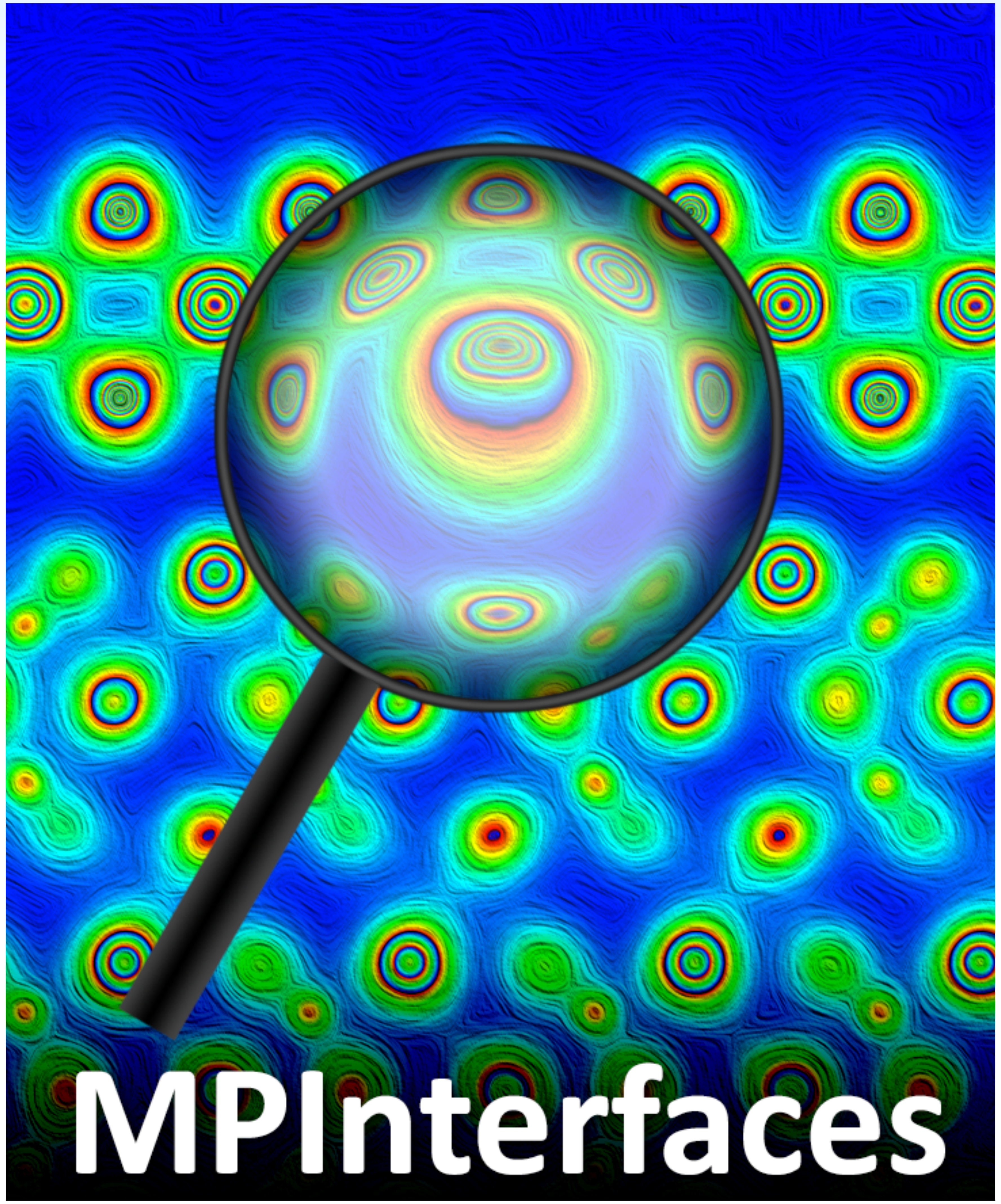


Powered by
MPInterfaces & materialsweb

H. L. Zhuang and RGH, JOM 66, 366 (2014)

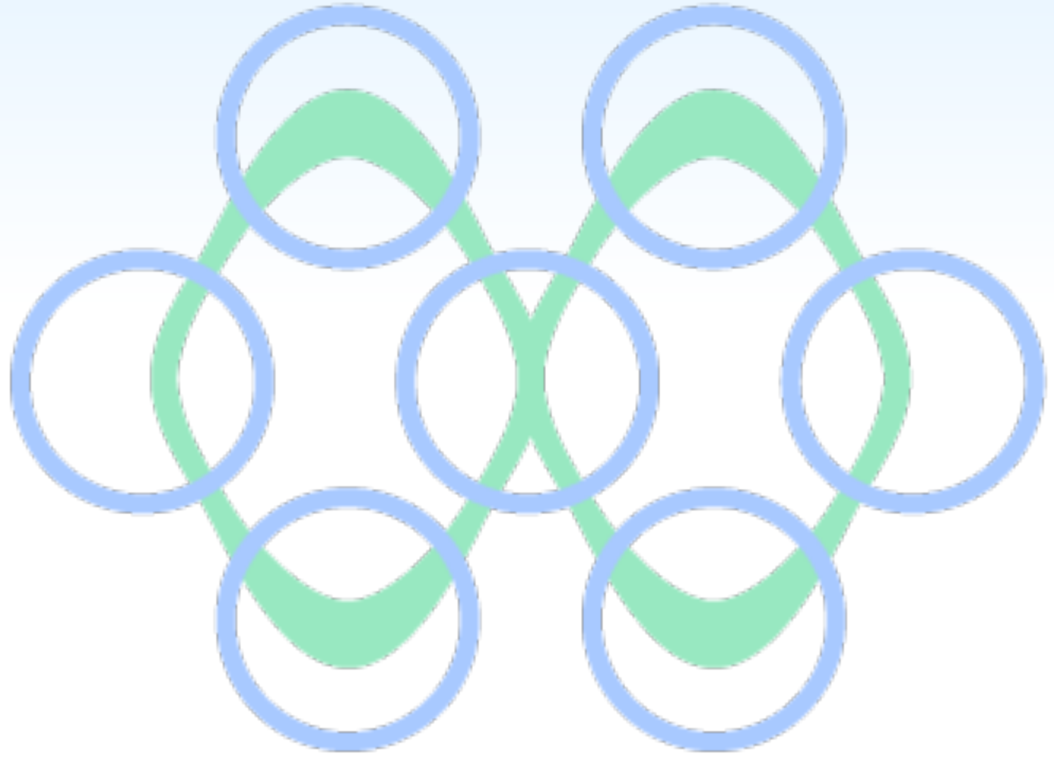
Structure and Stability of 2D Materials

- Classification of 2D materials
- Criteria for stability ΔE_f < 200 meV/atom
- Methods for 2D materials discovery
  - Datamining for exfoliation
  - Evolutionary algorithm searches
  - Chemical substitutions and etching
- Characterization of 2D materials
  - Pourbaix diagrams
  - Photocatalysis
  - 2D half-metals
  - Spin-orbit and 2D magnetism
  - Substrate control of phase stability



rhennig@ufl.edu
http://hennig.mse.ufl.edu

Datamining to Discover 2D Materials



```
from mpinterfaces.utils import
get_structure_type

layered = []
for s in structures:
    if get_structure_type(s) ==
"layered":
        layered.append(s)
```

Hennig *et al.*, arXiv:1610.07673 (10/2016)
Marzari *et al.*, arXiv:1611.05234 (11/2017)
Reed, *et al.*, Nano Lett. (2/2017)

Powered by
MPInterfaces & materialsweb

Ashton, Paul, Sinnott & Hennig. Phys. Rev. Lett. 118, 106101 (2017)
https://arxiv.org/abs/1610.07673 (2016)

2D Materials Databases

Data Mining

- Reed: Layered materials database
- Marzari: Layered materials and exfoliated 2D materials database
- Hennig: Exfoliated 2D materials, https://MaterialsWeb.org

Chemical Substitutions

- Thygesen: Substitution for known 2D materials structures, https://c2db.fysik.dtu.dk

Structure predictions:

- Hennig: Genetic algorithm prediction of 2D materials, https://MaterialsWeb.org

Need to develop a comprehensive 2D Materials Database (Crespi, Reed).

