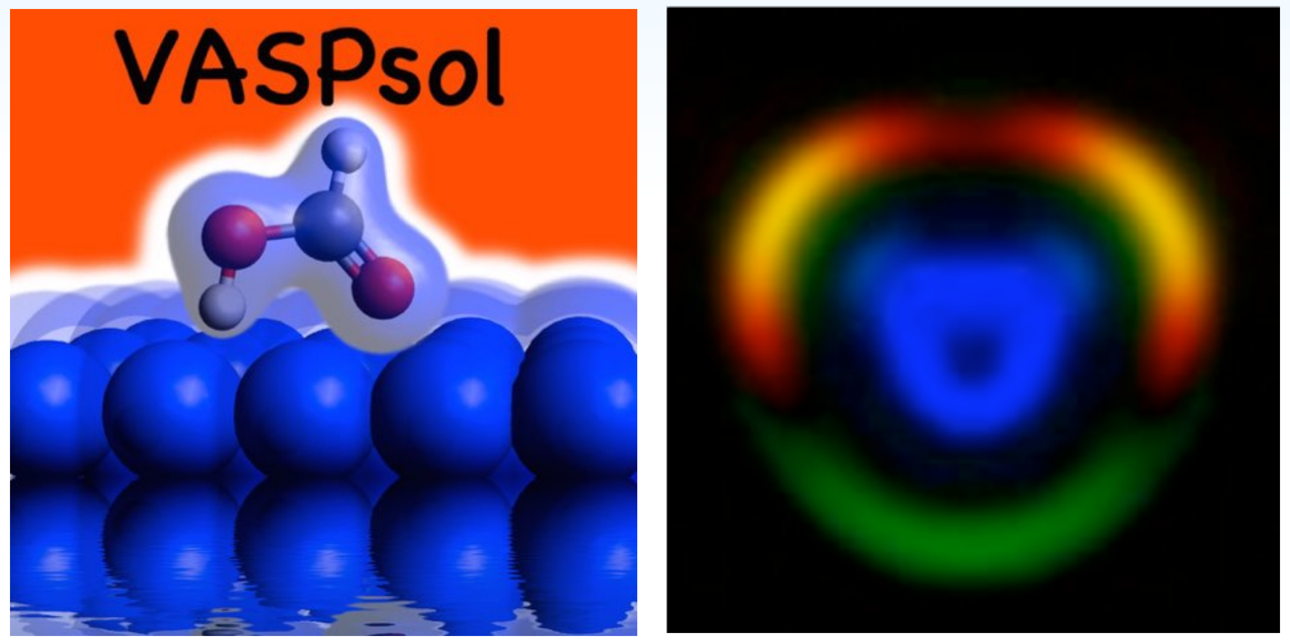
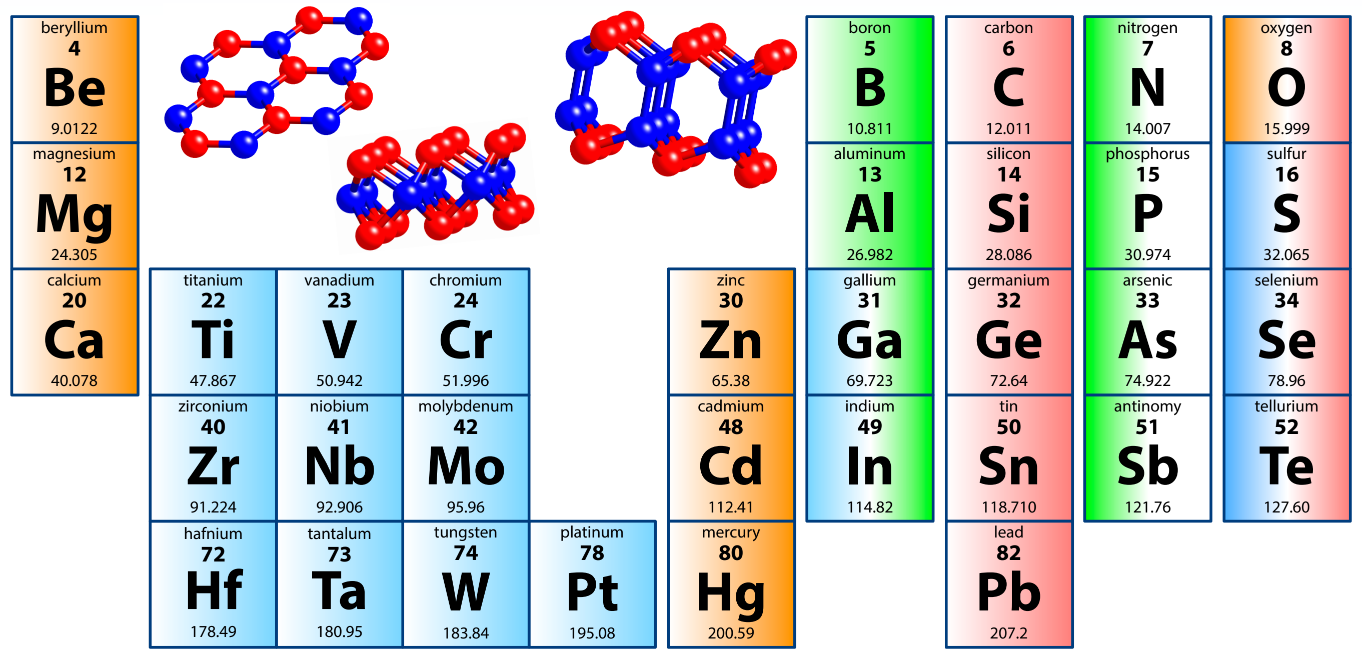
2D Materials Design for Production of Cold Electrons

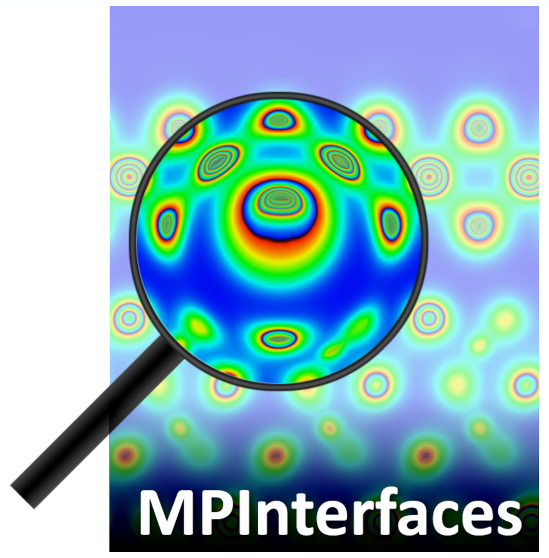
Richard G. Hennig, Joshua Paul, Michael Ashton, University of Florida