Online Database: https://materialsweb.org

materialsweb

Home | About | Docs | Contact

Use the topology-scaling algorithm on your own structures

VASP Workflow Builder

Structure Characterization

Bulk Materials

10891 Entries

2D Materials

~~00685~~ Entries

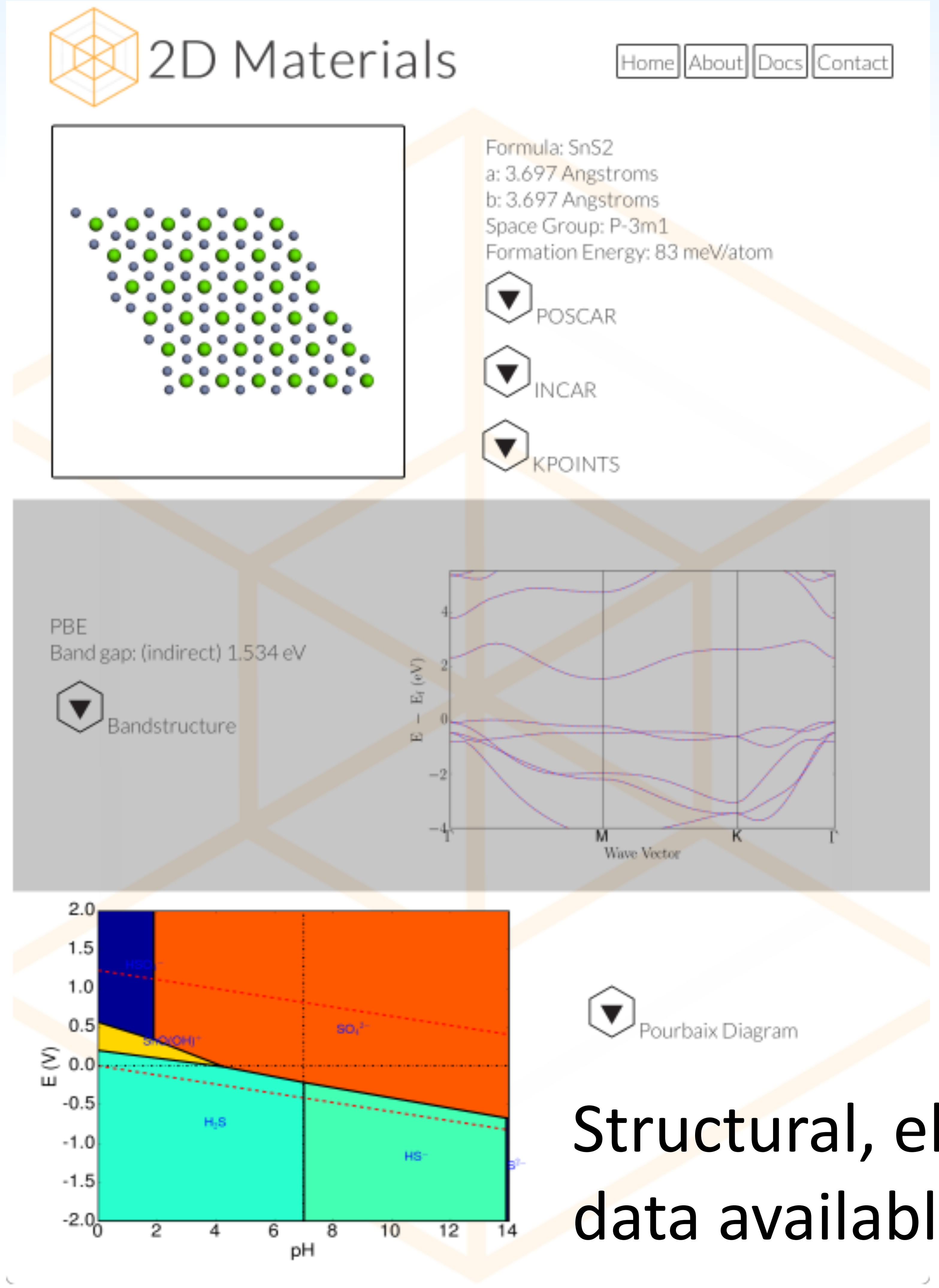
00765

Browse 2D materials

Powered by
MPInterfaces & materialsweb

Ashton, Paul, Sinnott & Hennig. *Phys. Rev. Lett.* 118, 106101 (2017)

Online Database: https://materialsweb.org



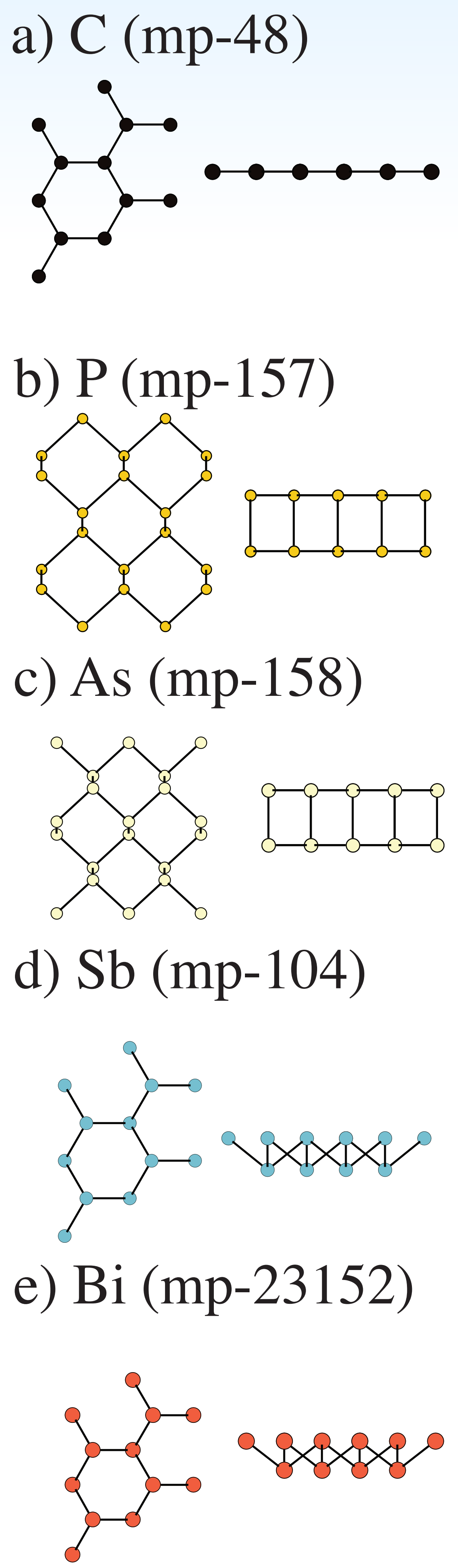
Unique crystal structures for each 2D material stoichiometry in the DB

Structural, electronic and thermodynamic data available for all materials

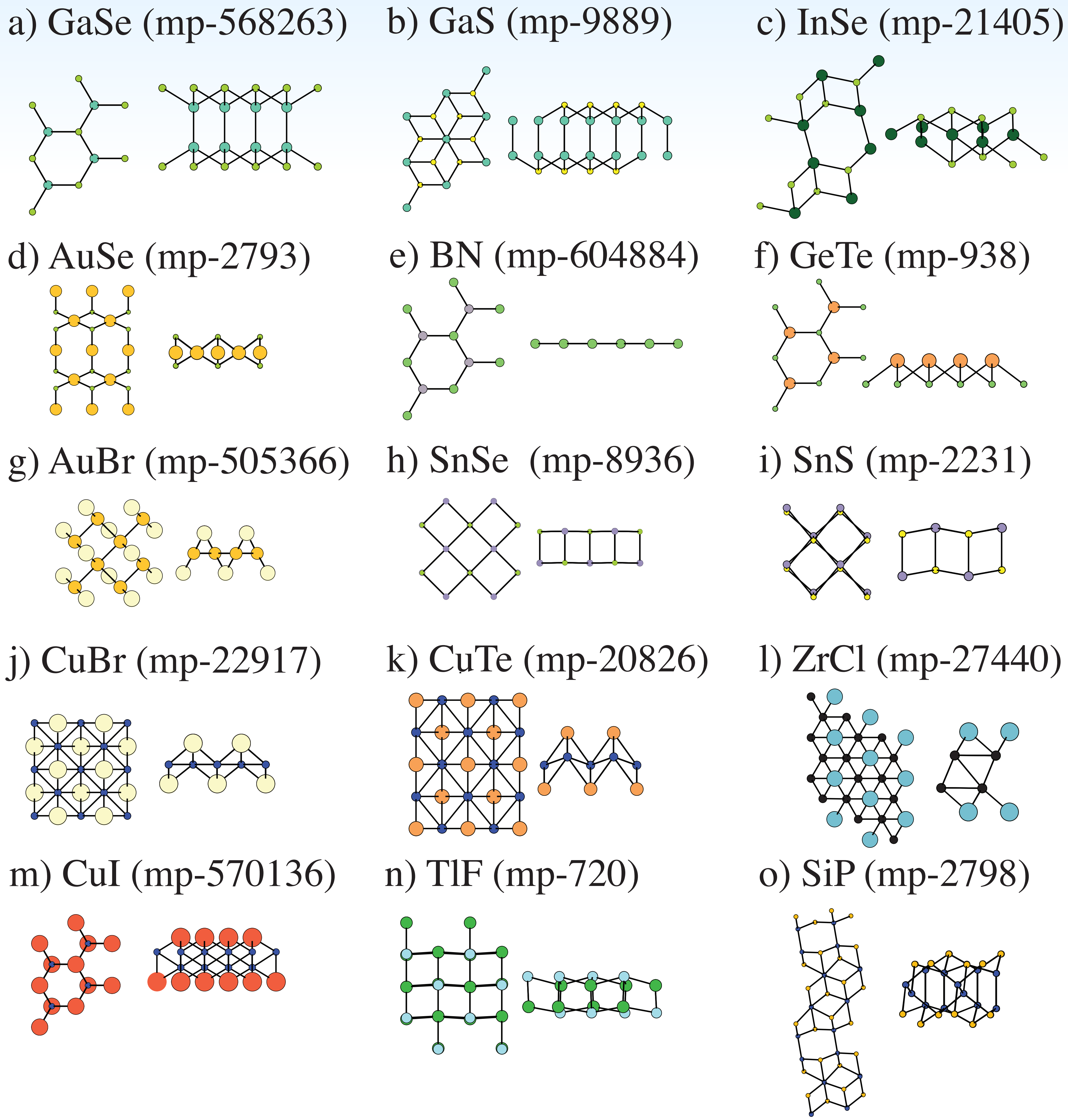
Need to add properties such as band offsets, excitons, magnetic order, …