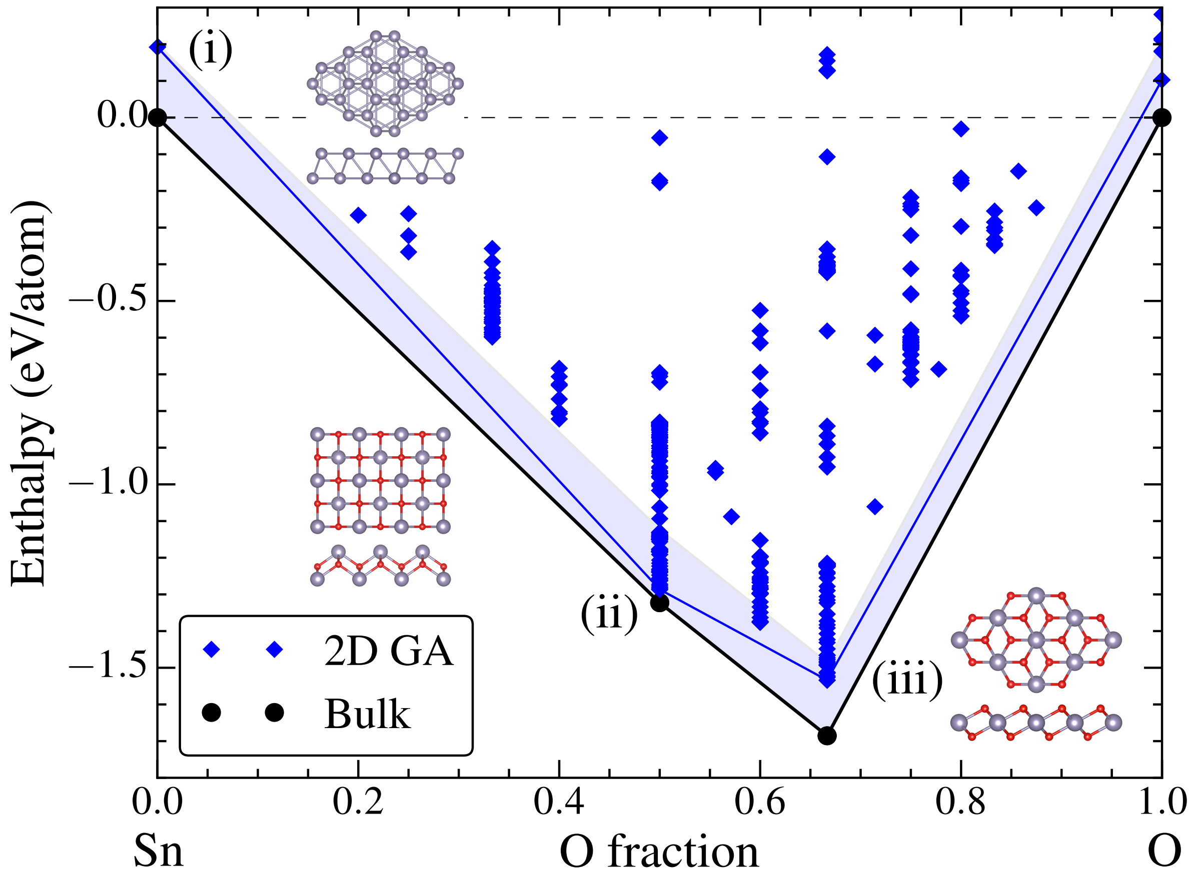


VASPSol - Ab initio methods for solid/liquid interfaces

MPInterfaces - High throughput framework for 2D materials

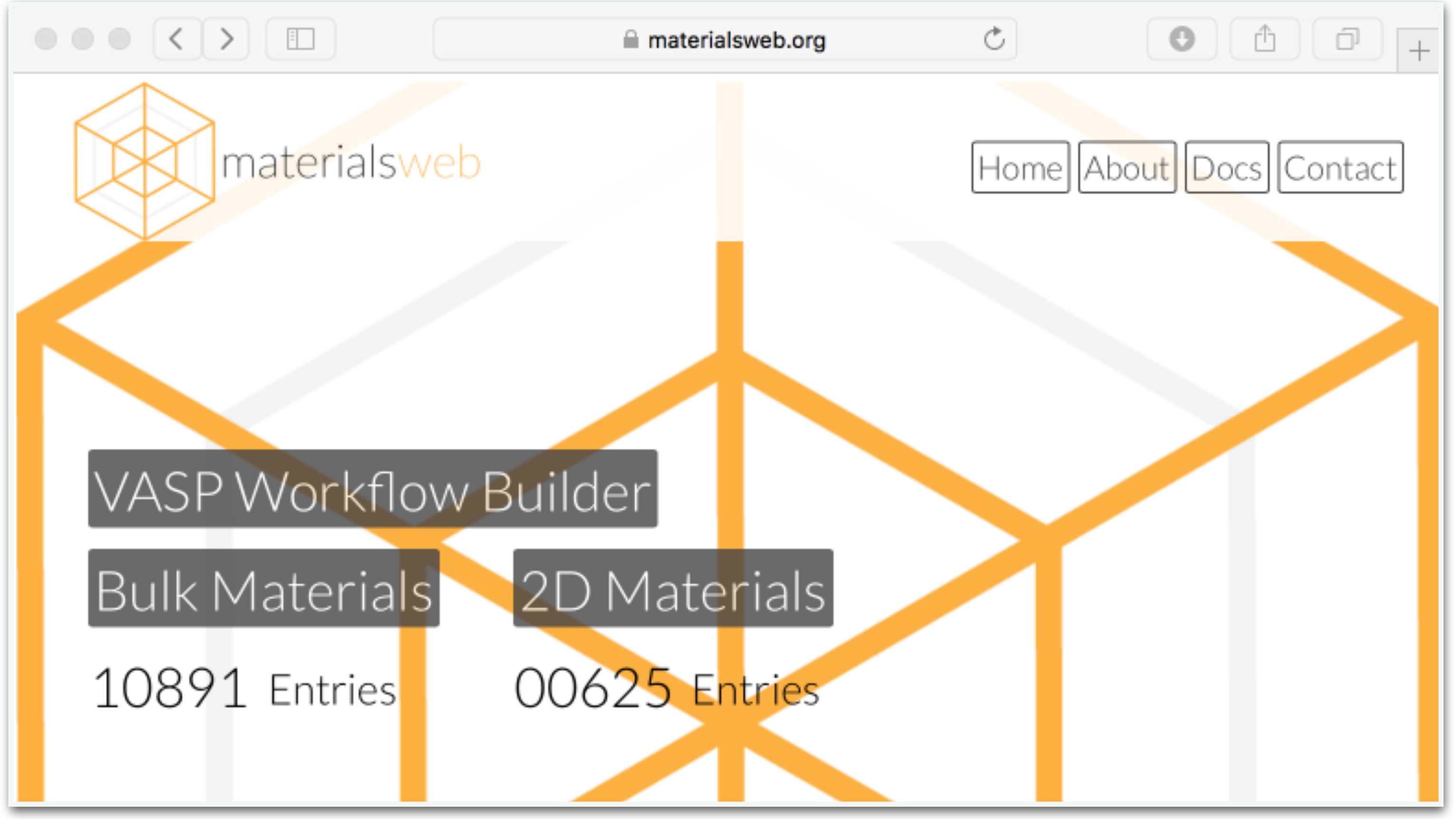






GASP - Genetic algorithm and machine learning for structure predictions

Data available at http://materialsweb.org



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

P3 Workshop
October 17-19, 2016 • Jefferson Lab

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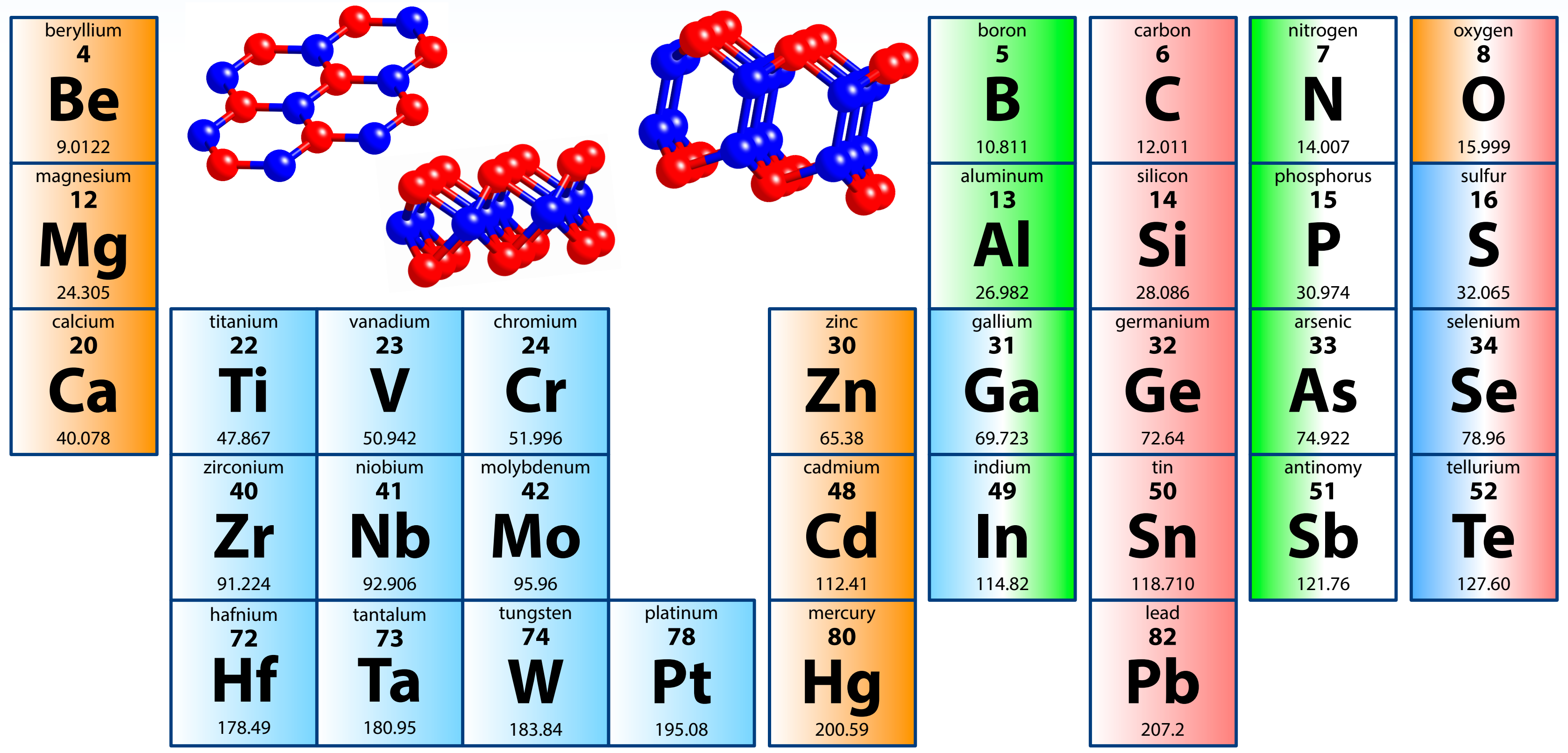
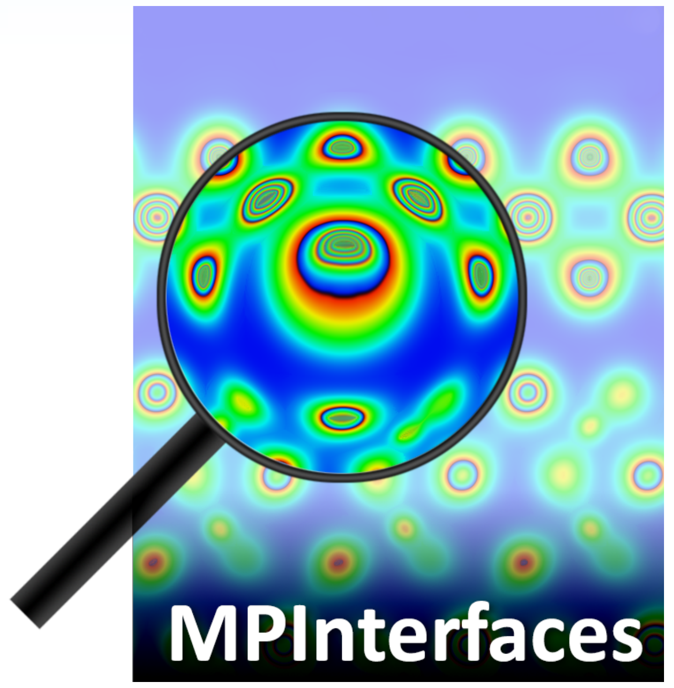
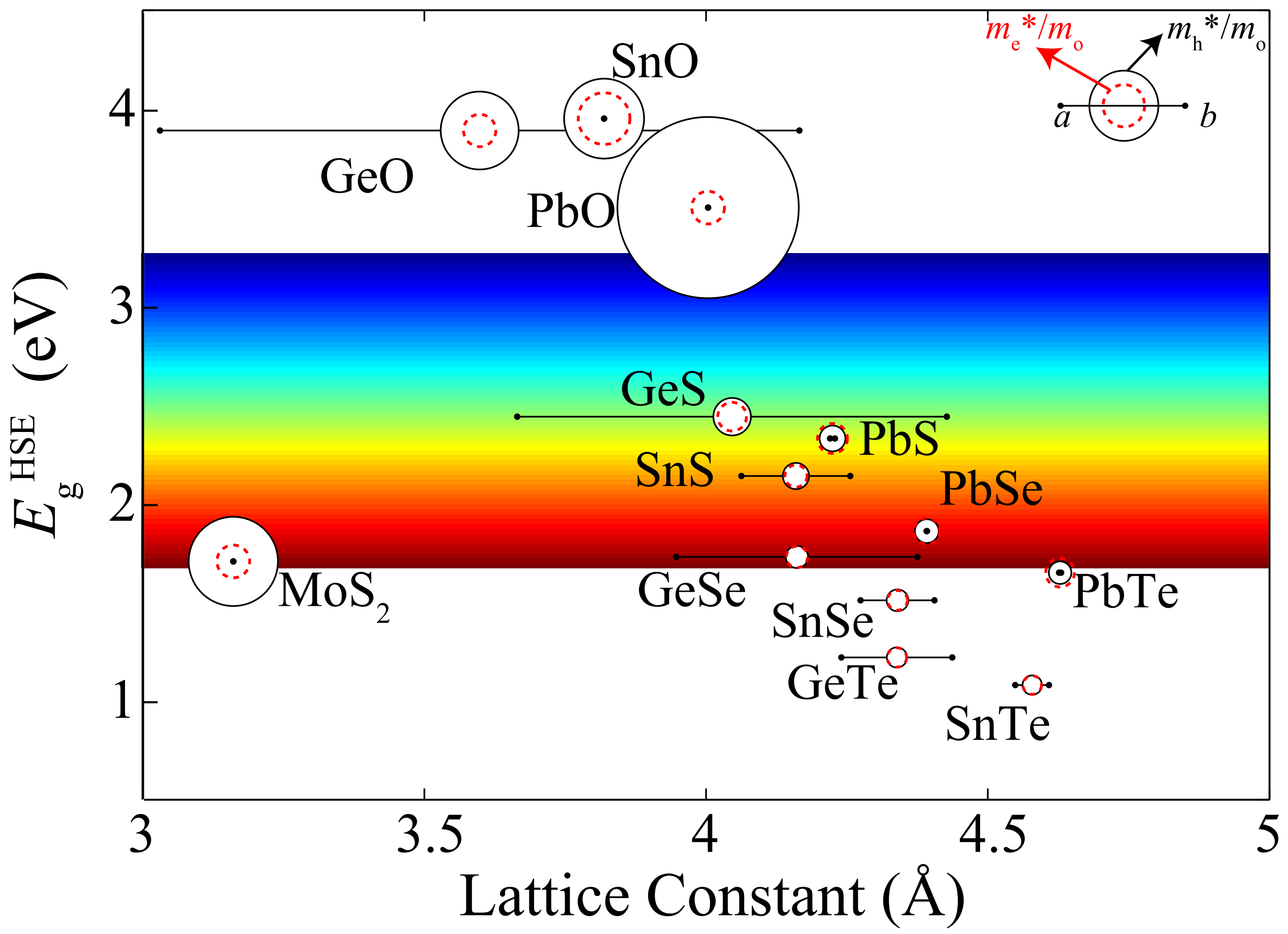
MPInterfaces - High throughput framework for 2D materials





Screen 2D materials for photocathodes

- Formation from layered bulk materials
- Semiconductors with small effective masses
- Promising family of group-IV monochalcogenides



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Acknowledgment

- MPInterfaces for novel 2D materials: **K. Mathew**, **A. Singh**, **M. Ashton**, **J. Paul**, J. Gabriel, H. Zhuang, M. Blonsky, M. Johannes, R. Ramanathan, R. Duan, Z. Ziyu
- VASPsol solvation model and nanocrystals: K. Mathew, J. Gabriel, C. Bealing
- GASP genetic algorithm and machine learning: **B. Revard**, W. Tipton, A. Yesupenko, B. Antonio, S. Honrao
- Financial support by NSF-CAREER, NSF-SSI, NIST, DOE-EFRC
- Computational resources provided by HiPerGator@UF and NSF XSEDE

NSF NIST emc2 XSEDE

HiPerGator 2.0
The University of Florida Supercomputer

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2D Materials Beyond Graphene

Materials interfaces

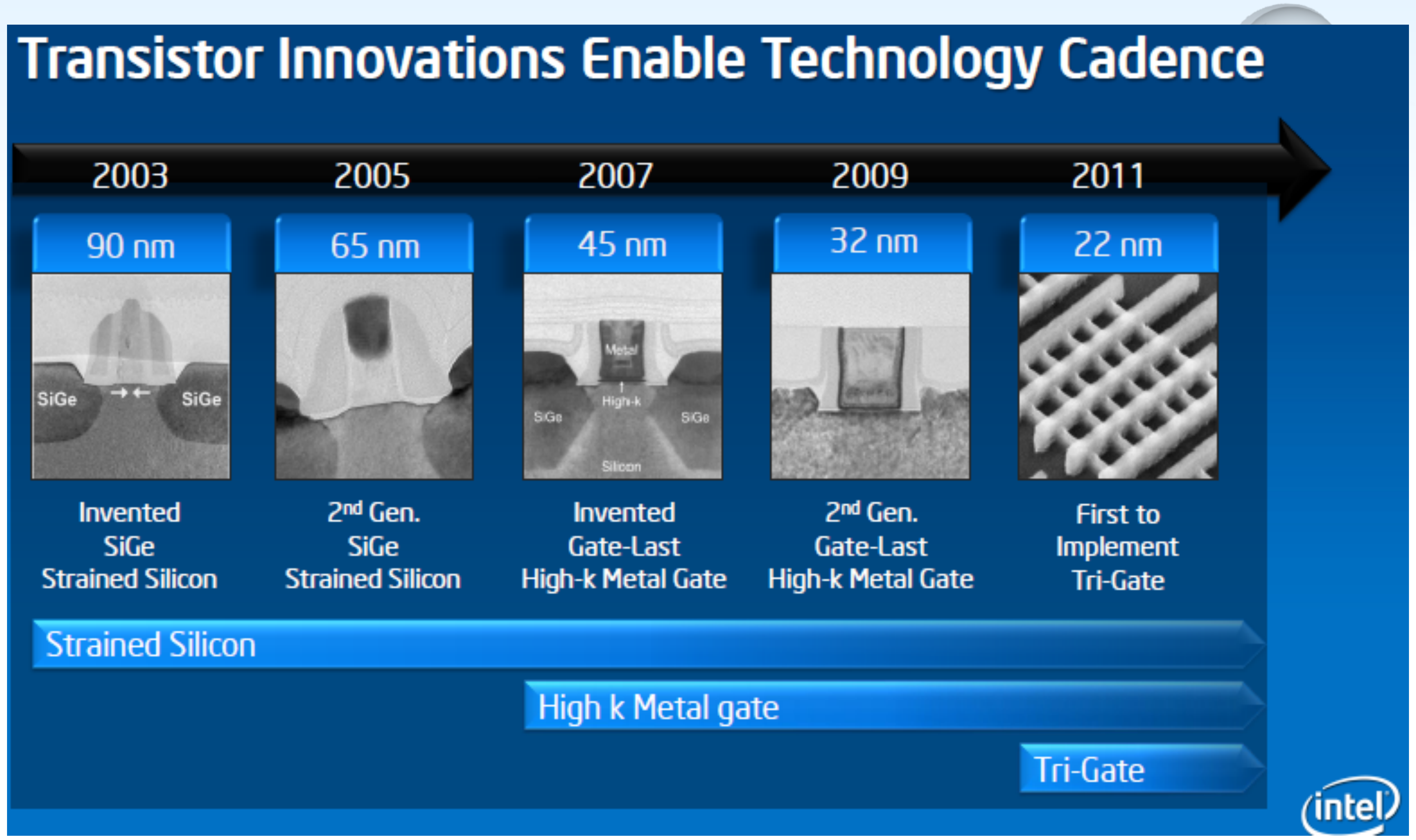
- At the heart of many modern-day critical technologies
- Importance in key industrial segments: Microelectronics, chemical and energy industries

Single-layer or 2D materials

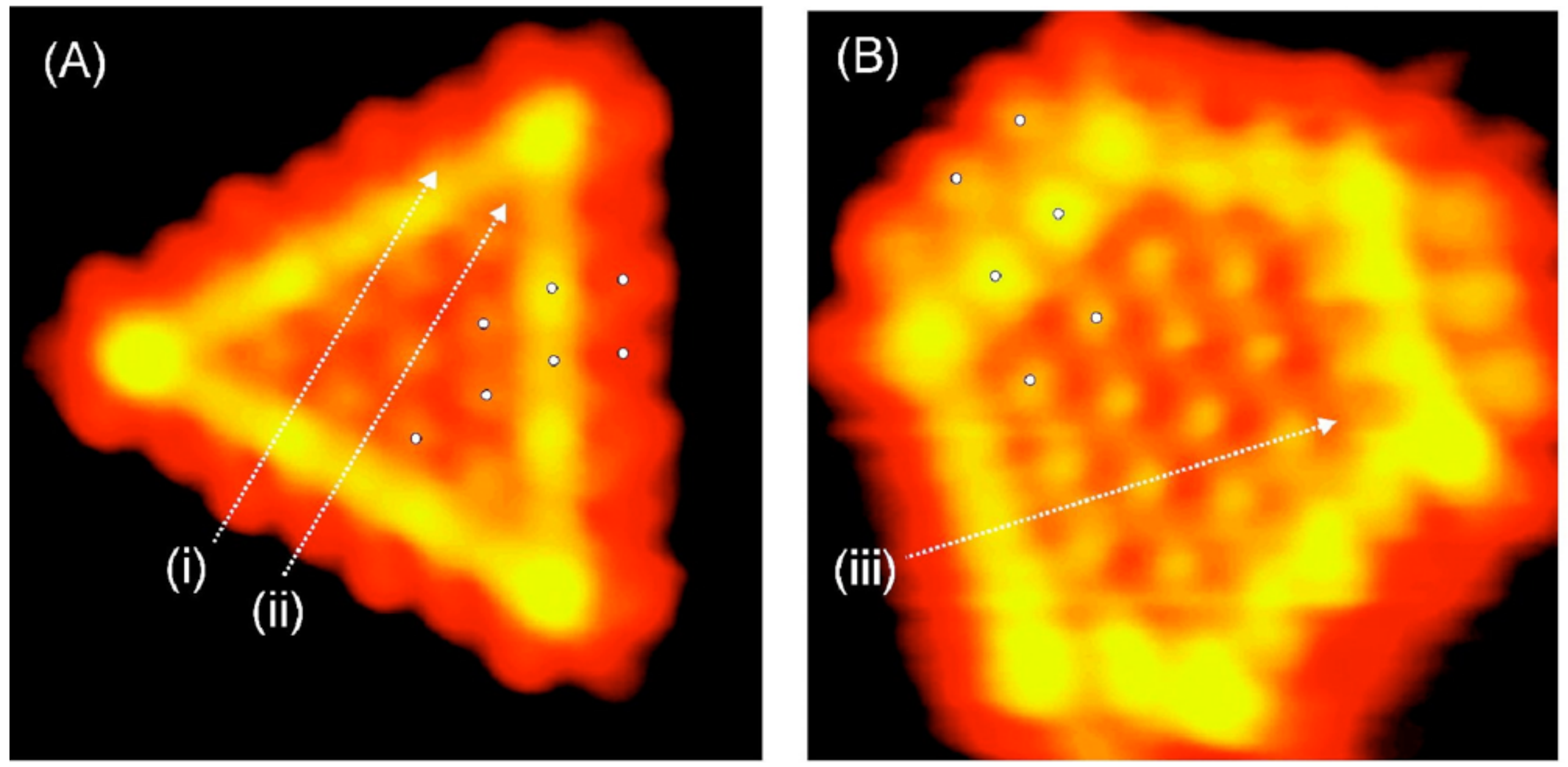
- Maximize their interfacial area
- Properties differ from 3D counterparts
- Potentially many more 2D materials awaiting discovery

Advantages for Photocathodes

- Atomically flat
- Low surface energy, hydrophobic, low reactivity
- Possibly weak interactions with substrates



http://newsroom.intel.com/docs/DOC-2032



Lauritsen et al., J. Catalysis 221 25 (2004)

Overview of 2D Materials

Definition: Two-dimensional materials are crystals with structures that are periodic in two dimensions and have finite extension in the third dimension.

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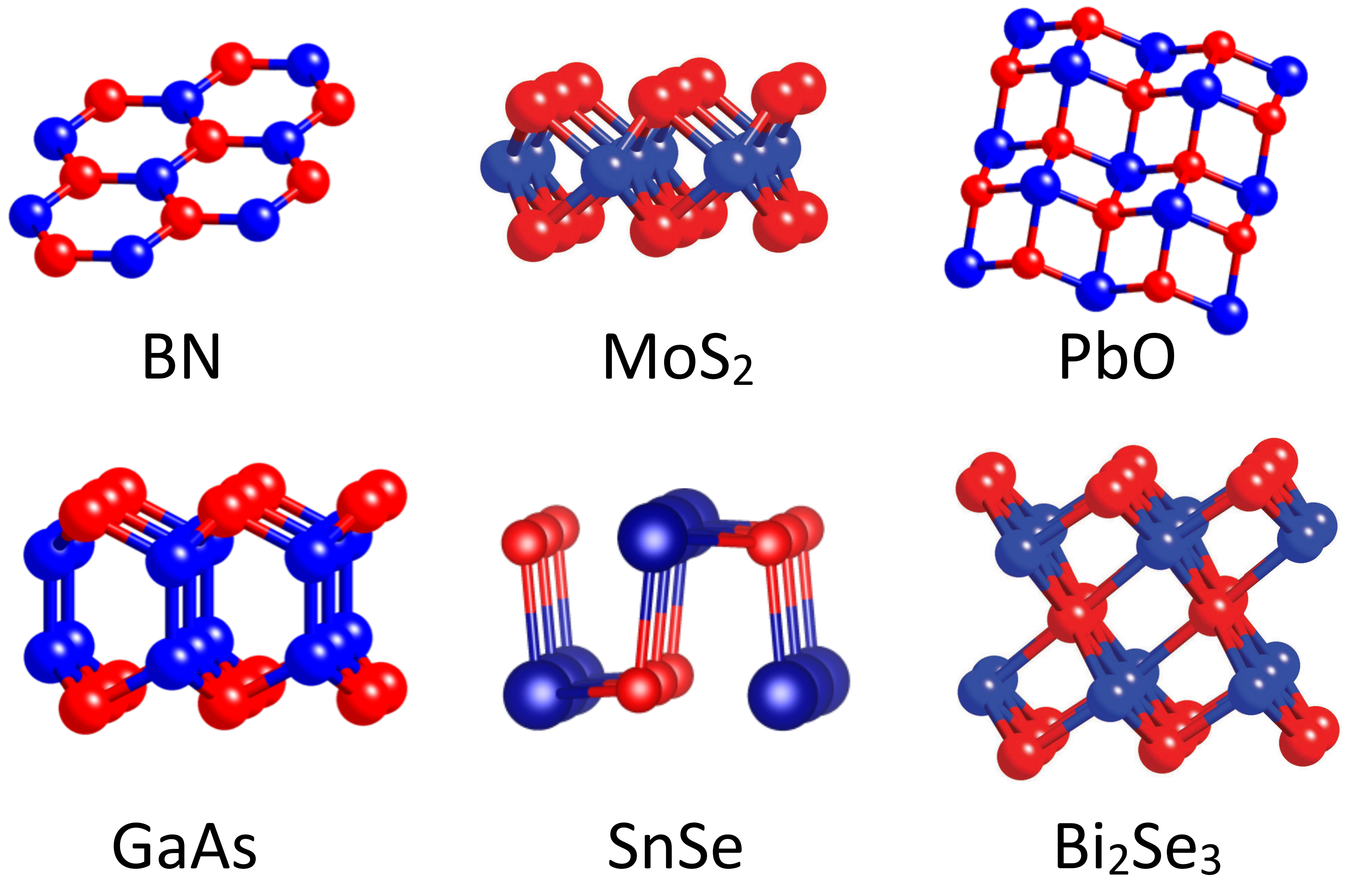
- 2D materials could consist of more than one atomic layer

Structure



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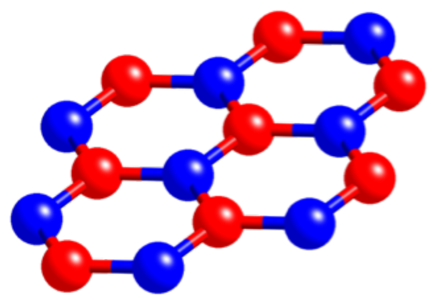
- 2D materials could consist of more than one atomic layer
- Electronic, magnetic, etc. properties for electronic and energy applications

Structure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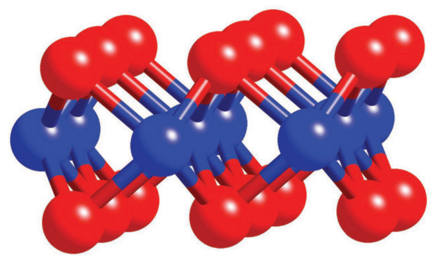
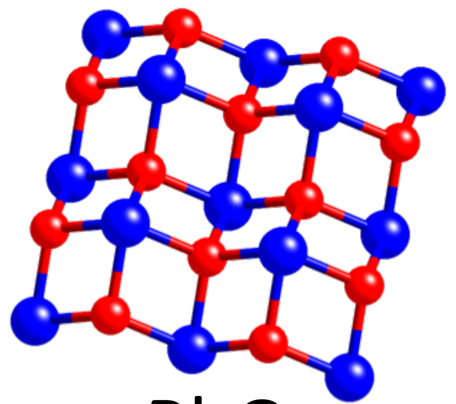
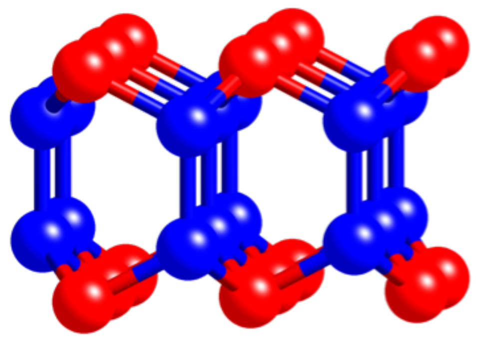
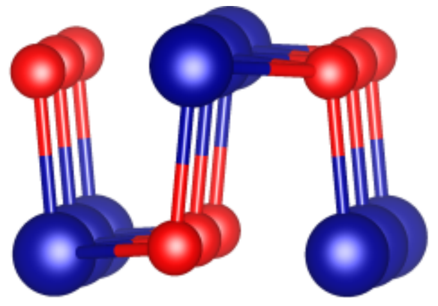
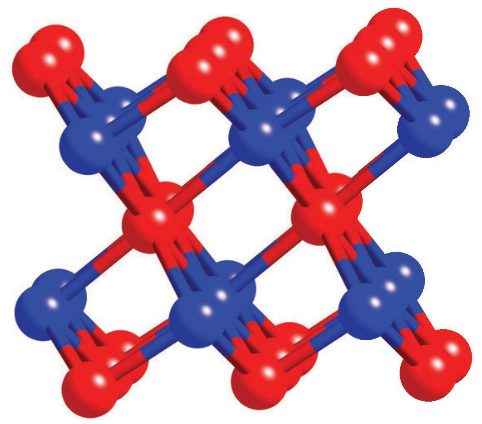

MoS_2

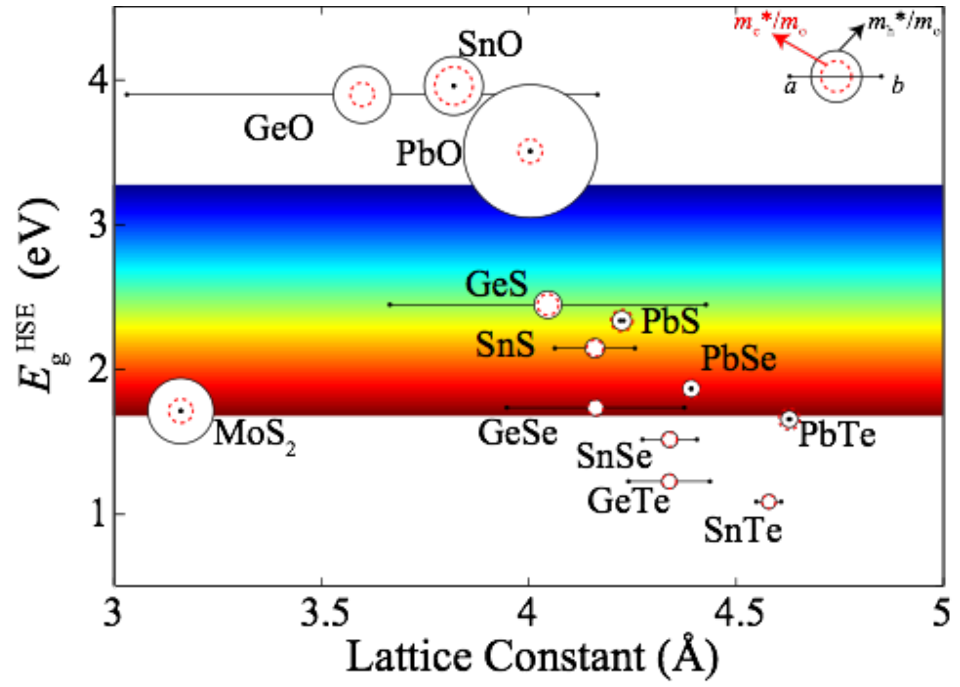

PbO

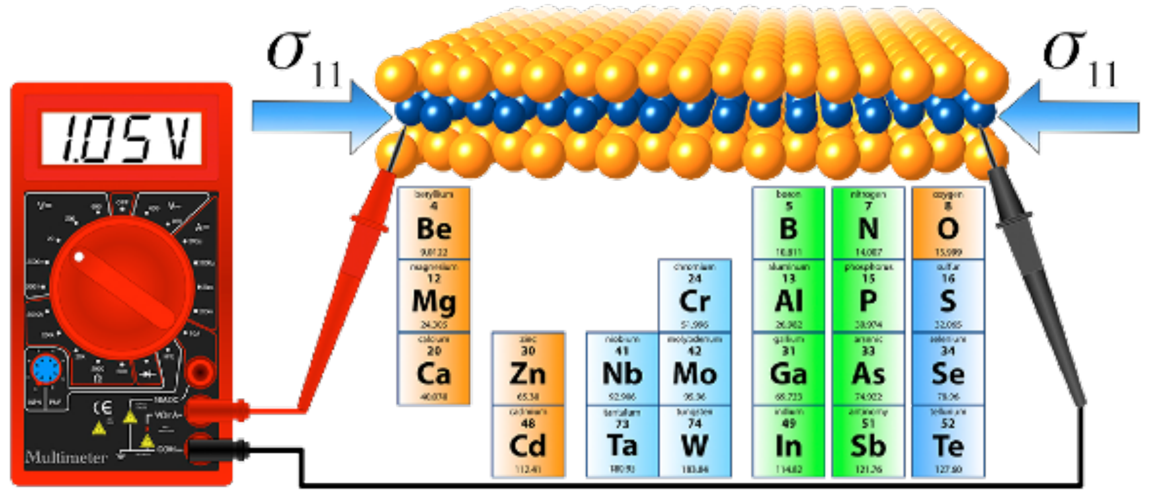

GaAs


SnSe


Bi_2Se_3

Properties





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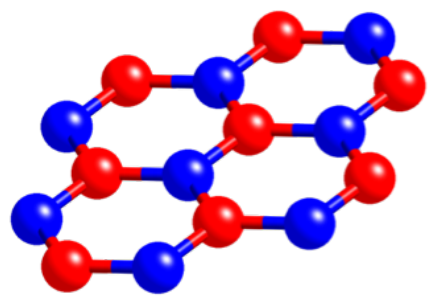
Overview of 2D Materials

Definition: Two-dimensional materials are crystals with structures that are periodic in two dimensions and have finite extension in the third dimension.

- 2D materials could consist of more than one atomic layer
- Electronic, magnetic, etc. properties for electronic and energy applications
- Substrates for synthesis and chemical properties for processing

Structure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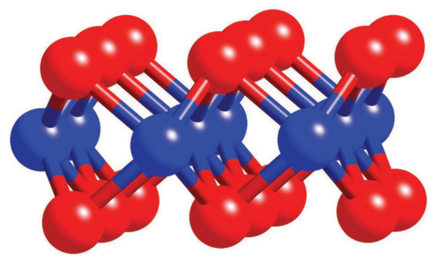
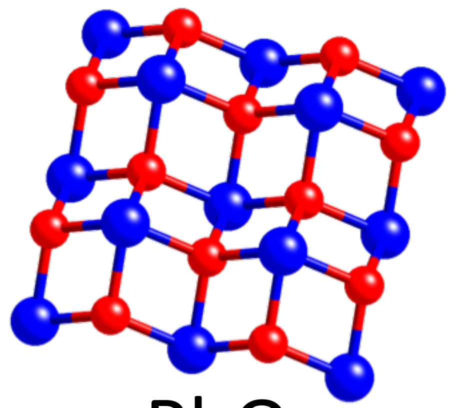
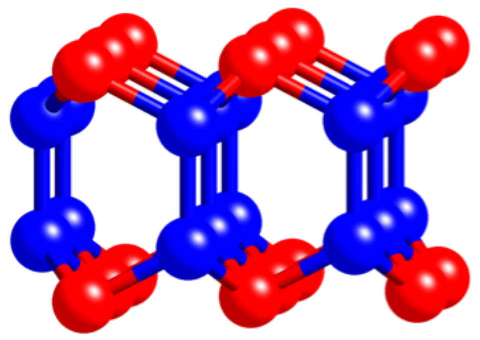

MoS_2


PbO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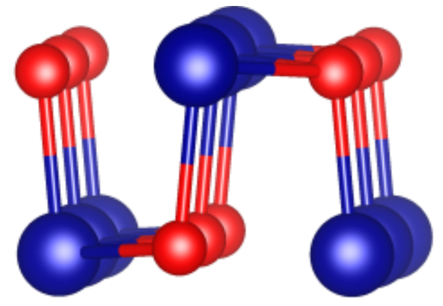
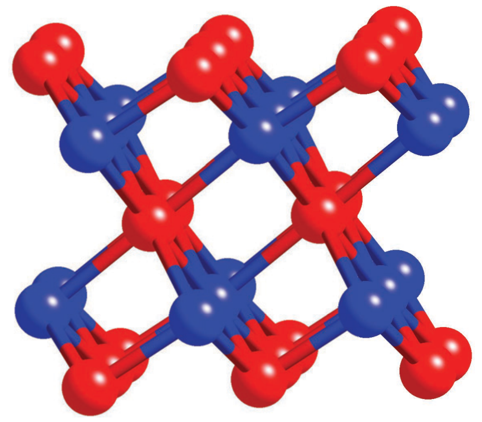

SnSe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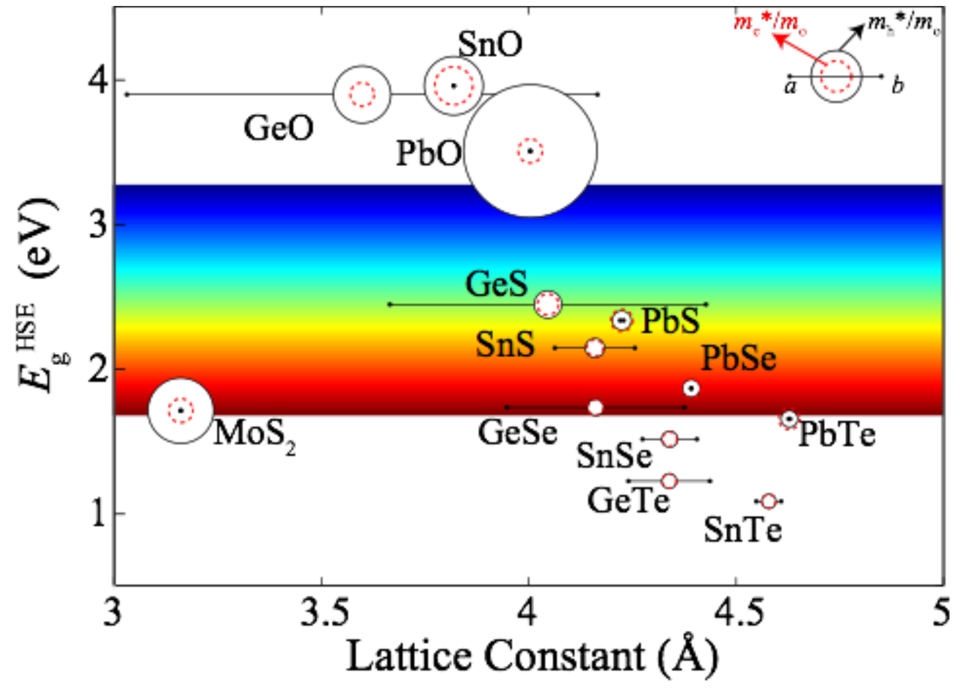