Structure Prototypes

Elementary 2D Materials



Binary A-B 2D Materials

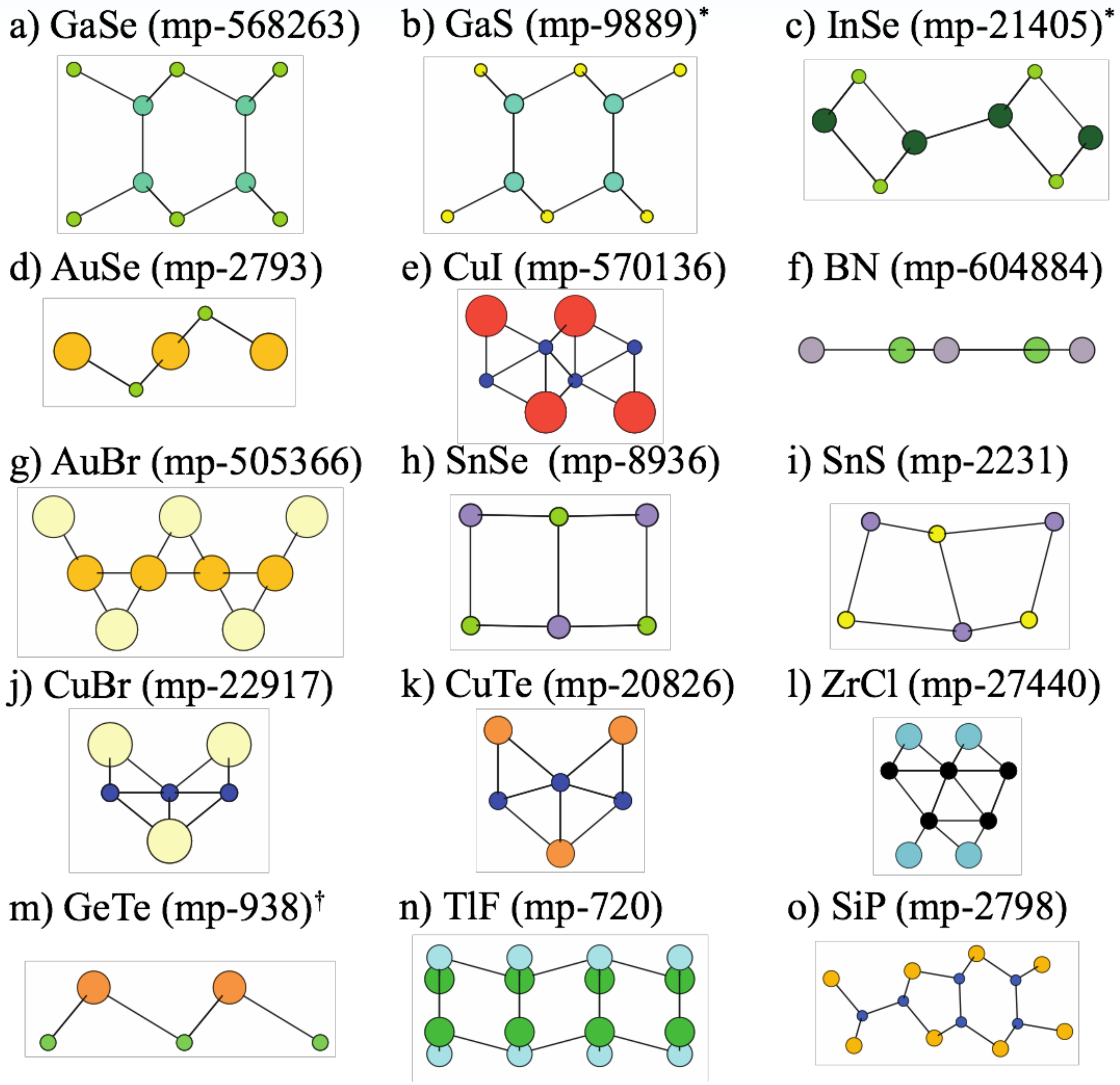


…

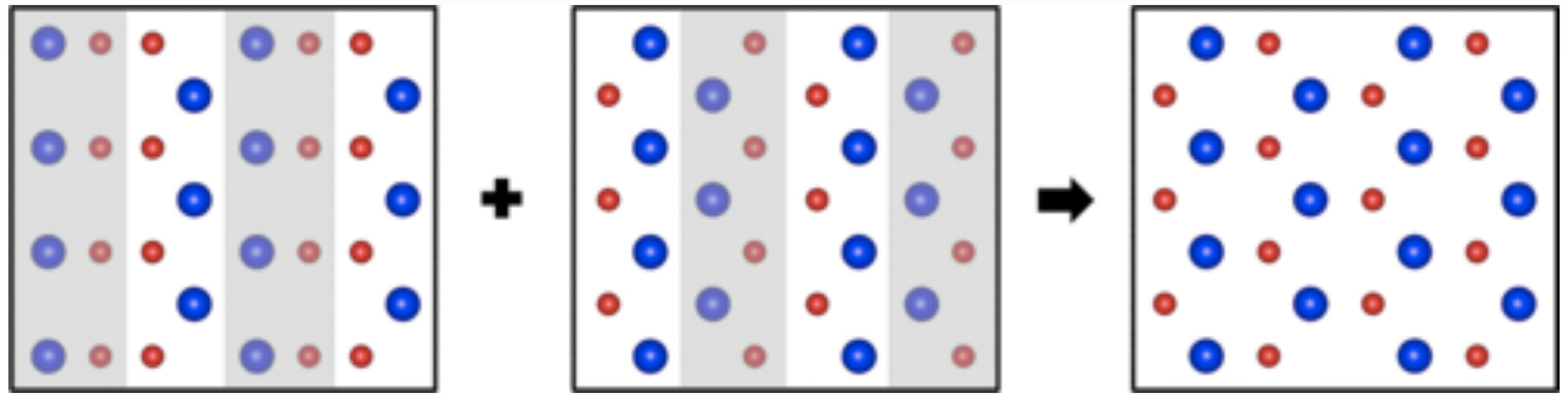
Ashton, Paul, Sinnott & Hennig. *Phys. Rev. Lett.* 2017

Using Crystal Structure Templates

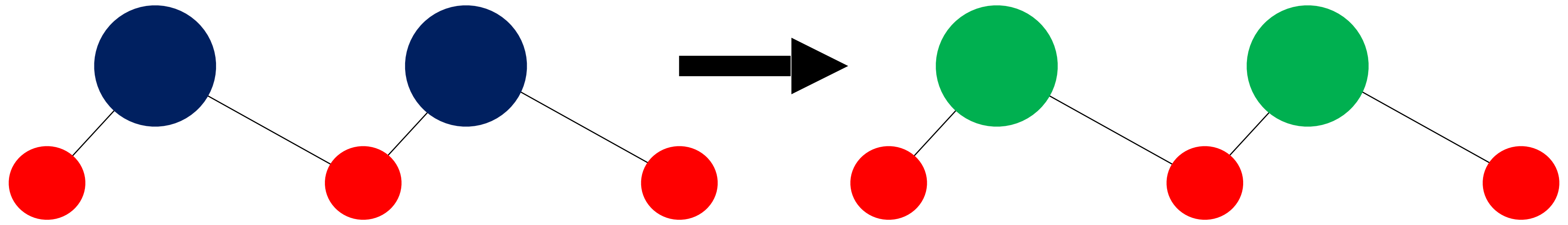
Unique AB crystal structures



Genetic algorithms

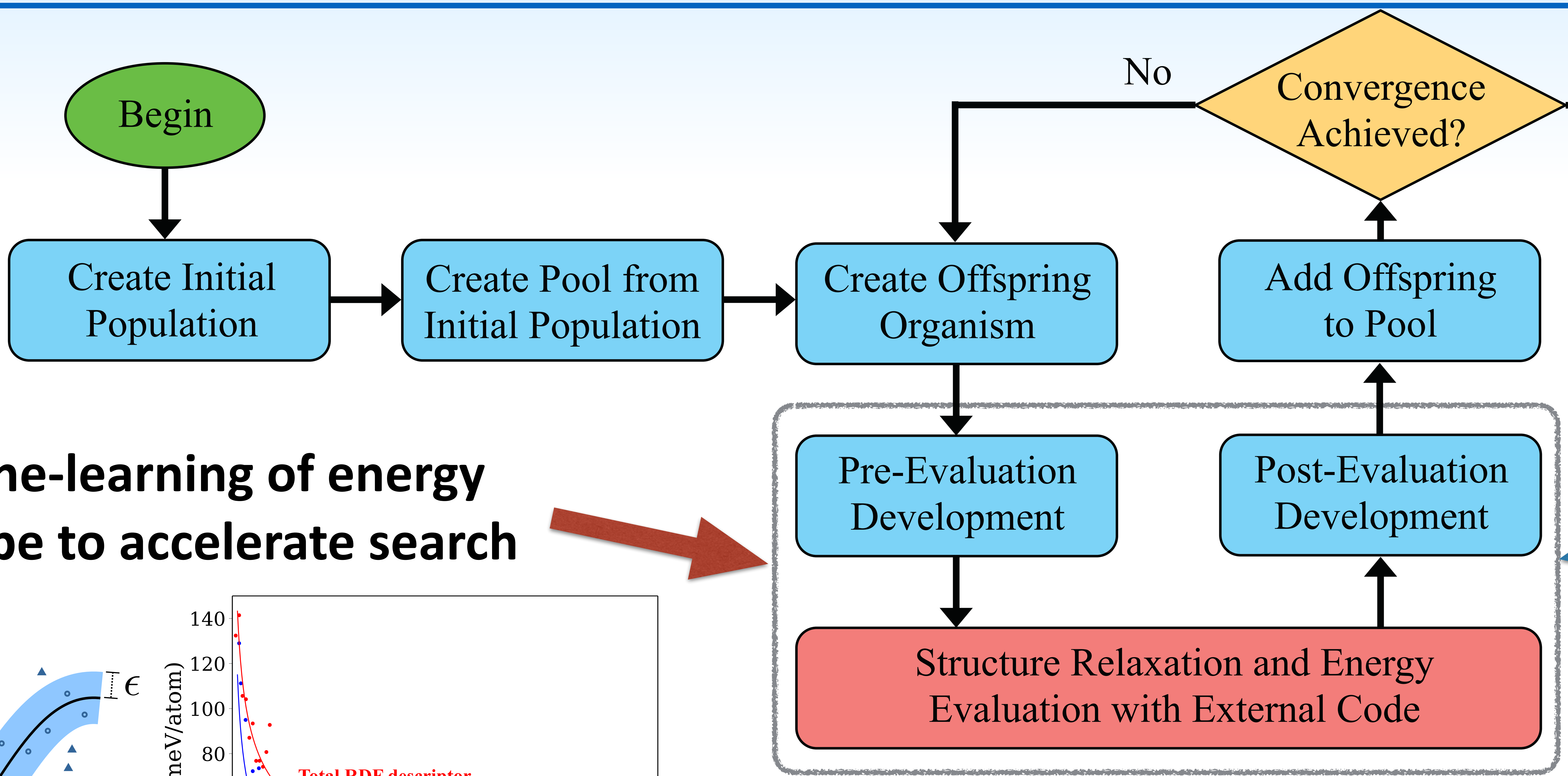


Element substitution



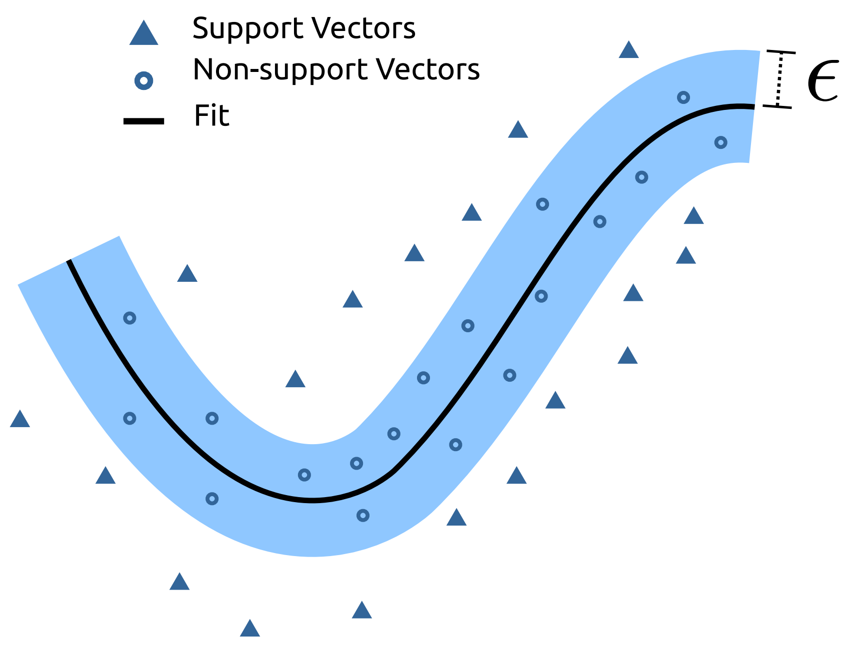
API for 2D materials and prototype structures accelerates materials search

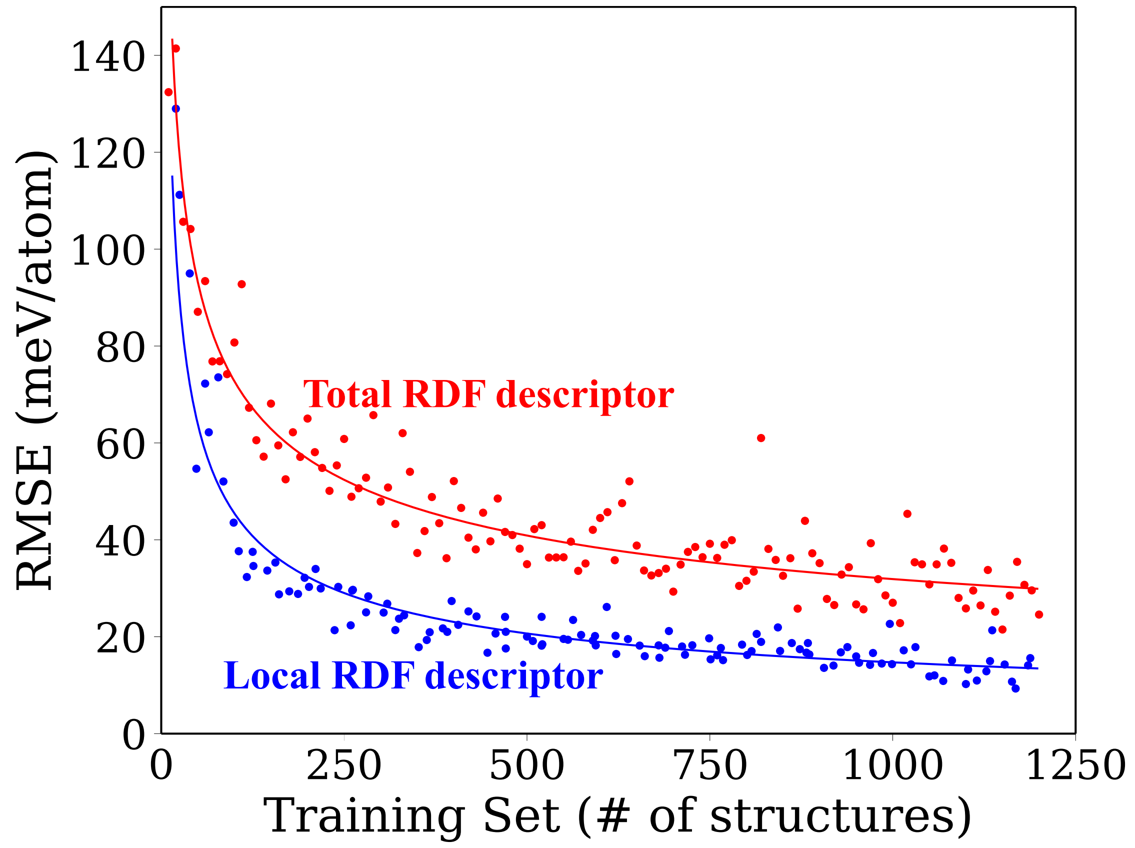
Genetic Algorithm and Machine Learning for 2D Materials



Machine-learning of energy landscape to accelerate search

Modification for 0D, 1D, 2D, materials and surface structures (Greeley)





Grand canonical genetic algorithm
Variable number of atoms and composition

https://github.com/henniggroup/gasp-python

Enables search for low-low-dimensional materials with unknown structures

Part III: 2D Materials Data Framework for Dopants, Impurities, and Defects

rhennig@ufl.edu
http://hennig.mse.ufl.edu

Charged Defect Database Interface

Defects in semiconductors and insulators

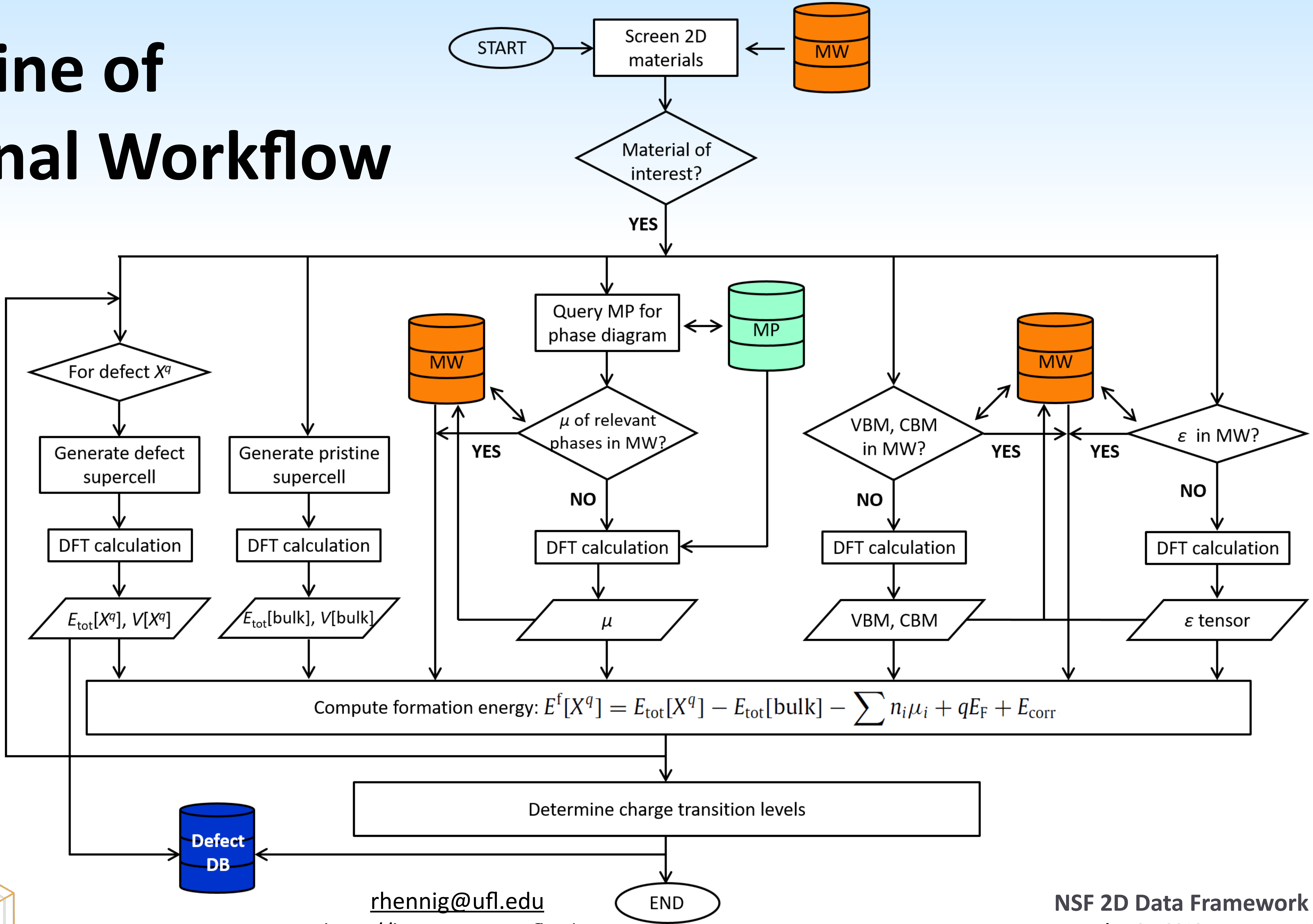
- Defects can carry charge (useful notation: Kröger-Vink)
- Change of charge state ⇒ Charge transition levels
- Important for optoelectronic devices, spectroscopy
- Calculation of charged defects in 3D materials is well established

$$E^f[X^q] = E_{\mathrm{tot}}[X^q] - E_{\mathrm{tot}}[\mathrm{bulk}] - \sum_i n_i \mu_i + qE_{\mathrm{F}} + E_{\mathrm{corr}}$$

- Similar approach works for 2D materials, but requires with periodic boundary conditions
- Generalized dipole correction developed by Freysoldt and Neugebauer
- Theory can also provide optical absorption, band edge positions, etc.