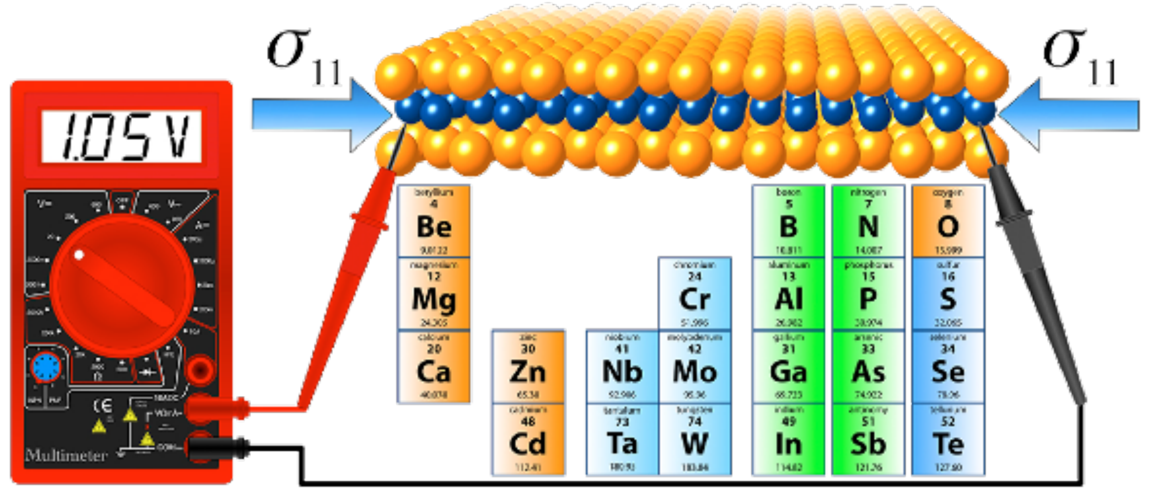

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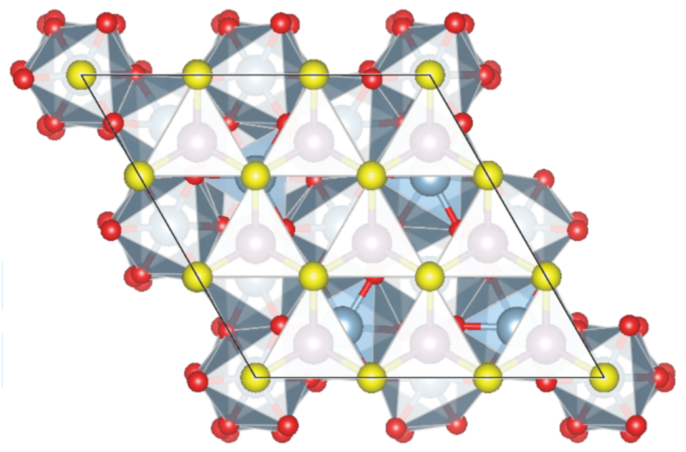
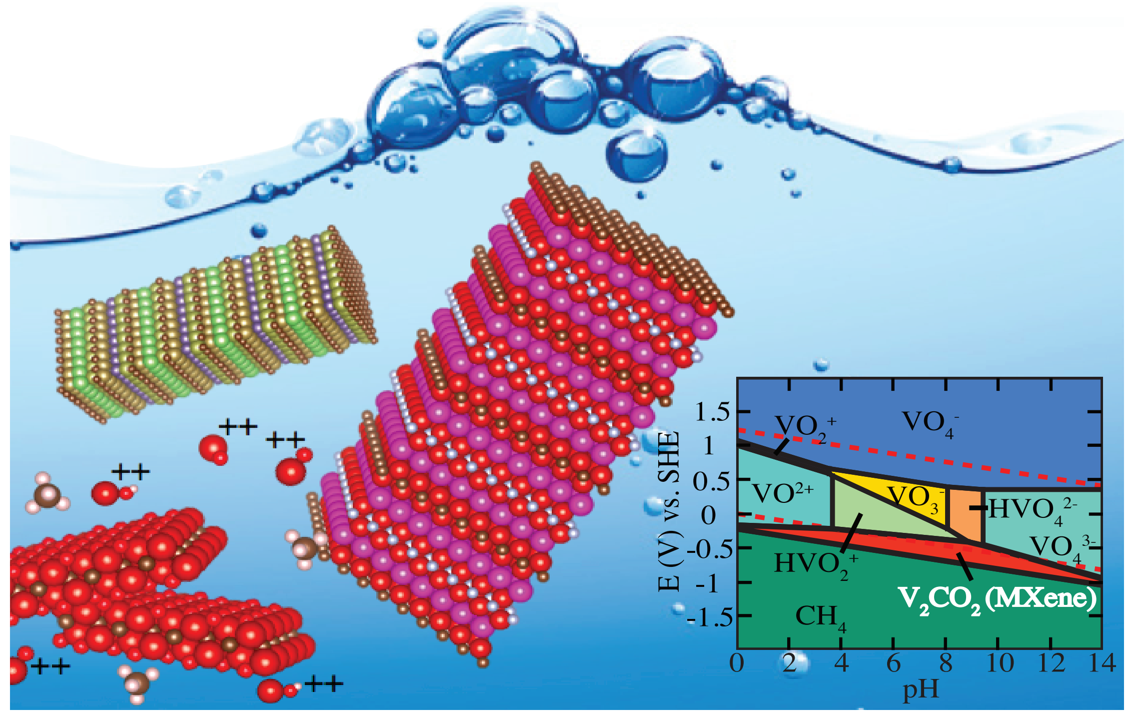
Processing





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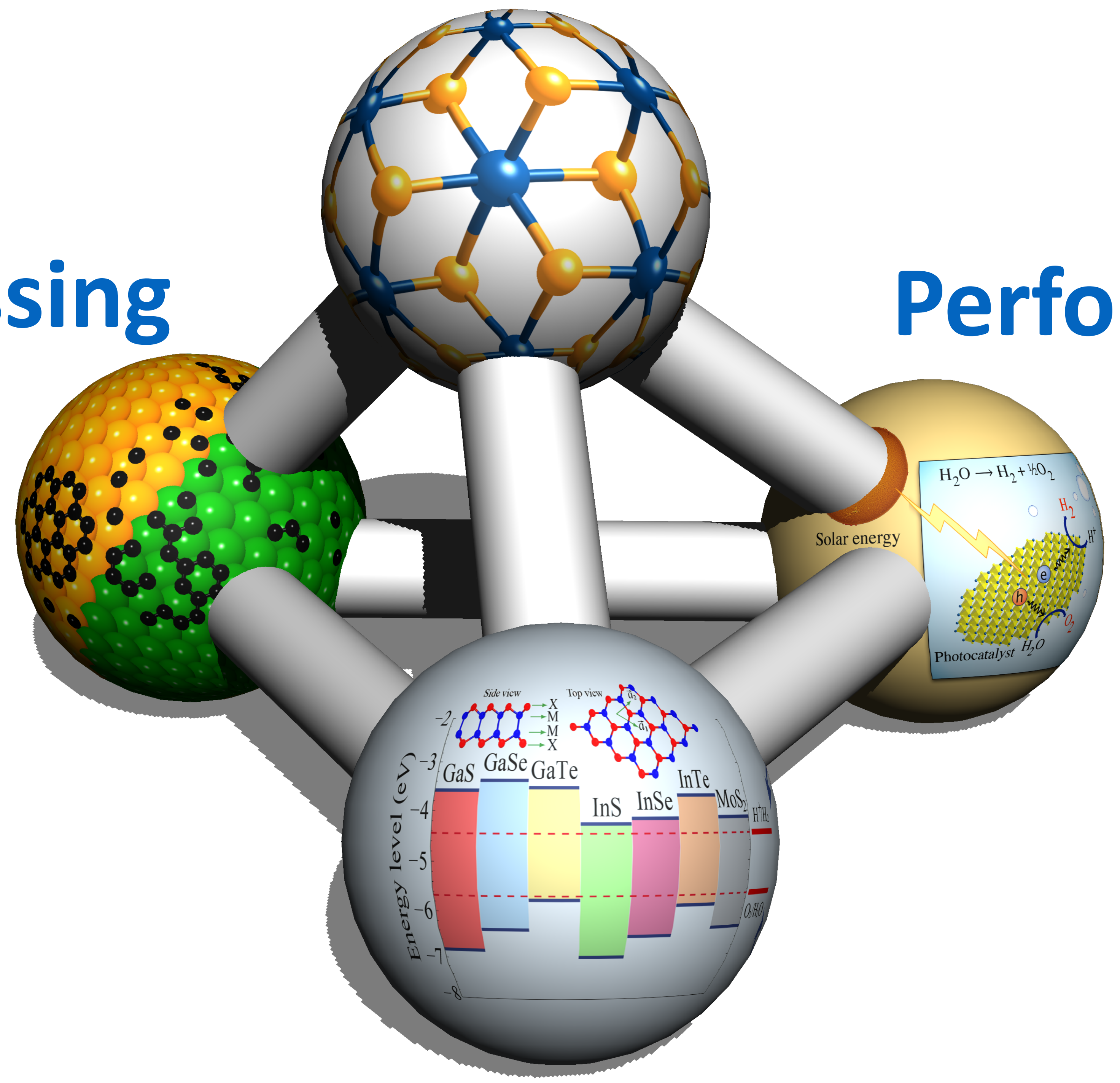
Materials Informatics of 2D Materials

Structure

Processing

Performance



Properties

Materials Selection	Data Mining	Layered bulk materials
	Chemical Substitutions	New Compositions and Structures
	Genetic Algorithm	
Structure	Structural Stability	Formation Energy
	Dynamic Stability	Phonon Spectrum
	Chemical Stability	Pourbaix Diagrams
Properties	Optotelectronics	Bandgap, Offsets, Absorption, Excitons
	Magnetism	Domains, Critical T
Processing	Substrates	Adsorption, Strain, Doping
	Electrochemistry	Etching, Solutions
Performance	Electronic Devices	I-V Characteristic Carrier Mobility
	Energy Applications	Light conversion, Catalytic Activity

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

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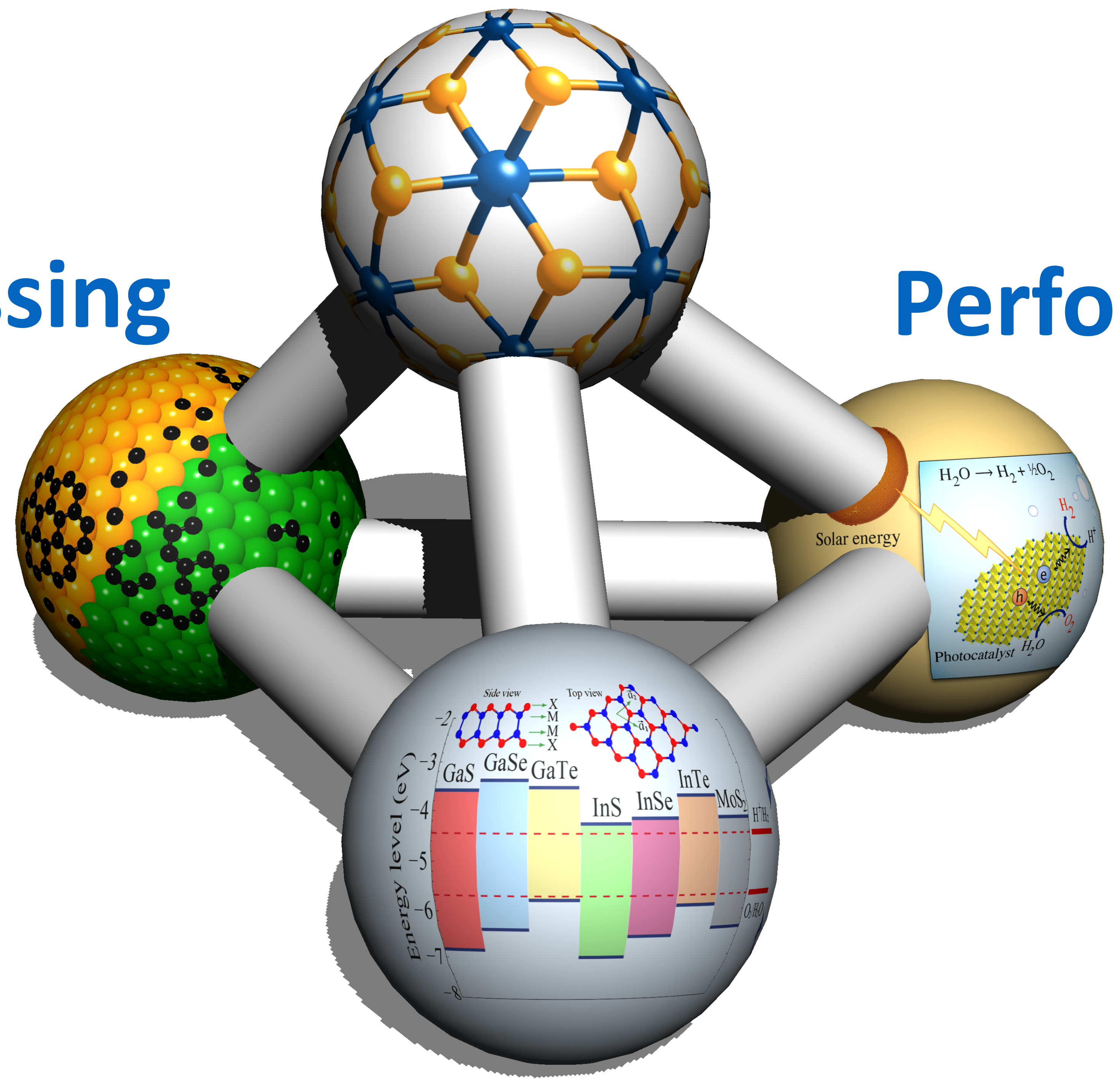

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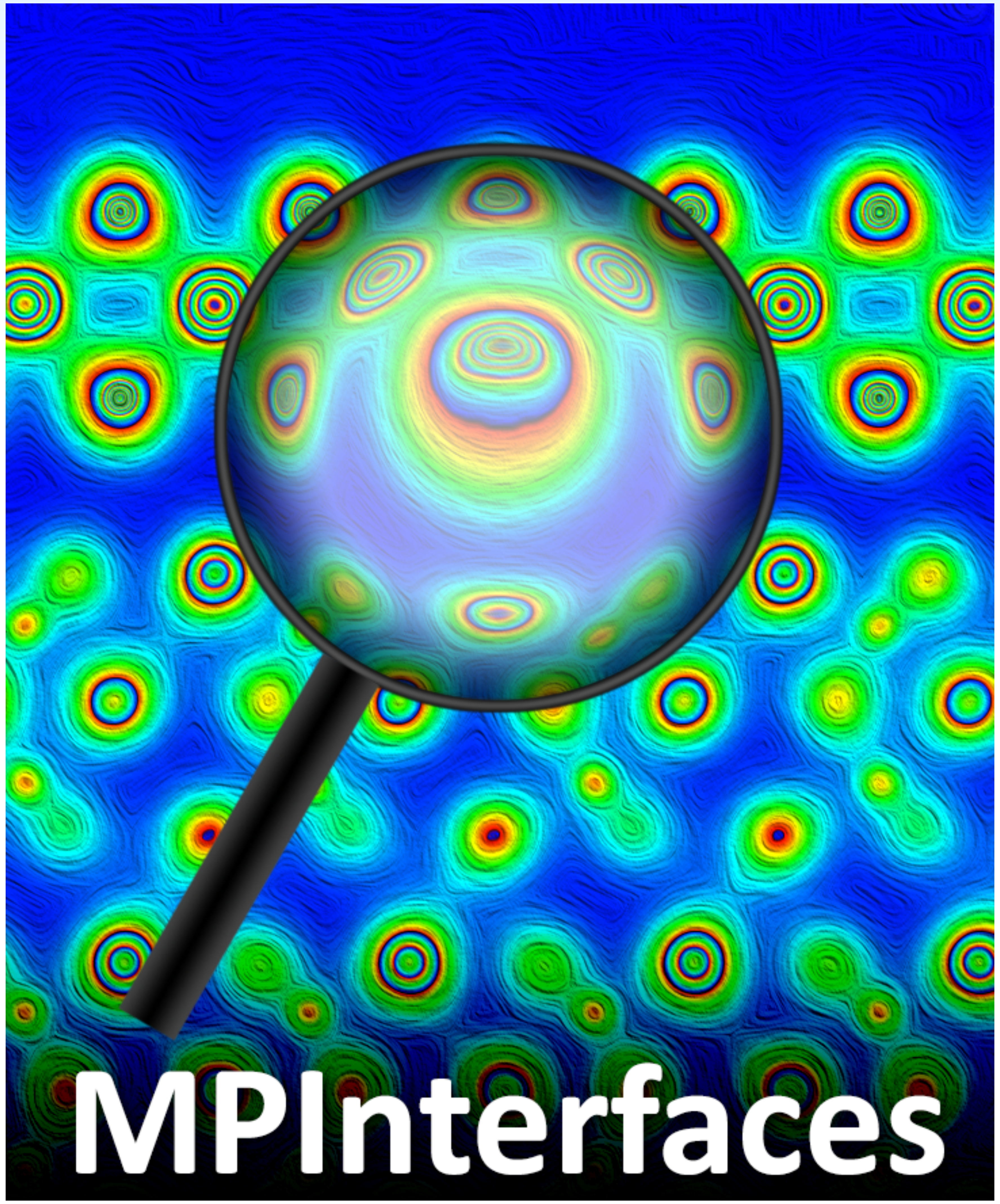

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Information from DFT for Photocathodes

Information from DFT for photocathodes

- Band structures (gaps, effective masses)