Need for high-throughput framework for 2D defect database

Outline of Computational Workflow

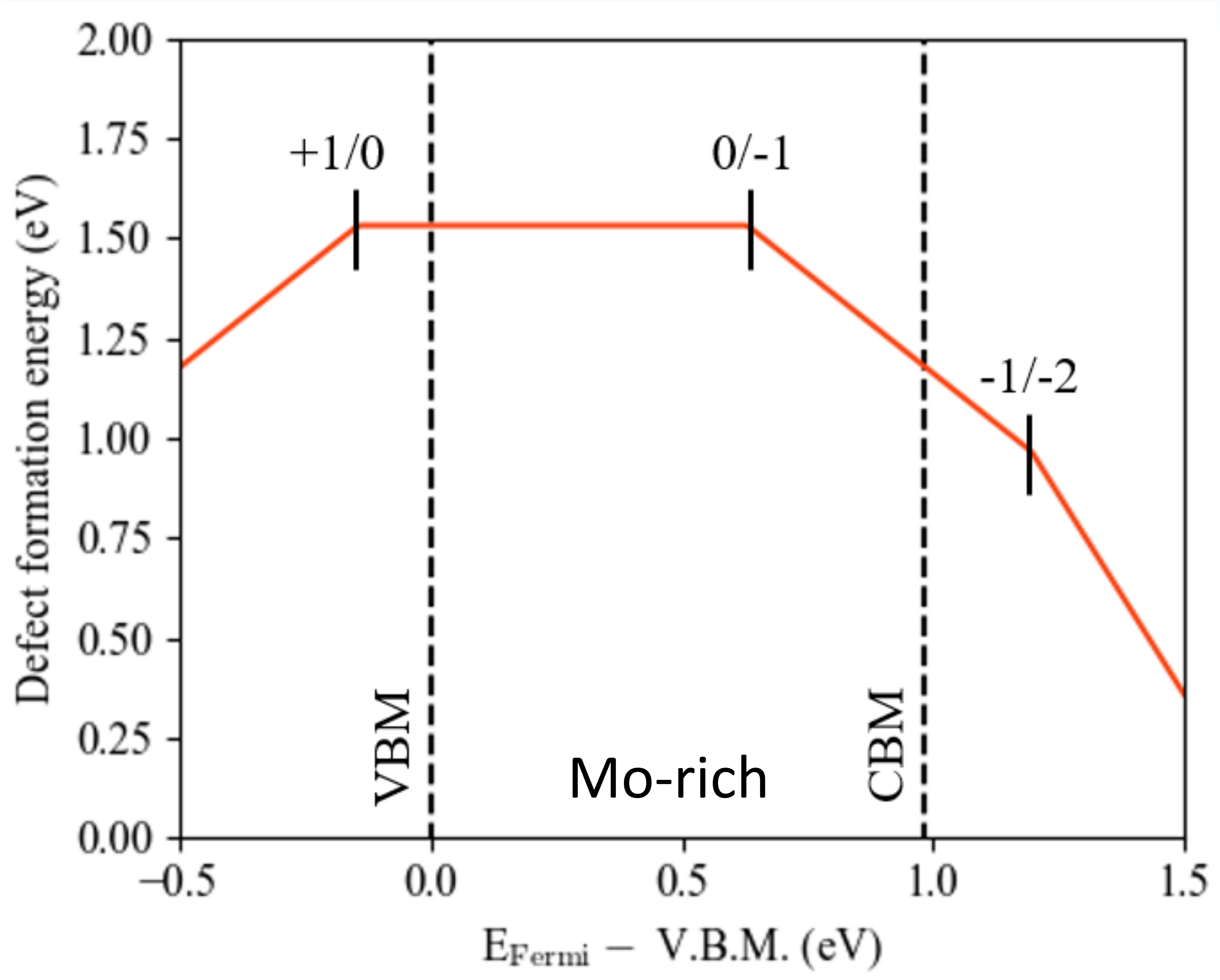


Powered by
MPInterfaces & materialsweb

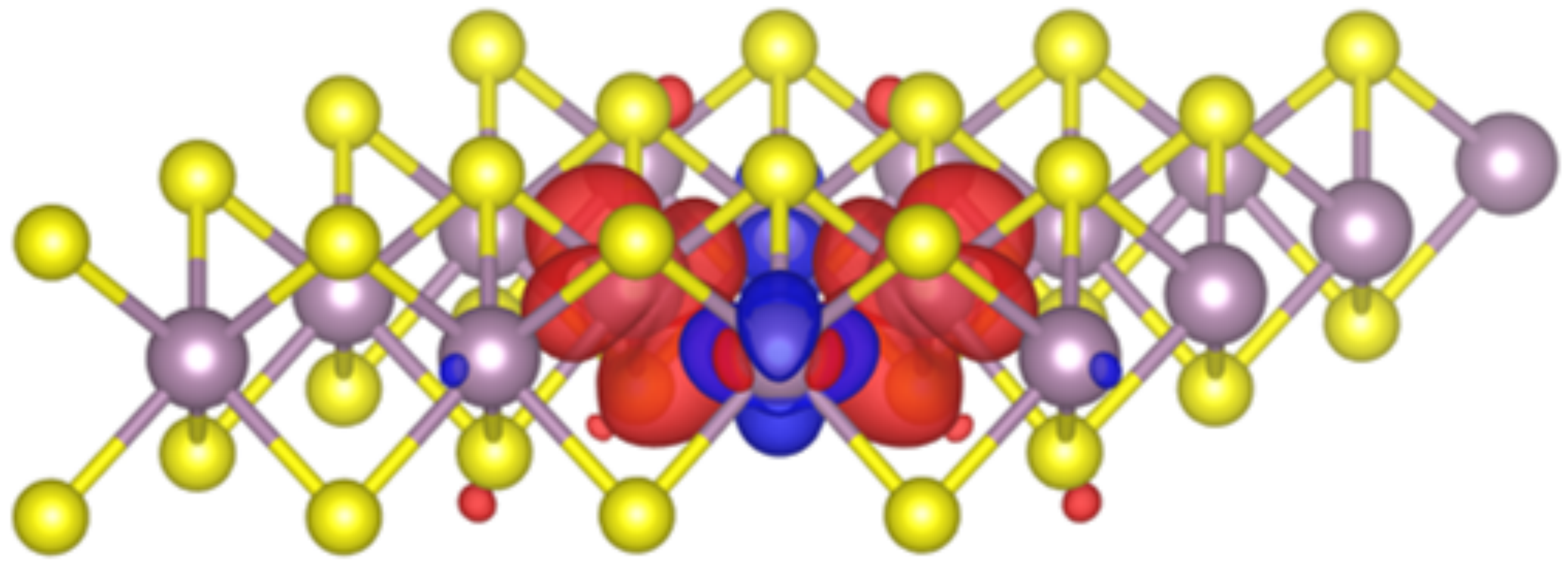
rhennig@ufl.edu
http://hennig.mse.ufl.edu

Example: Charged Vacancy in MoS_2

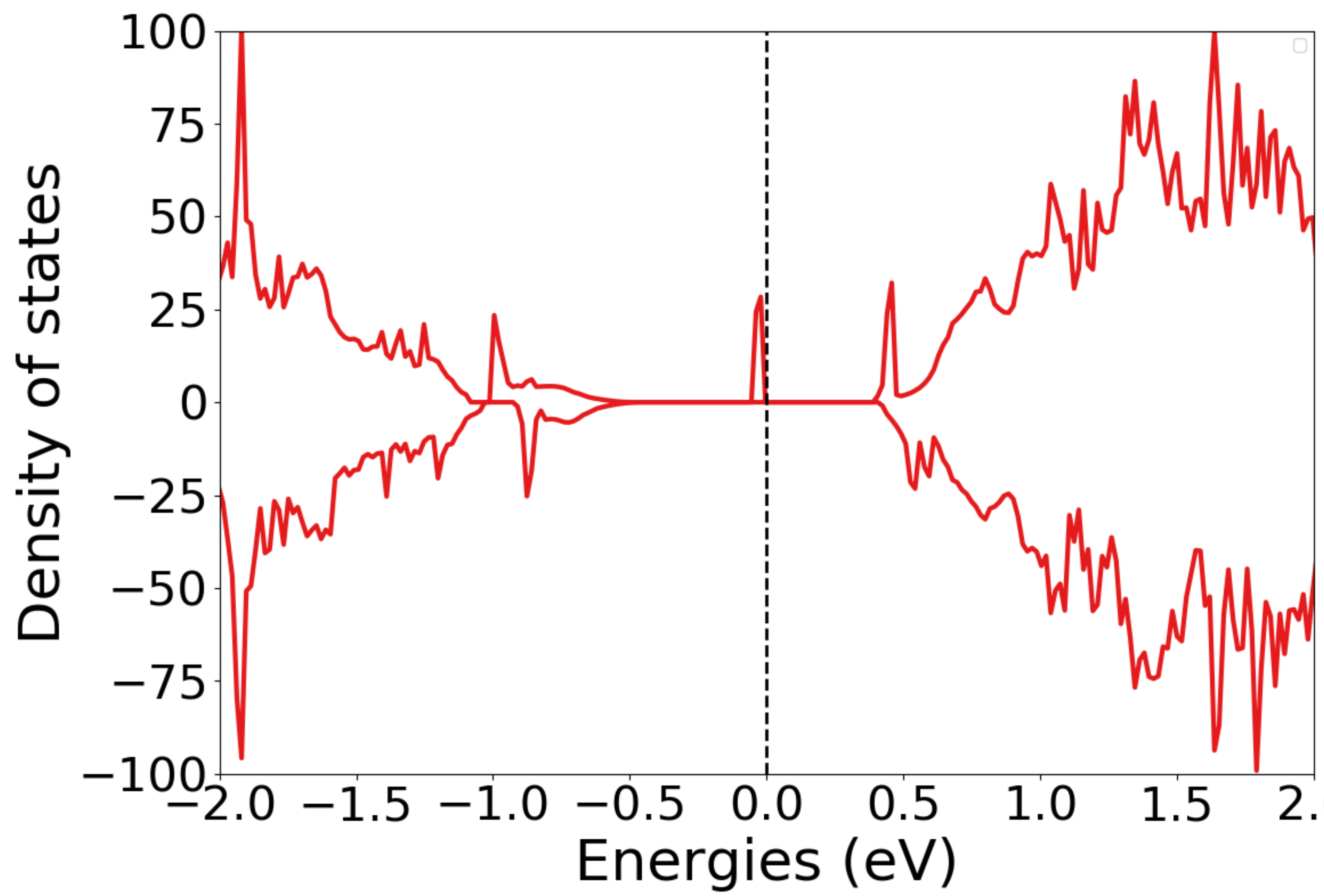
Defect formation energies and charge transition levels