A. K. Singh & RGH
Appl. Phys. Lett. 105, 042103 (2014)

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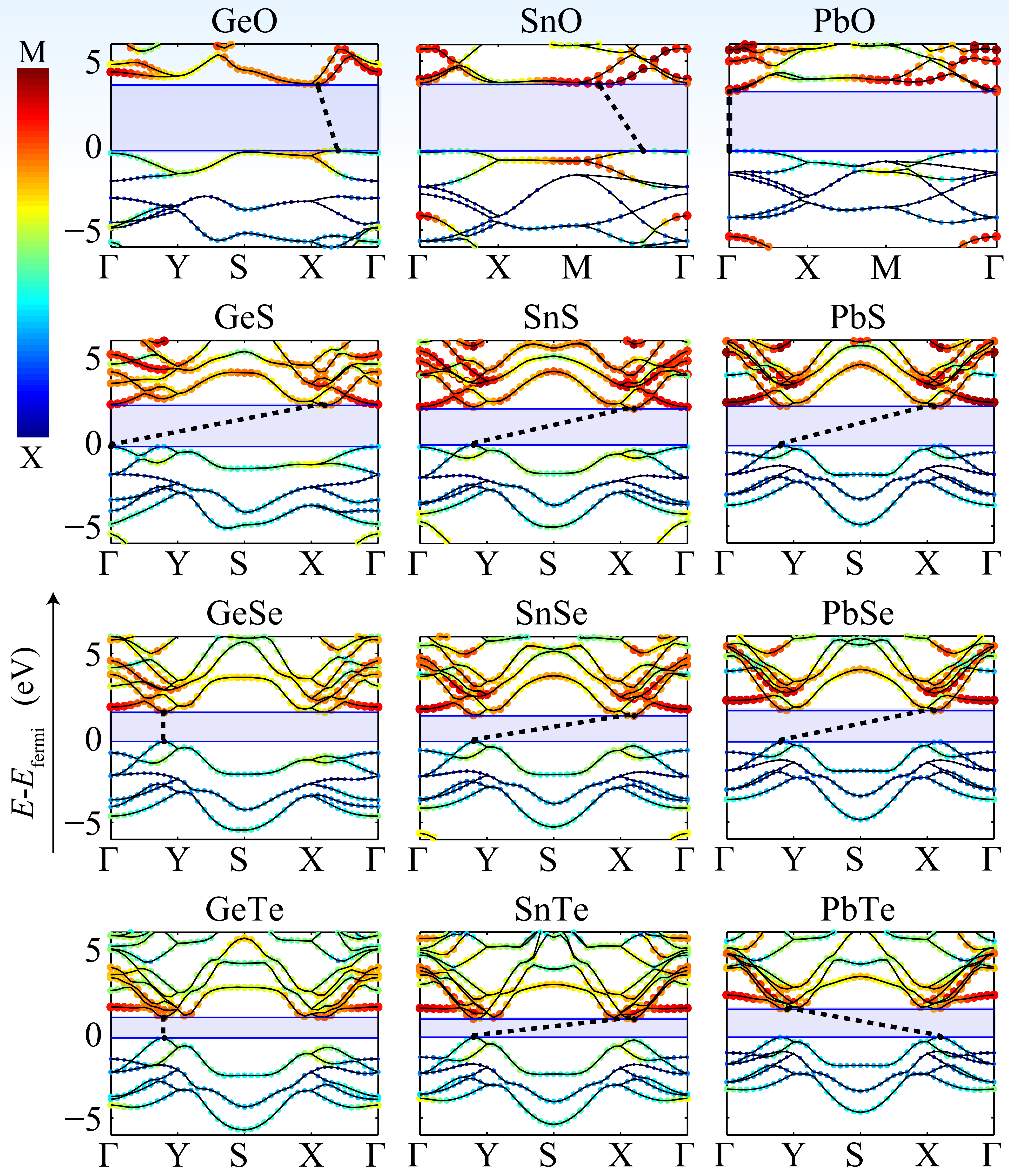

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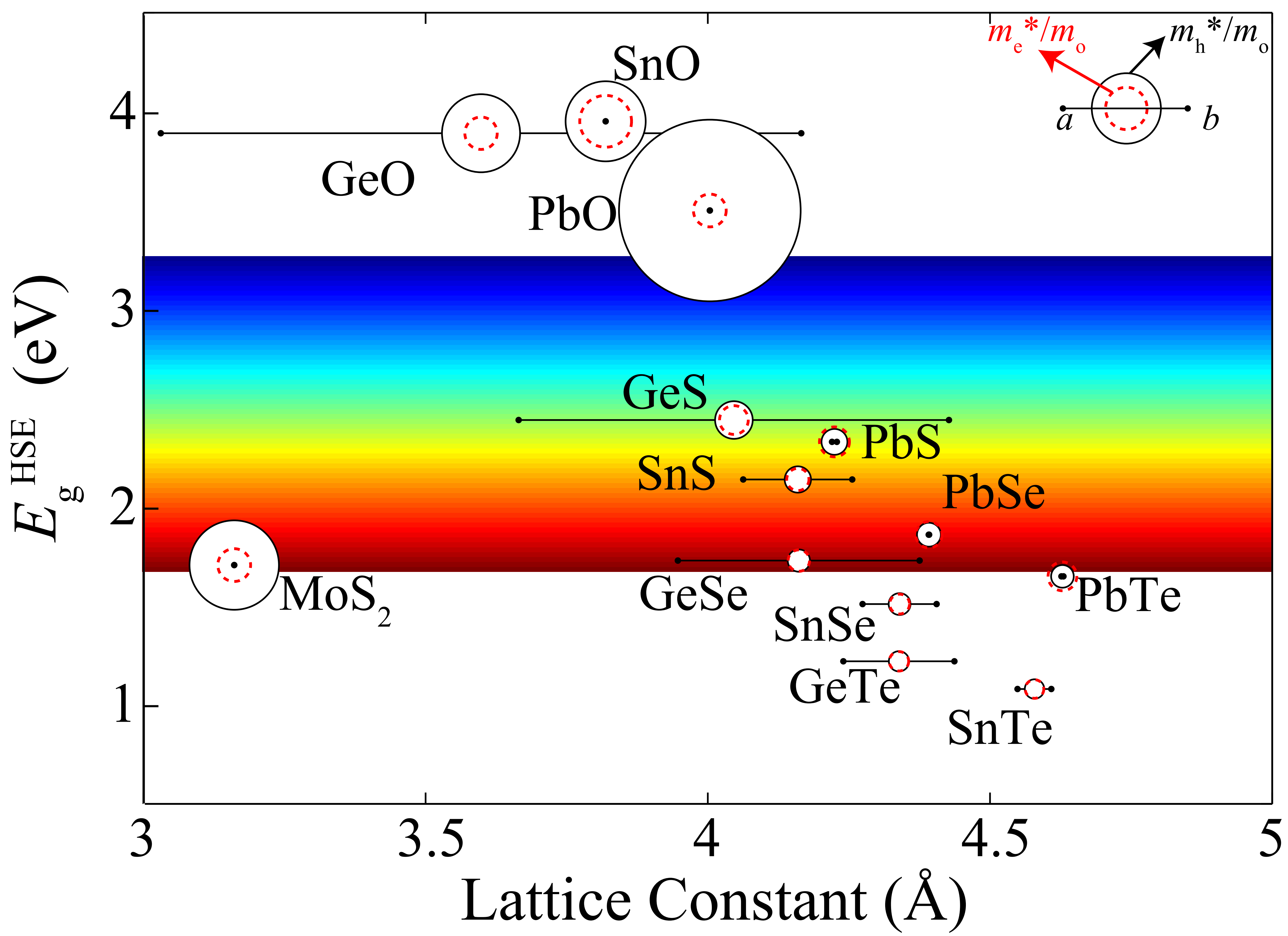

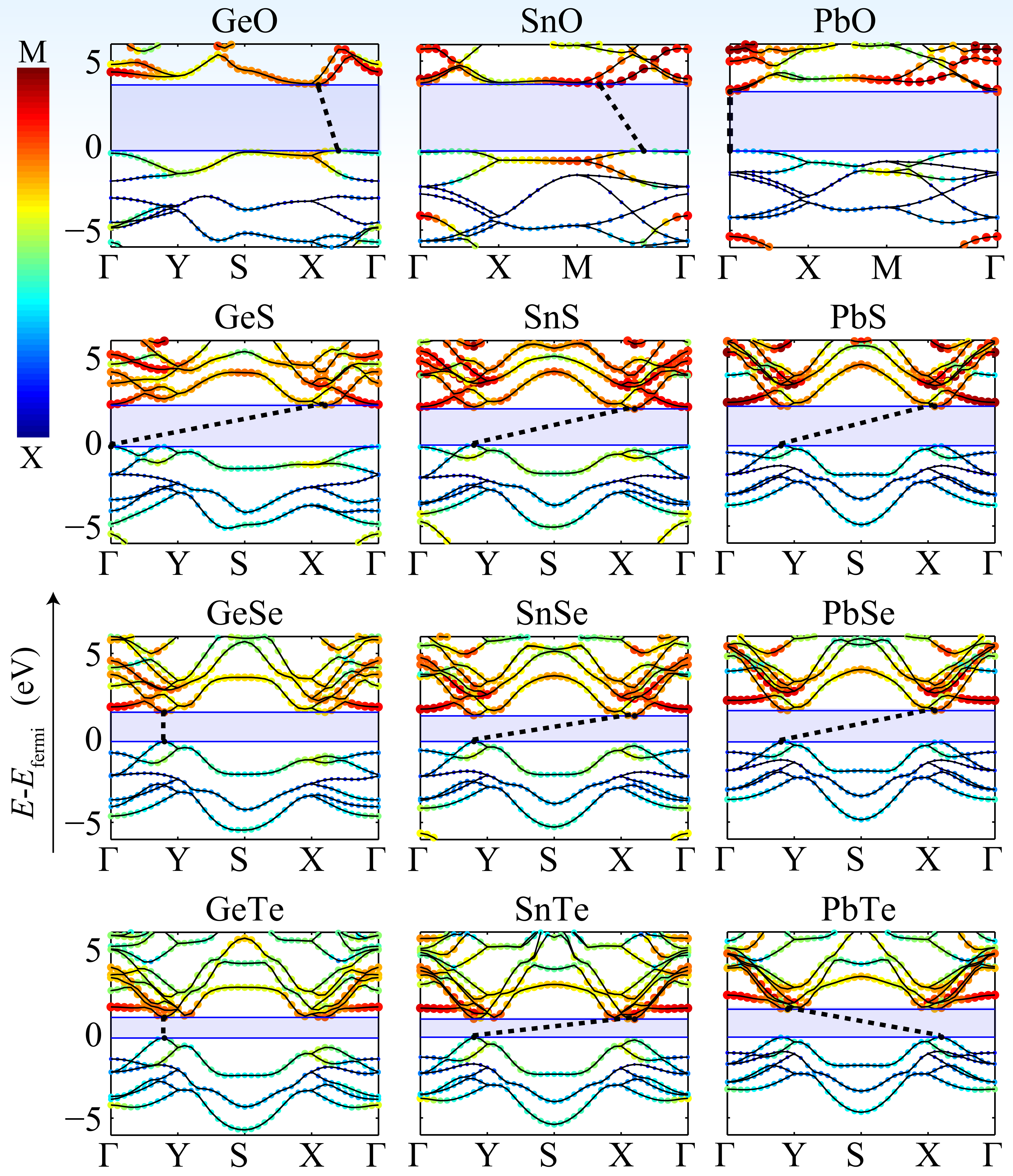

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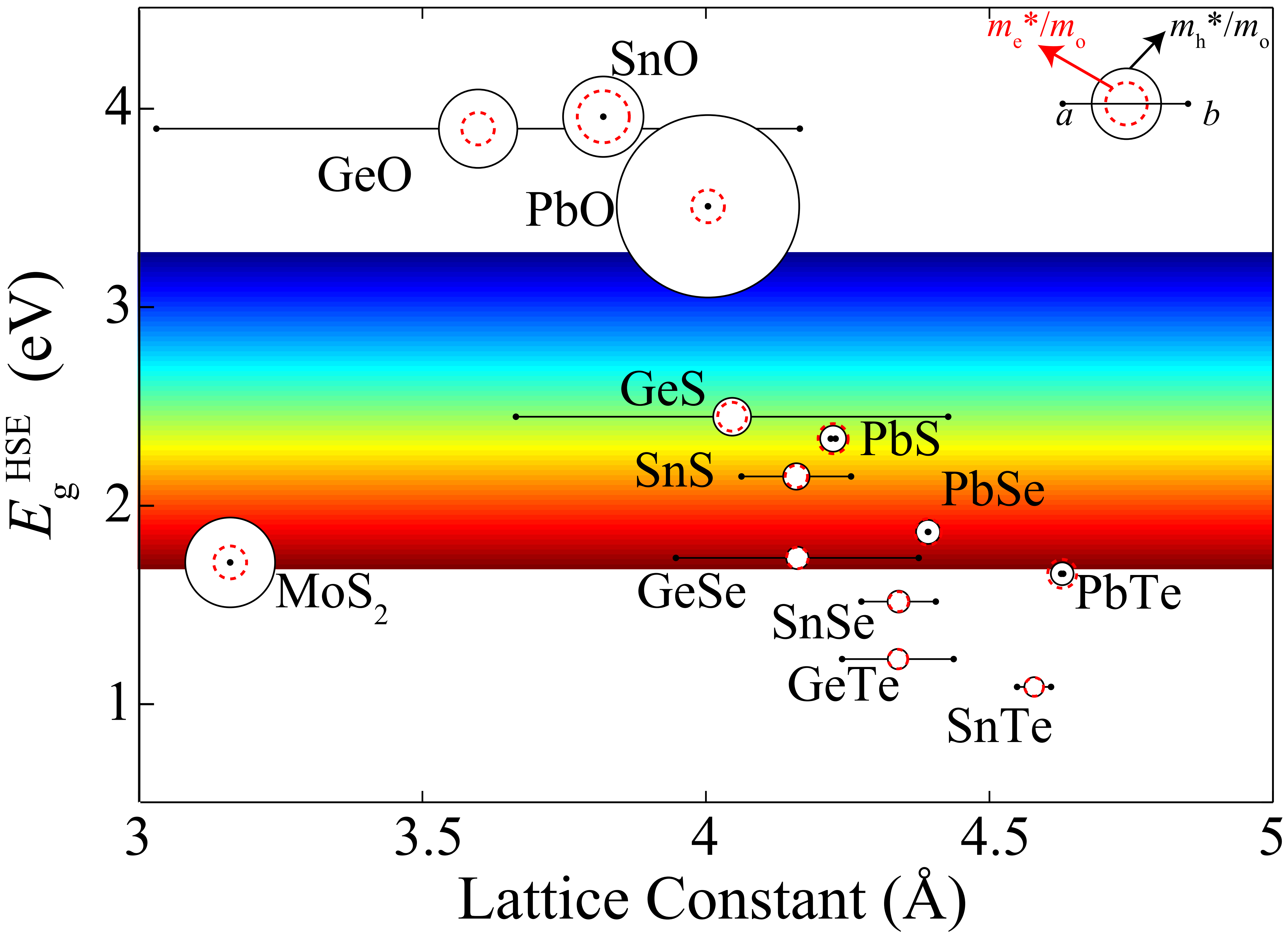

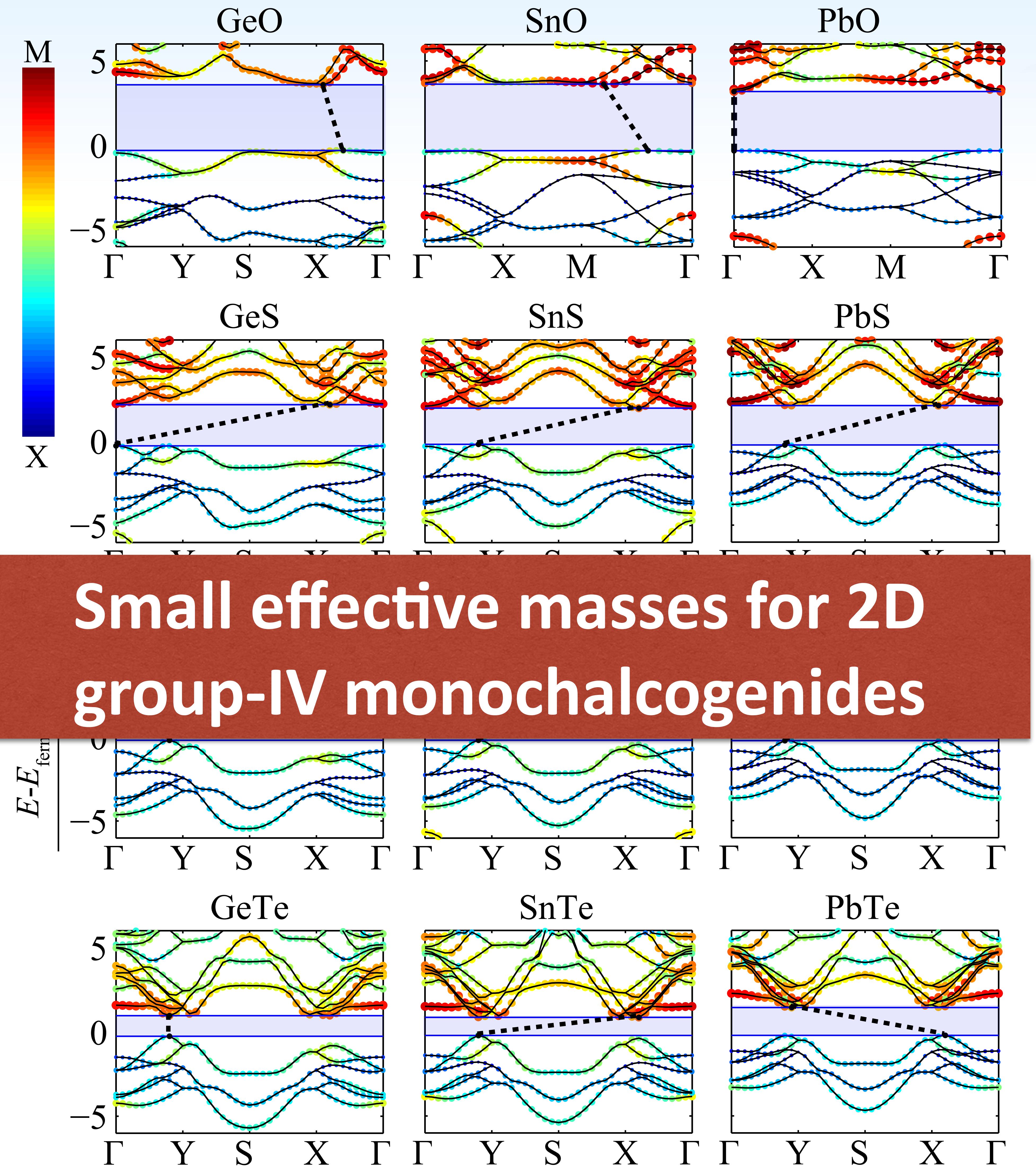

Small effective masses for 2D group-IV monochalcogenides

A. K. Singh & RGH
Appl. Phys. Lett. 105, 042103 (2014)

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- Workfunction and electron affinity

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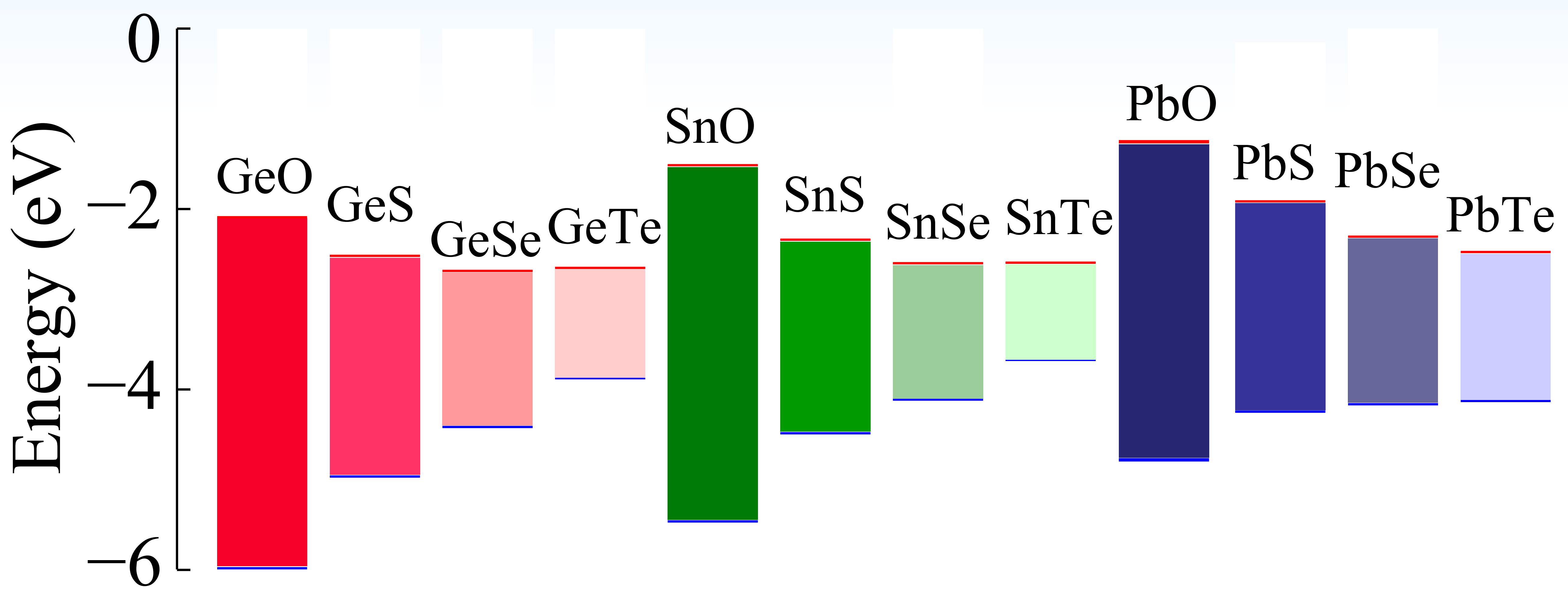

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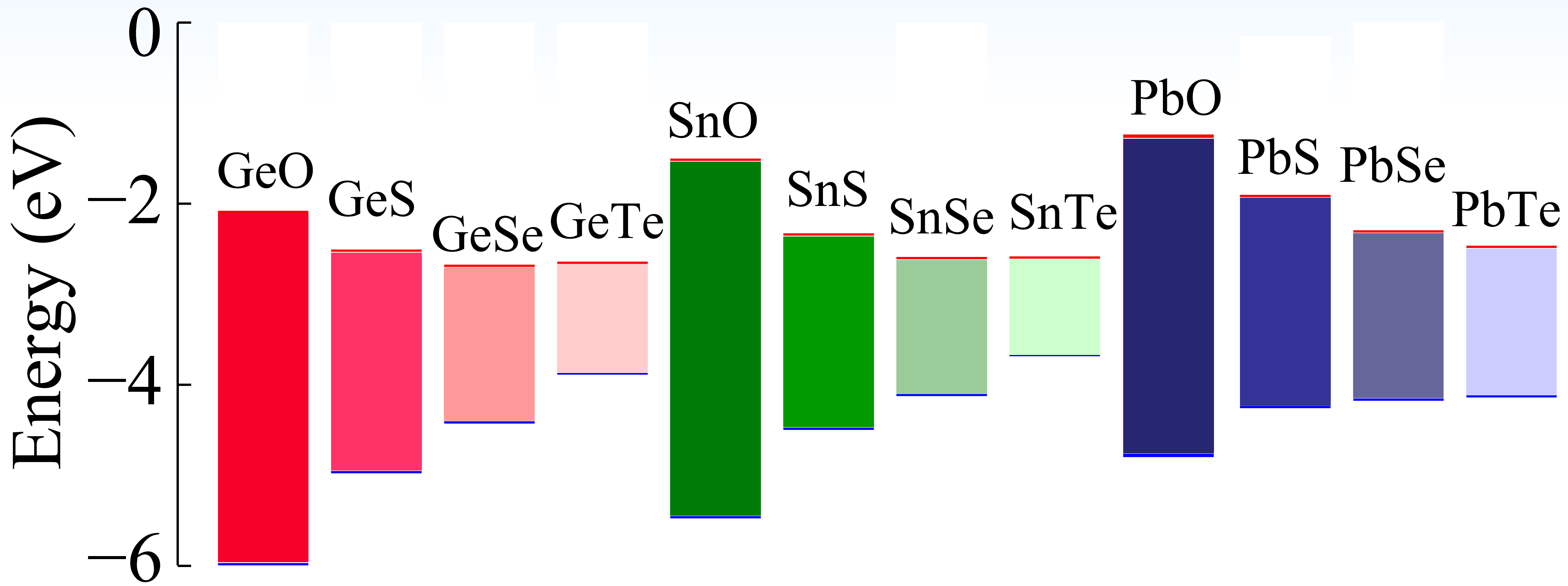

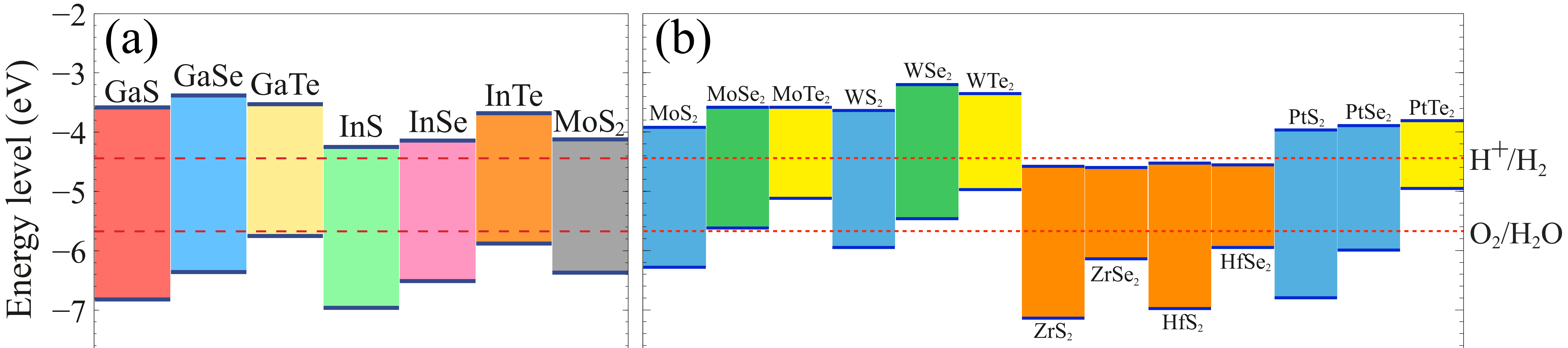

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- Band structures (gaps, effective masses)
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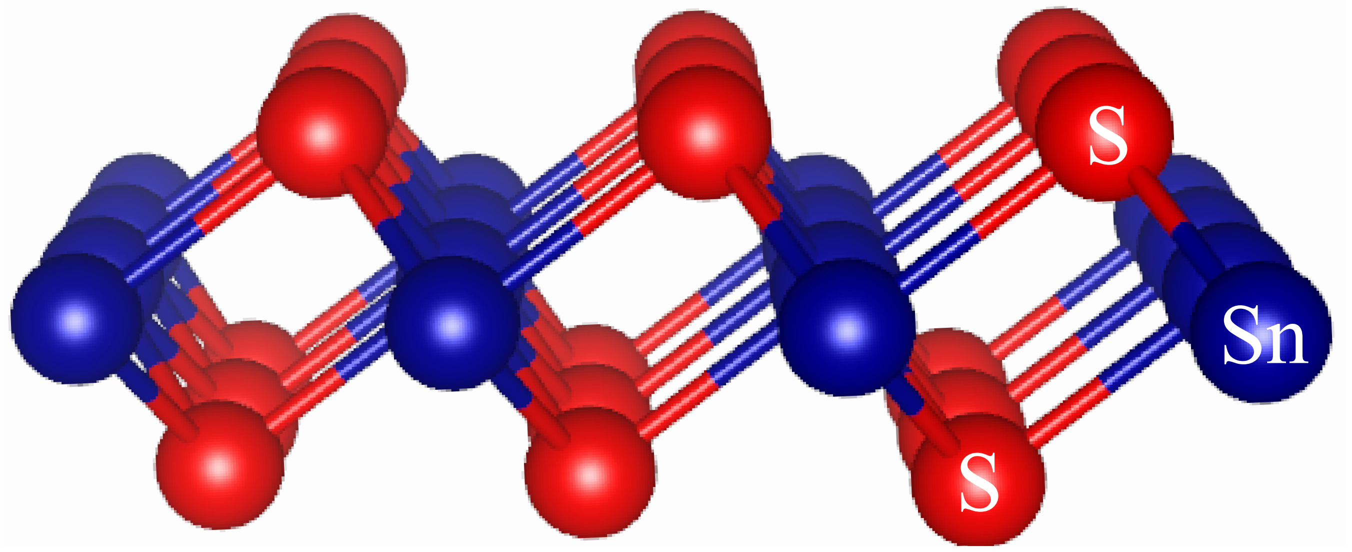
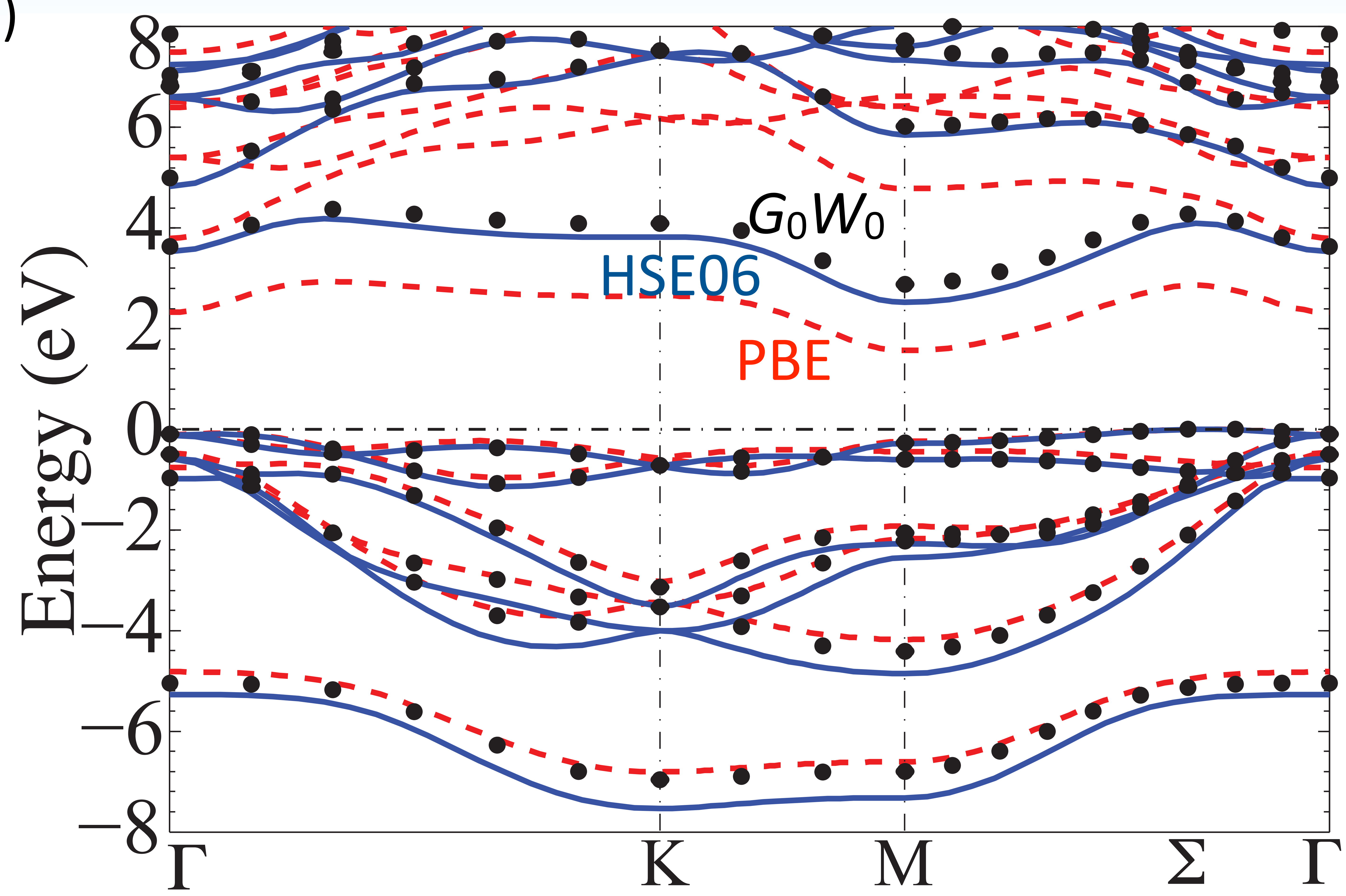
- Quasiparticle energies
  (corrections to band structure)

2D SnS_2





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- Optical transitions and excitons