Spin density difference between $(V_S)^x$ and $(V_S)^{-1}$



Electronic density of states



rhennig@ufl.edu
http://hennig.mse.ufl.edu

Needed Experimental Input

Most desirable 2d materials

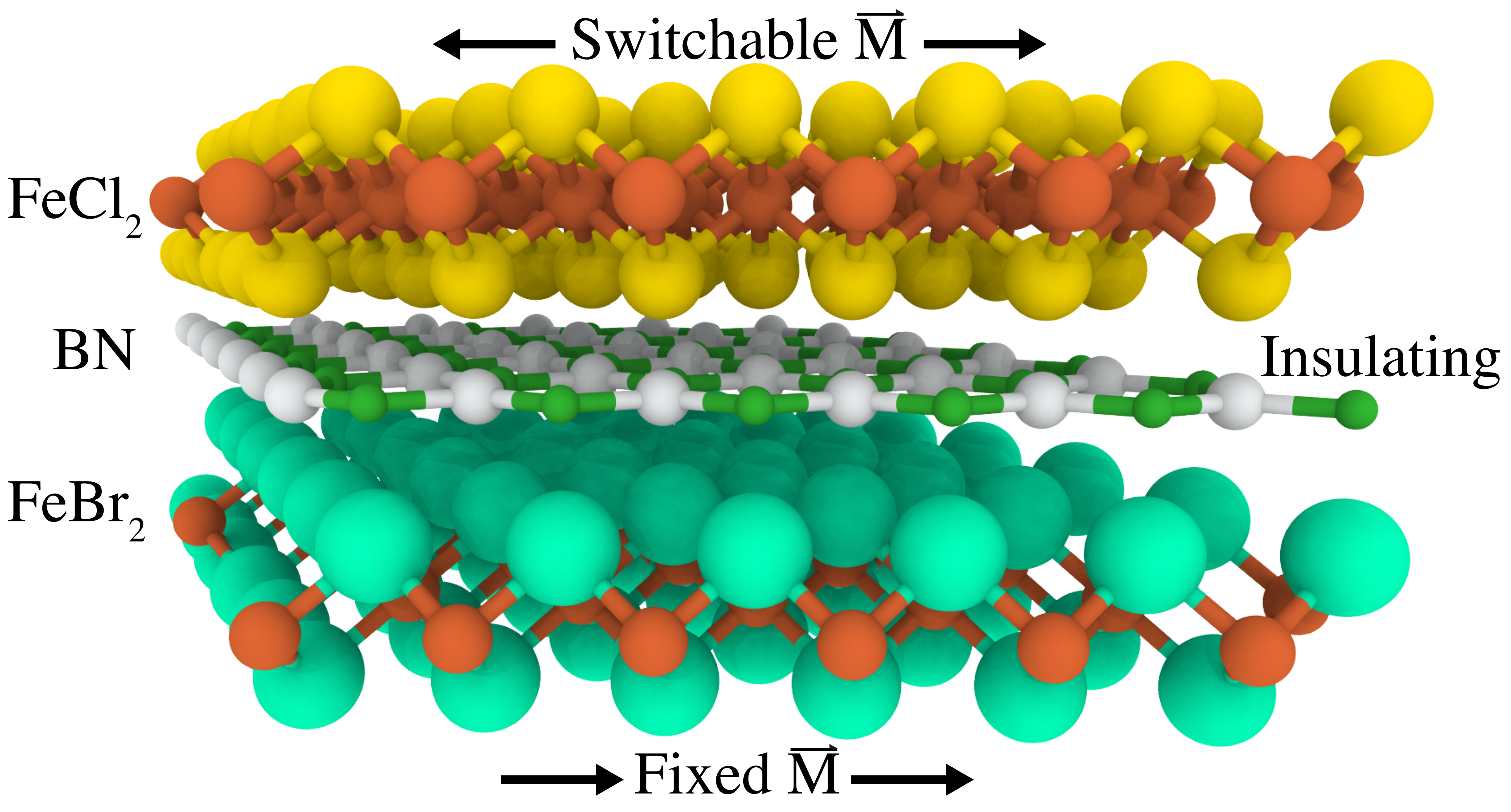
- List of experimentally synthesizable materials: **possible elements and combinations**
- Application goals: optoelectronics, spintronics, quantum devices, etc.
  determines **desired materials properties**, e.g. band offsets, and defect properties
- Synthesis conditions: **precursors, temperature profiles, partial pressures of components**

Relevant impurities and dopants

- List of **usable dopant species and relevant impurities**
- Desired **doping levels, p or n-type**

Other microstructure defects

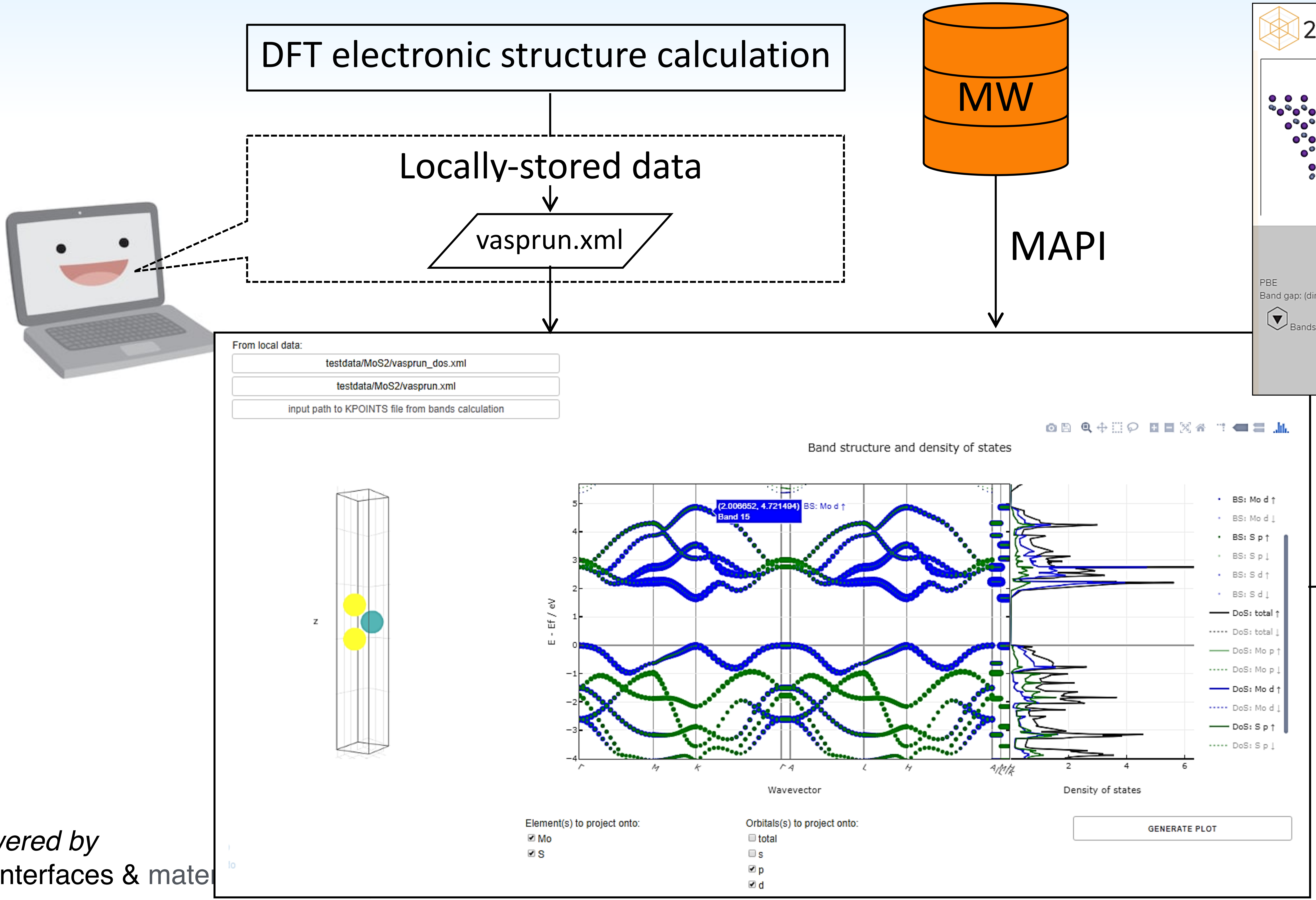
- Edges and grain boundaries
- Lateral and vertical hetero interfaces