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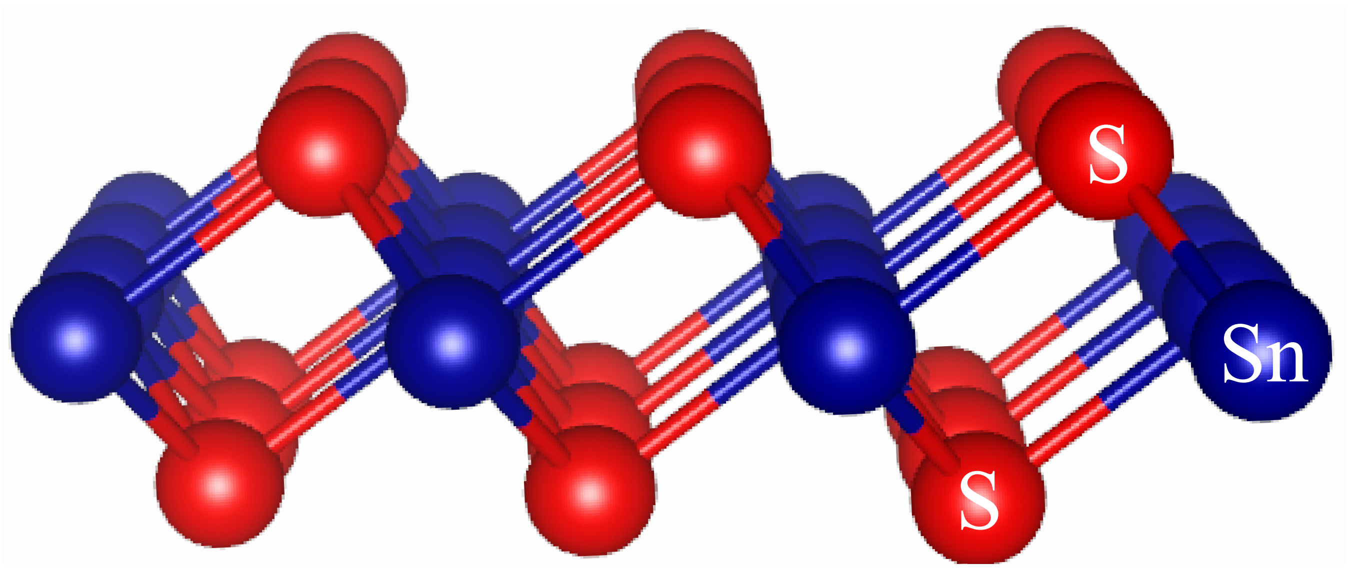

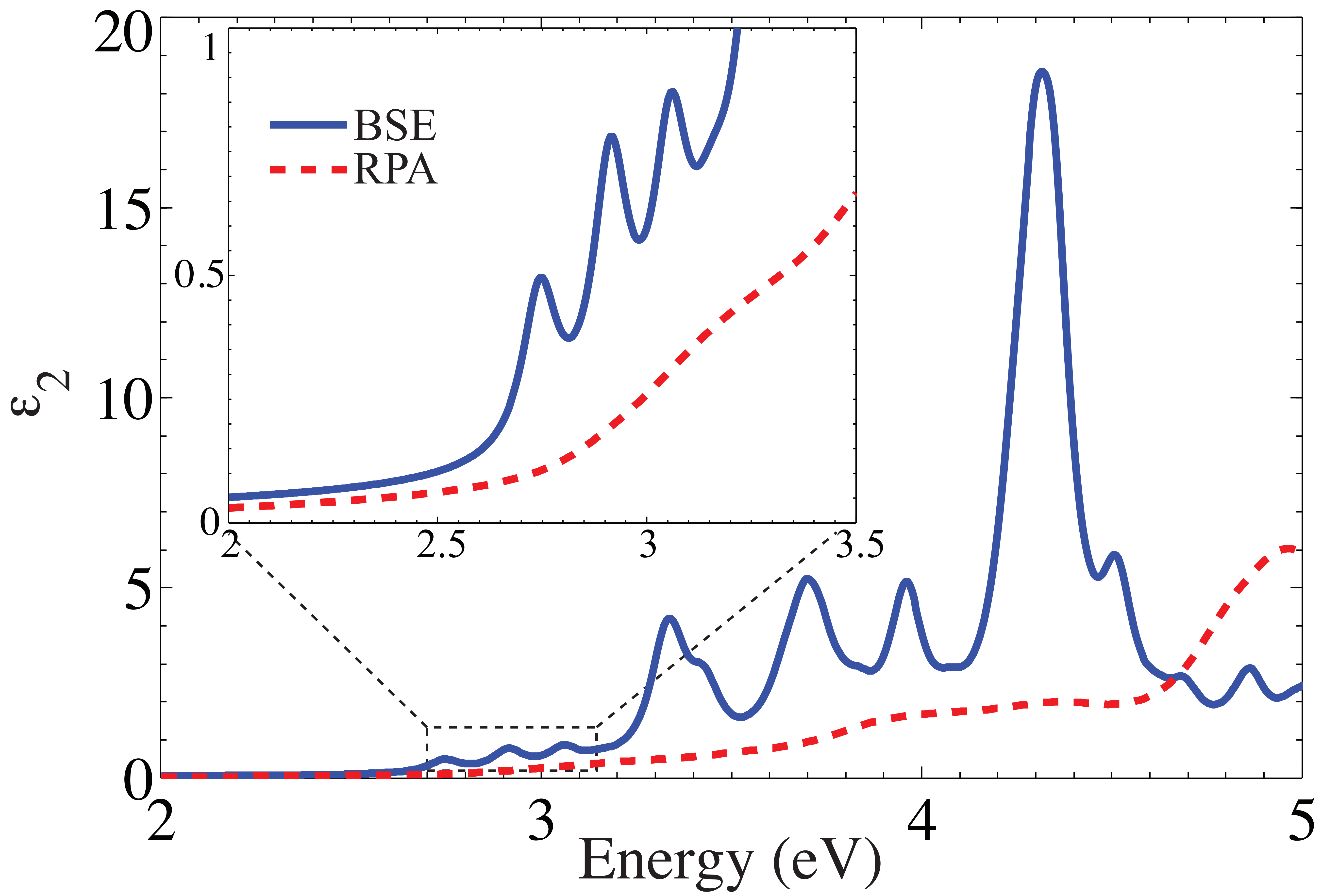

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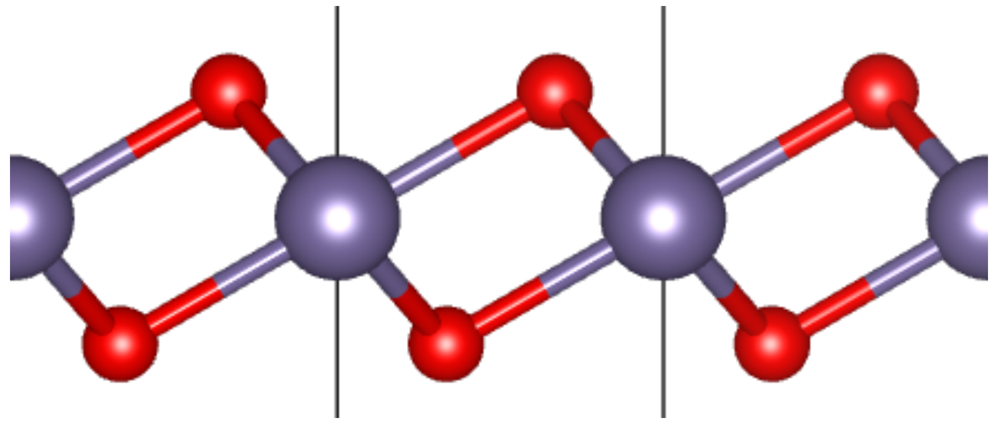
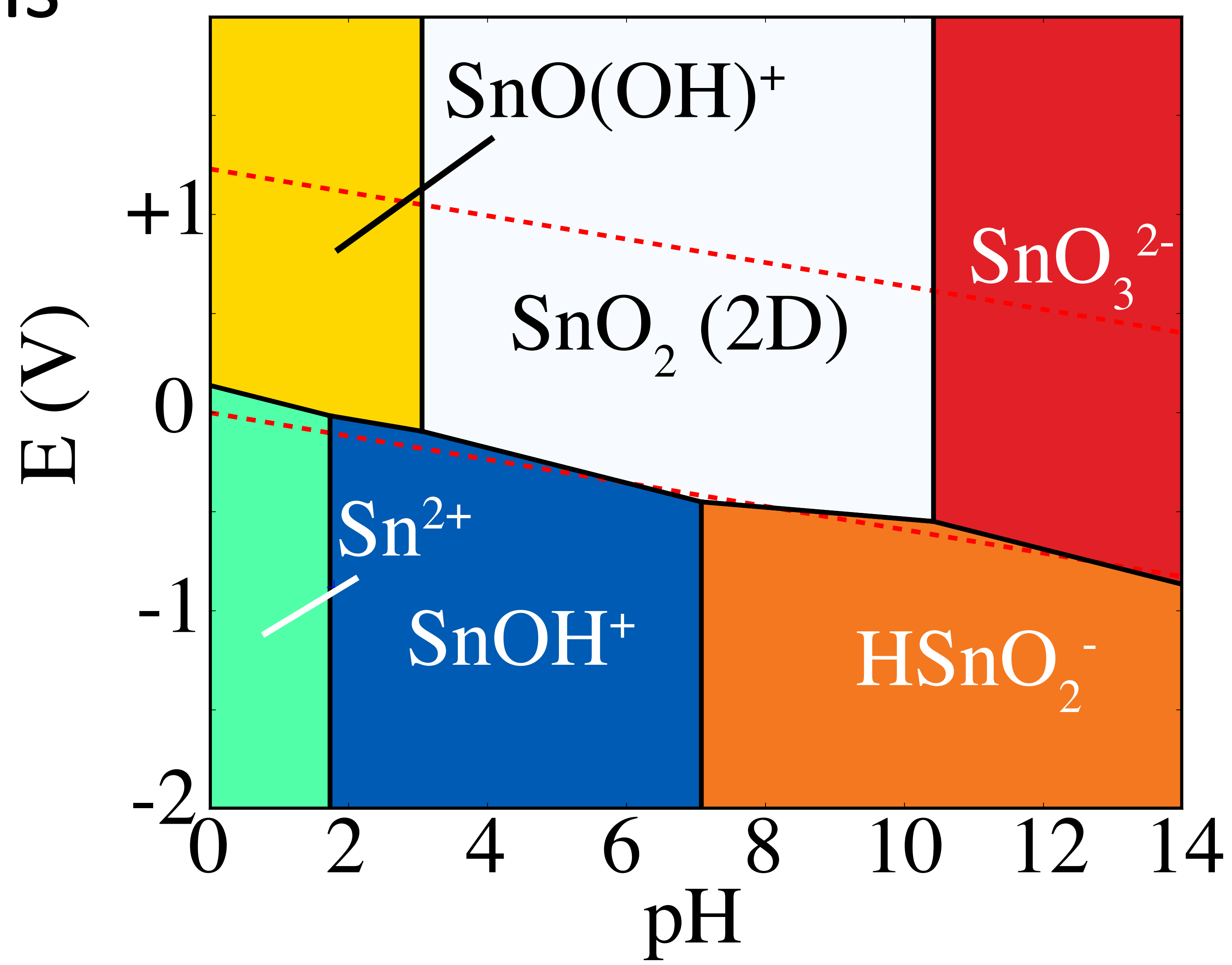
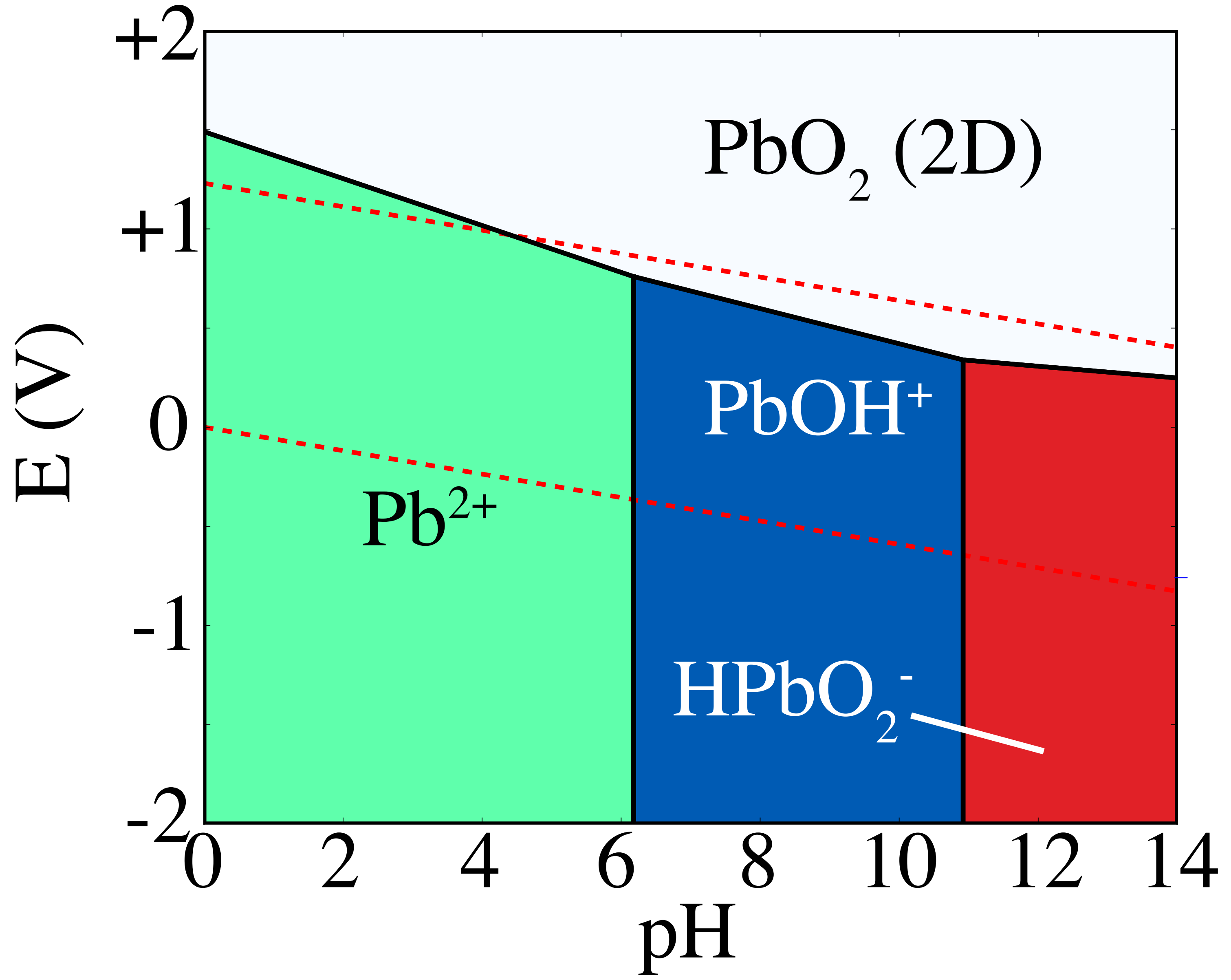
- Quasiparticle energies (corrections to band structure)
- Optical transitions and excitons
- Materials stability, Pourbaix diagrams



2D Sn-O Phases



2D Pb-O Phases



Screening of 2D Materials for Photocathodes

Screening of 2D materials:

1. Identify layered bulk materials ⇒ 826 monolayer candidates
2. Formation energy relative to bulk ⇒ 625 stable monolayer
3. Monolayers ⇒ 282 semiconductors ($0 < E_{gap} \leq 3$eV)
4. Semiconductors ⇒ 81 with direct gap
   ⇒ 201 with indirect gap
5. Semiconductors ⇒ 21 with $m_{effective} < 1\ m_e$
6. Additional consideration: Dirac-cone 2D materials