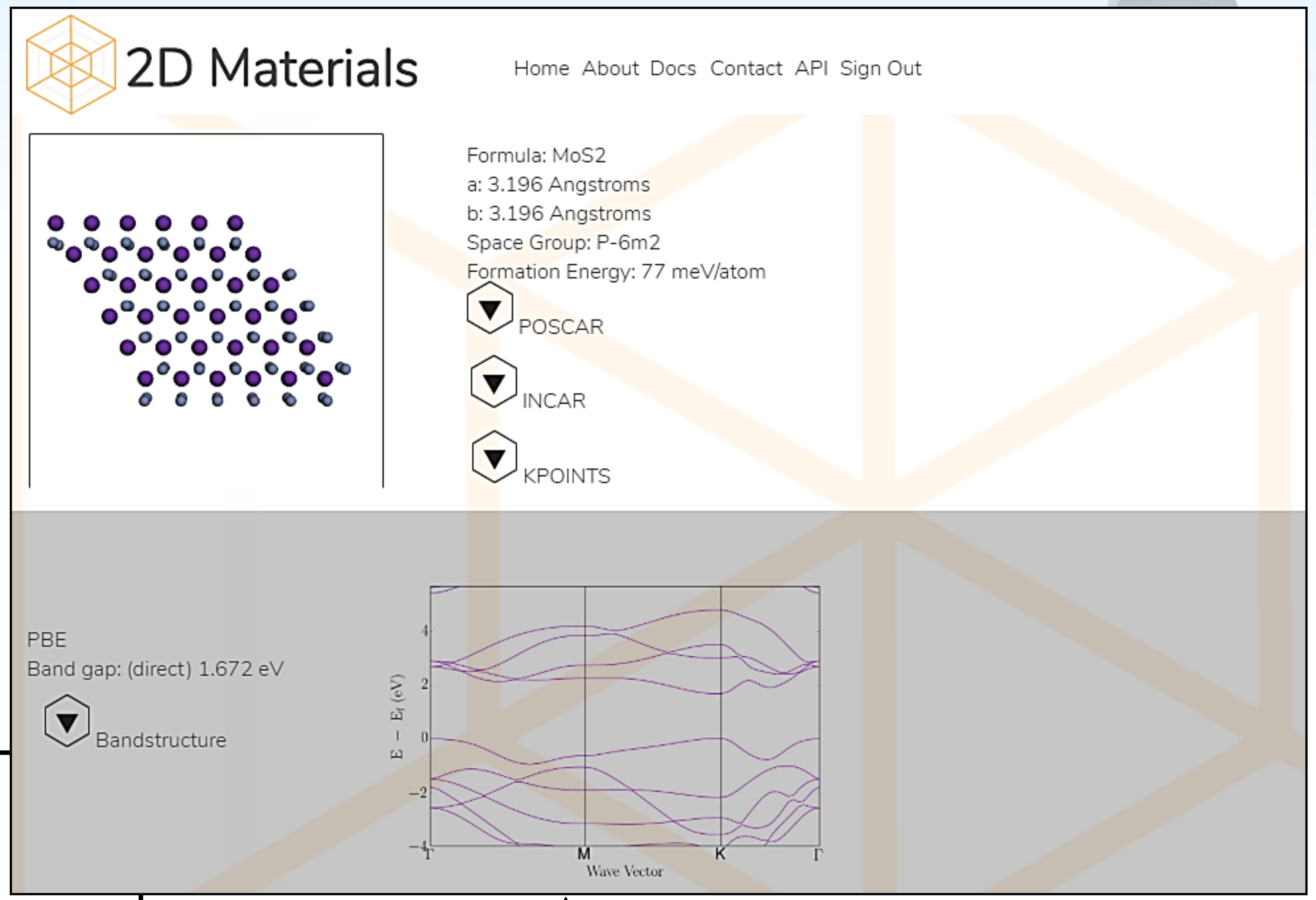


Need for experimental input (2DCC, Crespi).

Part IV: 2D Materials Data Framework for Data Representation of Band Structures

Band Structure Visualization Tool





Replace static band structure diagrams currently on the MaterialsWeb and other databases

Powered by
MPInterfaces & mater

From local data:

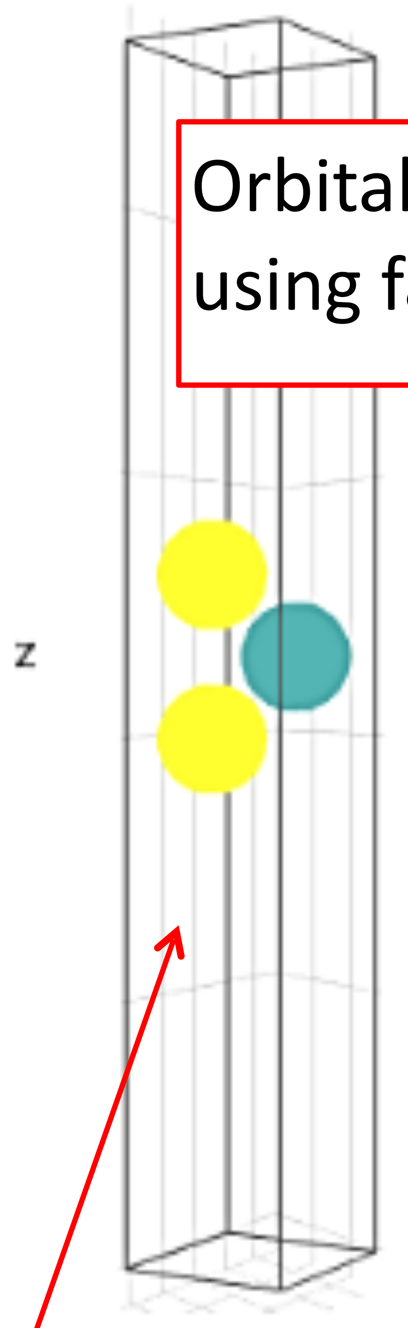
testdata/MoS2/vasprun_dos.xml

testdata/MoS2/vasprun.xml

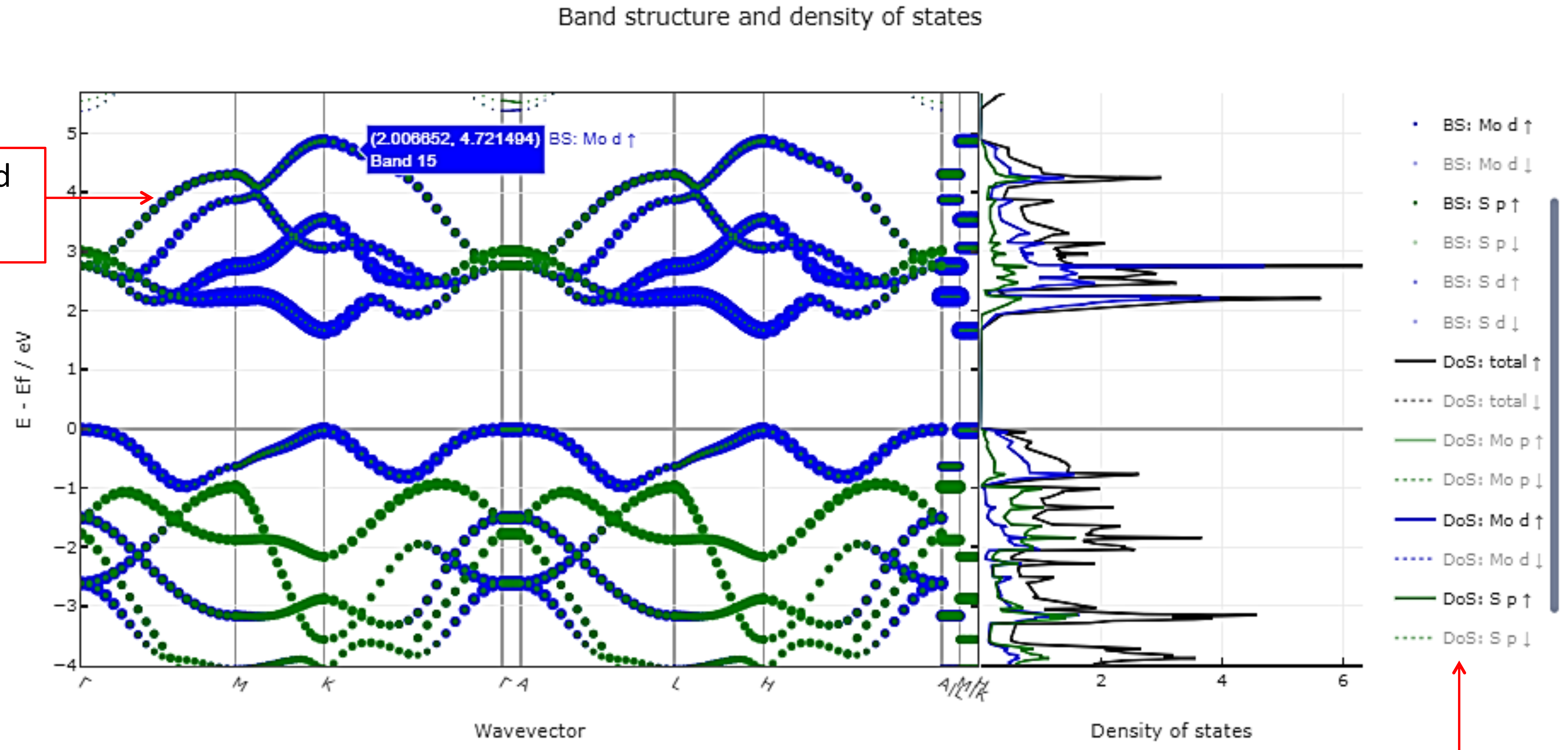
input path to KPOINTS file from bands calculation

Input paths to vasprun.xml files from DOS and band structure calculations
If no KPOINTS file is given, it looks in directory as the bands vasprun.xml file

Chart options: zoom, pan, view data on hover, etc.



Orbital projections visualized using fat bands



Atoms colored by element, Clicking on an atom to select for projection

Element(s) to project onto:

- [x] Mo
- [x] S

Orbitals(s) to project onto:

- [ ] total
- [ ] s
- [x] p
- [x] d

Select element(s) and

GENERATE PLOT

User can turn on and off specific traces by clicking

Coupling of website and MongoDB database, and other codes (Lambrecht, Rabe, Birol)

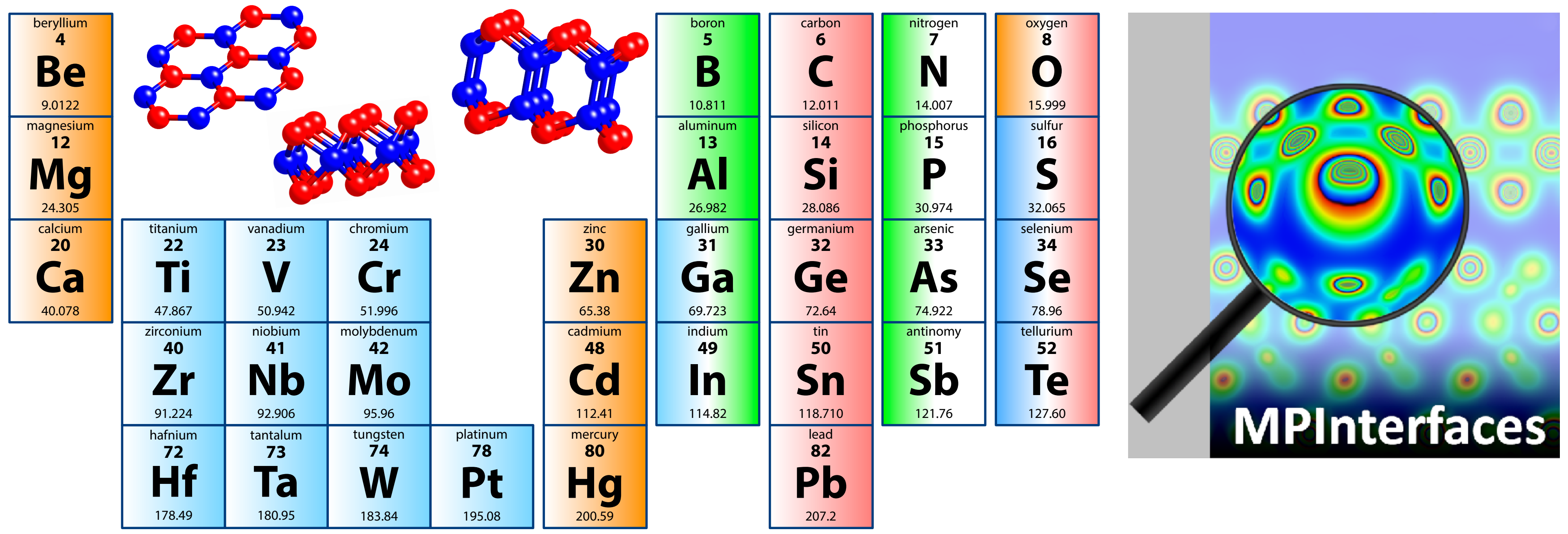
Data Analytics for Discovery and Design of 2D Materials

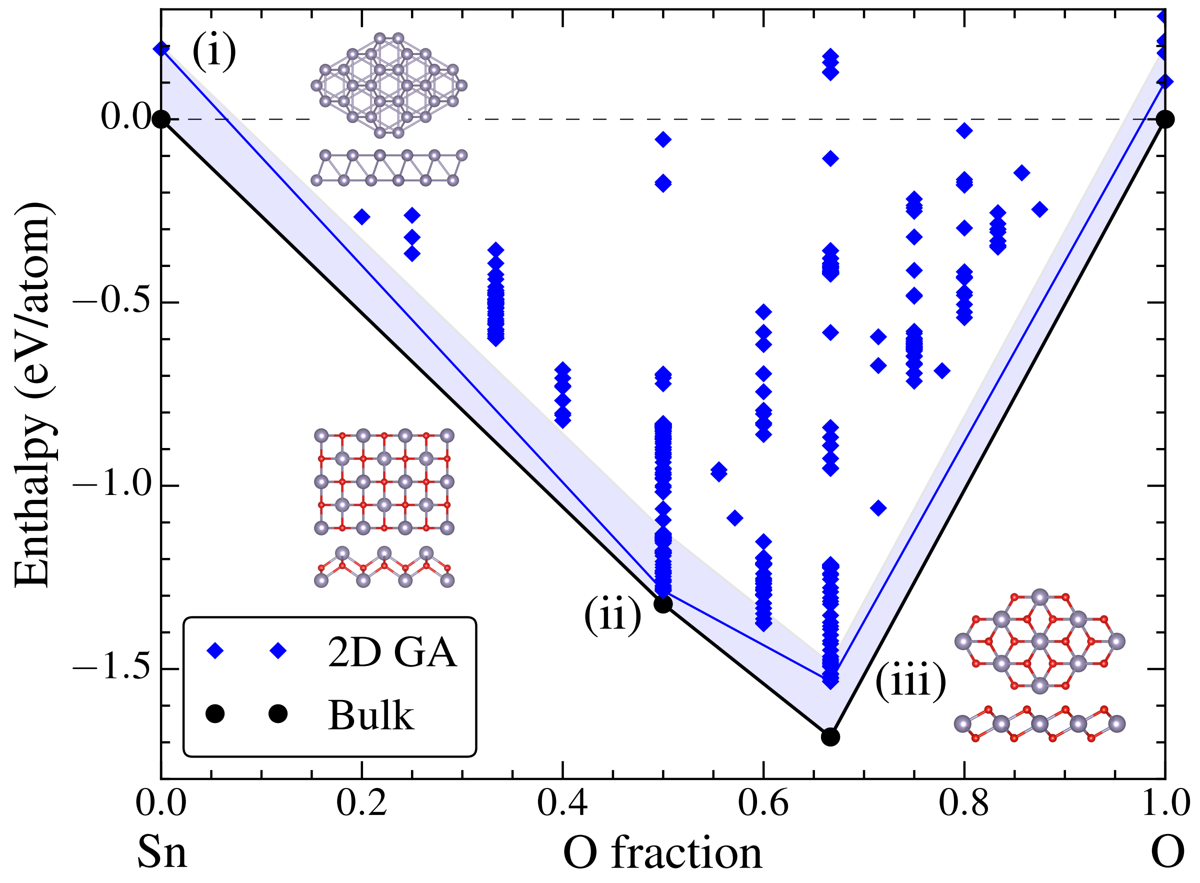
Richard G. Hennig, University of Florida

Search for 2D Materials

- Materials structure and microstructure
- Input from experiment required
- Need for new methods for non-equilibrium defects and processing
- Role of ML for dimensionality reduction

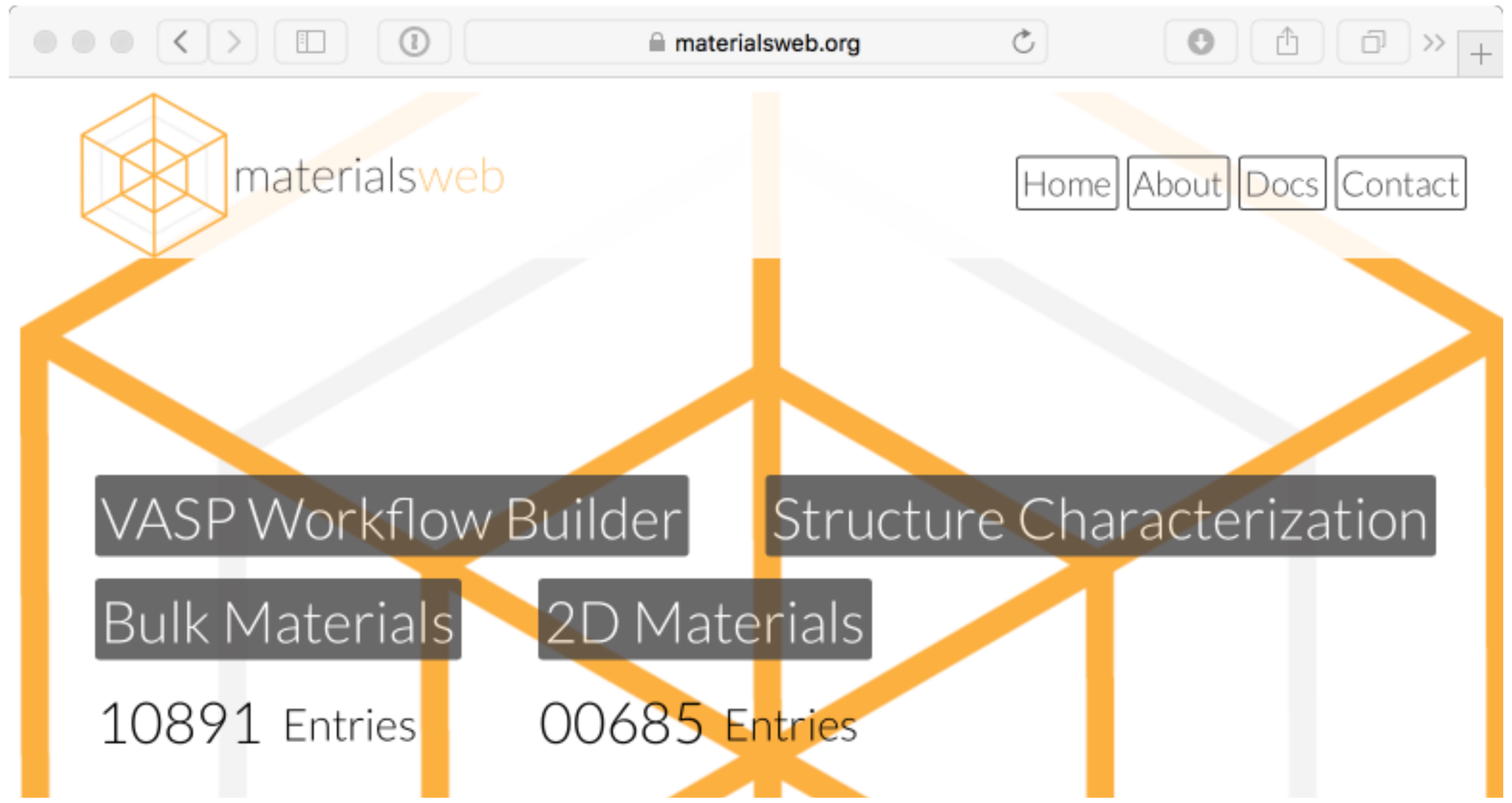
MPInterfaces - High throughput framework for 2D materials





GASP - Genetic algorithm and machine learning for structure predictions

Data available at http://materialsweb.org



Powered by
MPInterfaces & materialsweb

Open source available at https://github.com/henniggroup