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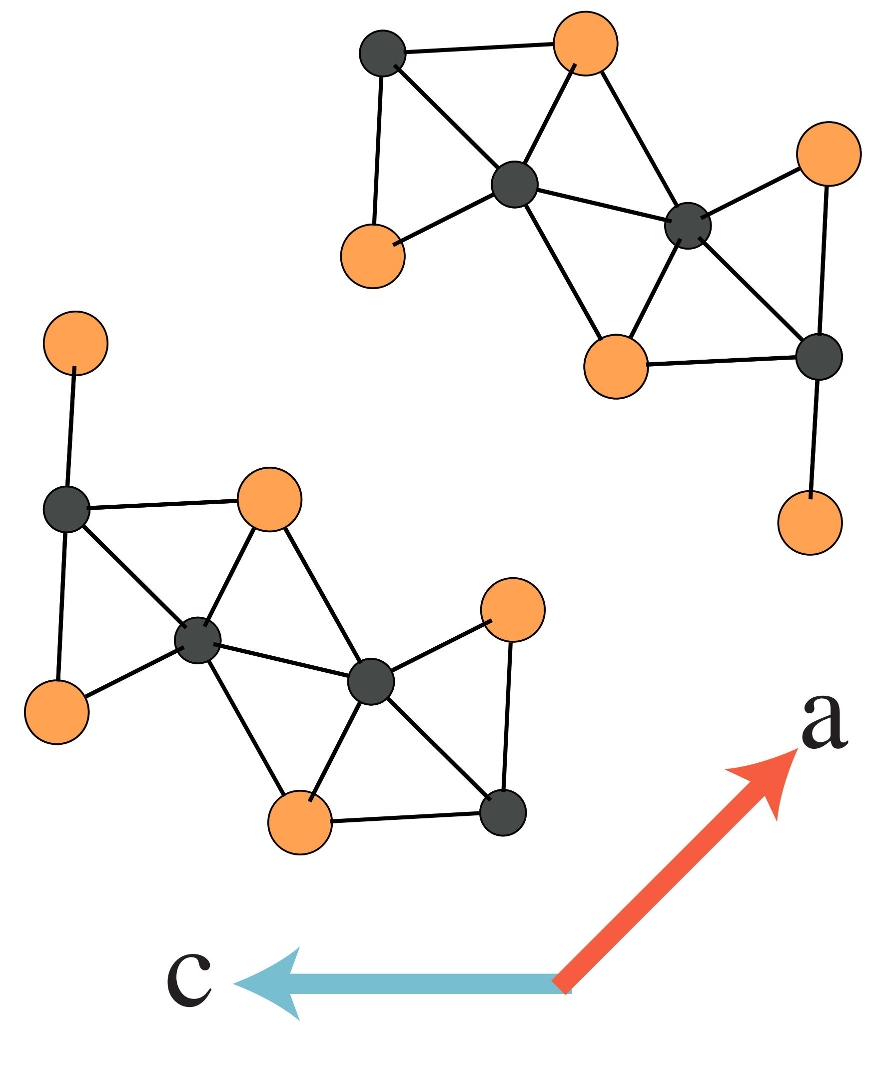
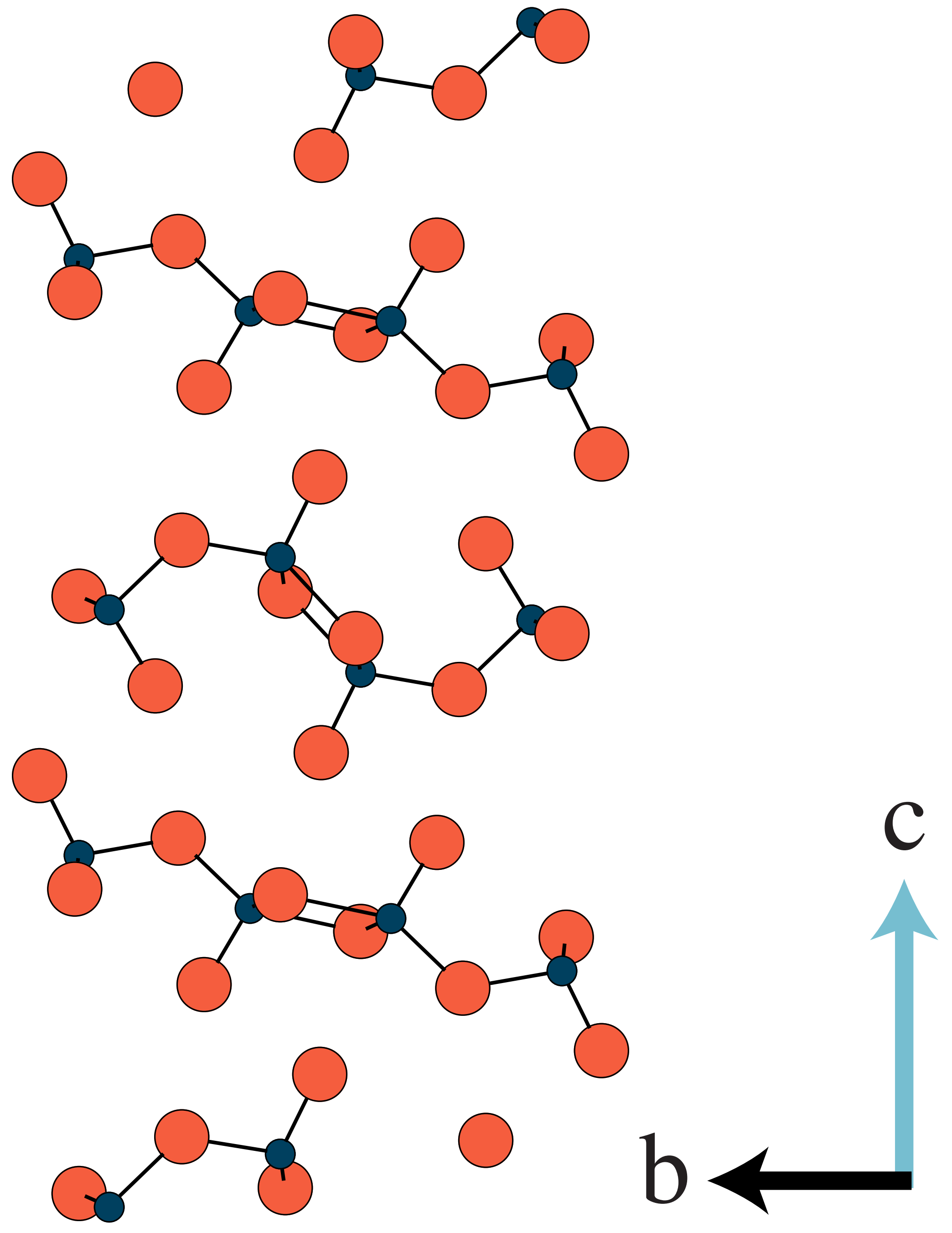
Datamining to Discover Layered Bulk Materials

- Many layered structures exist in materials that can be used to synthesize monolayers
- Identifying layered compounds using data from MaterialsProject.org using bond topology

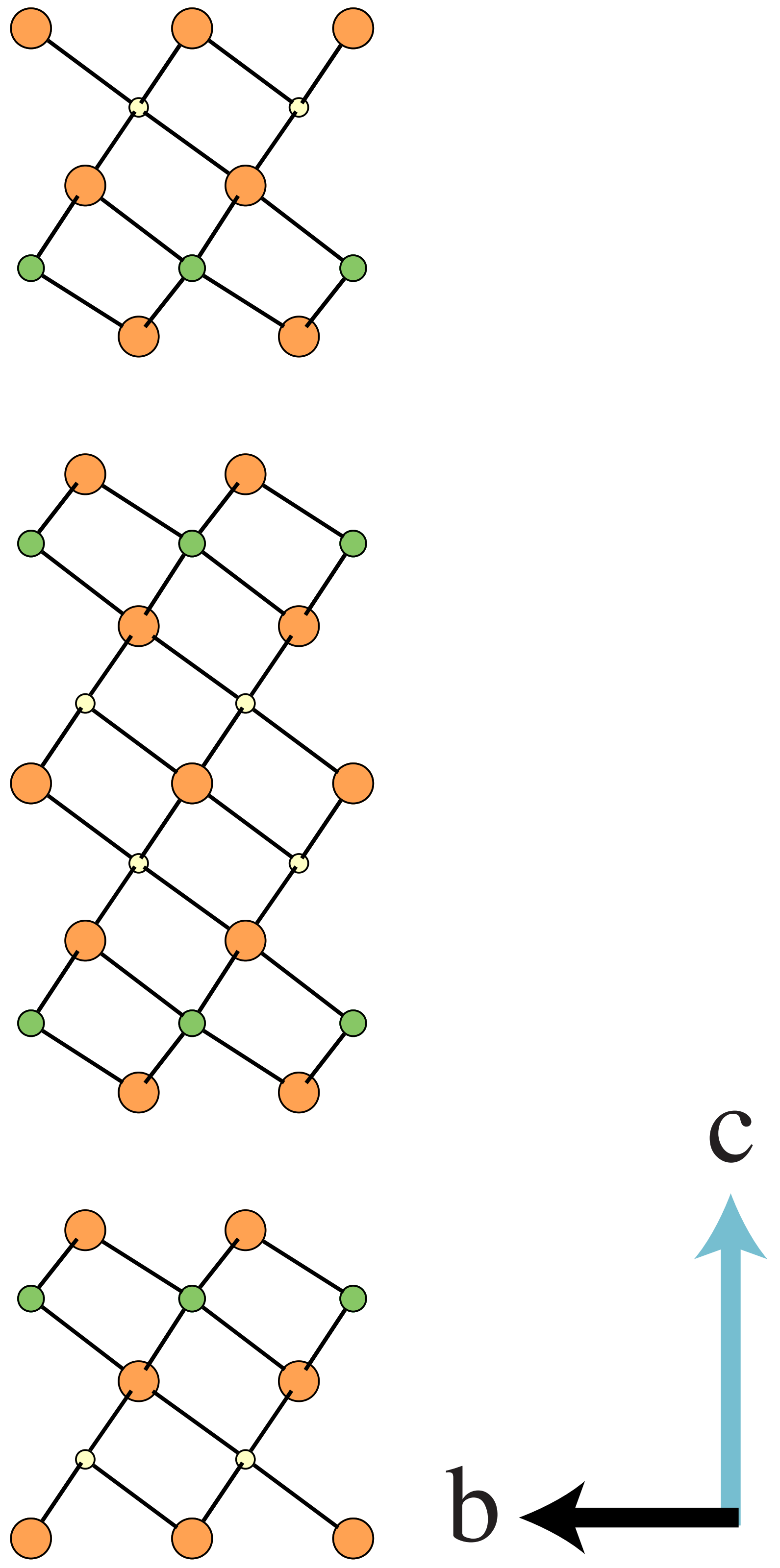
a) Ta_2Te_3 (mp-542634)



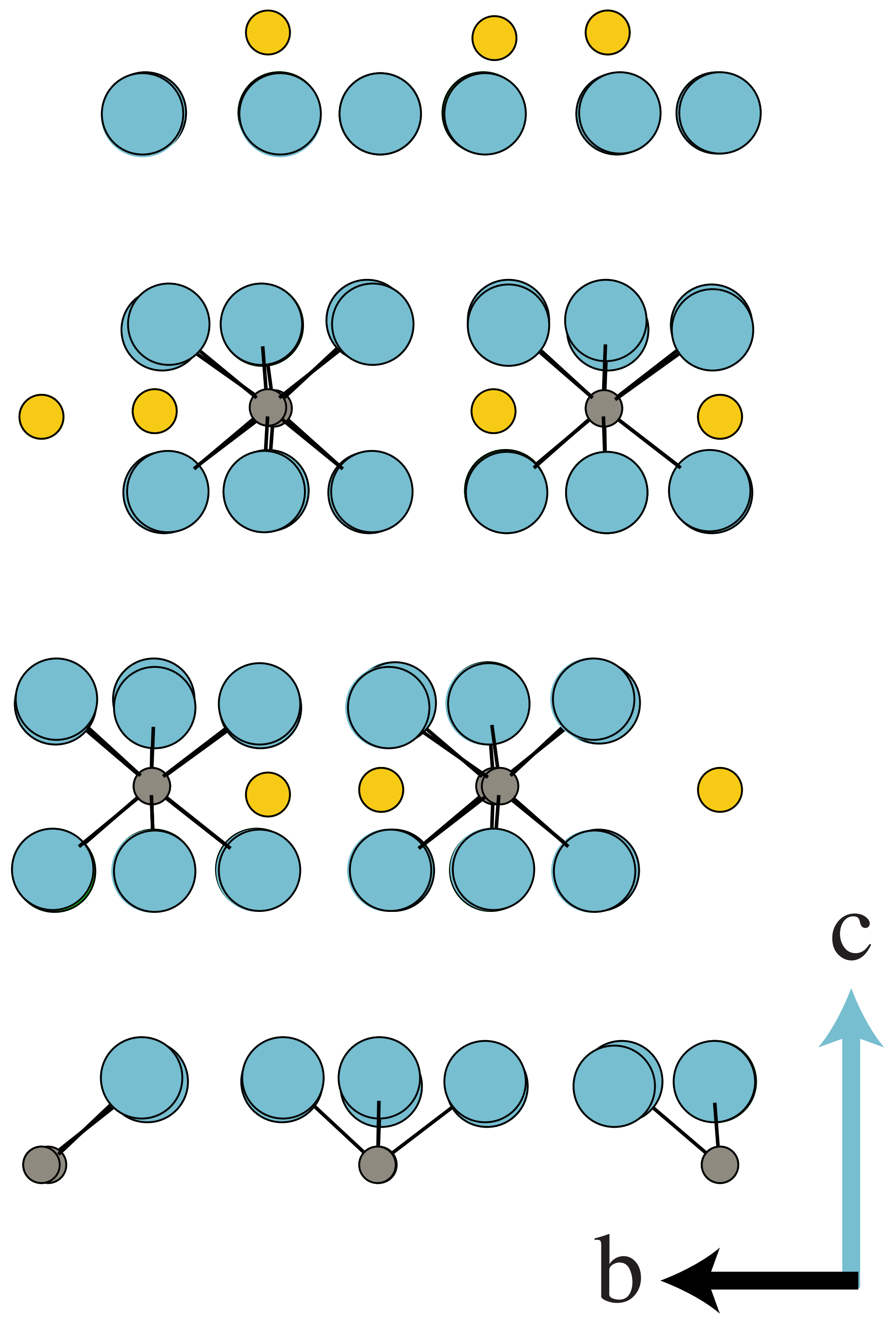
b) V_2O_5 (mp-25643)



c) $Ge_2Te_5As_2$ (mp-14791)



d) Li-WCl_6 (mp-570512)



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submitted (2016)

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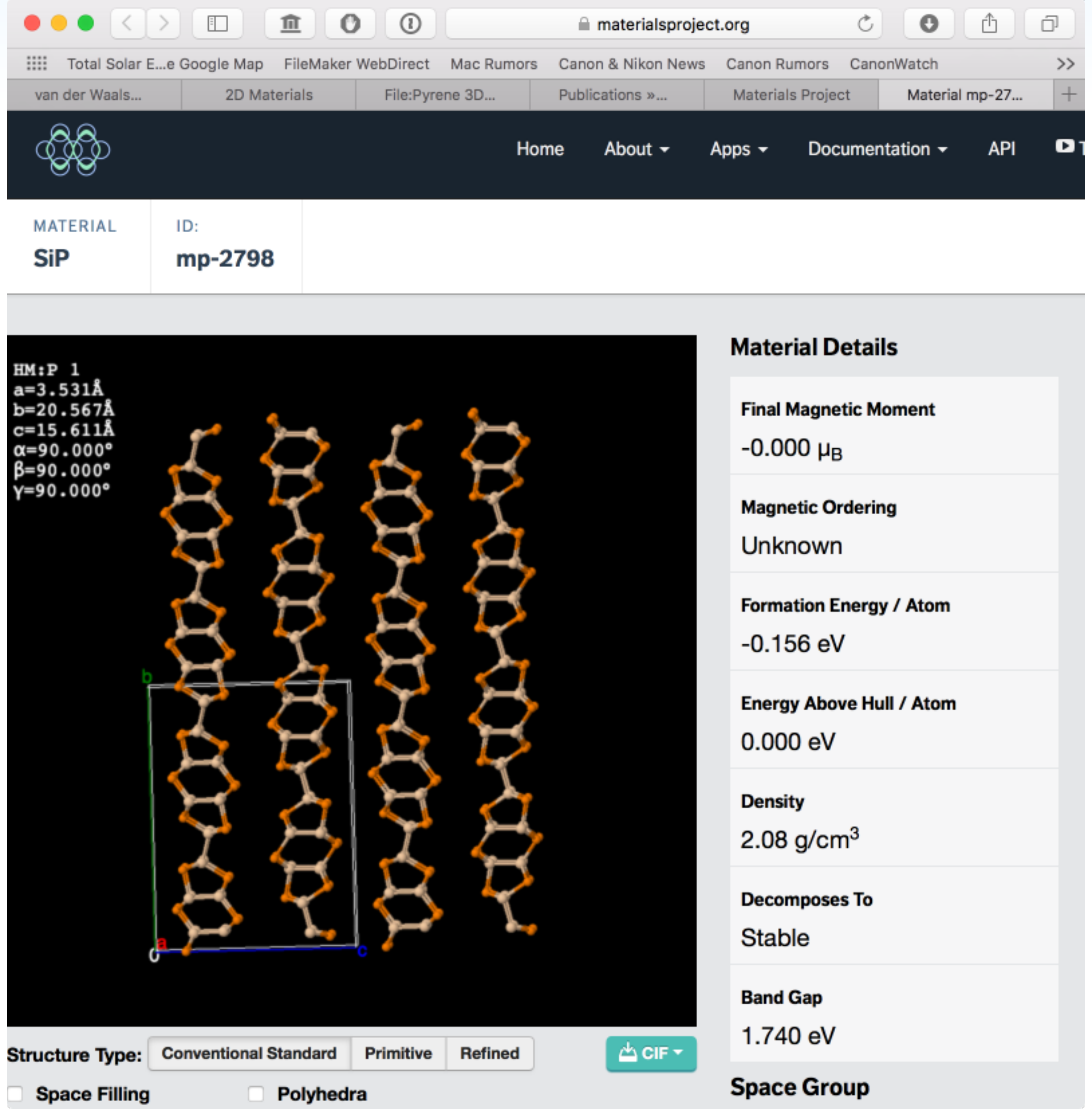
- Search MaterialsProject Database for layered 3D structures with van der Waals gap



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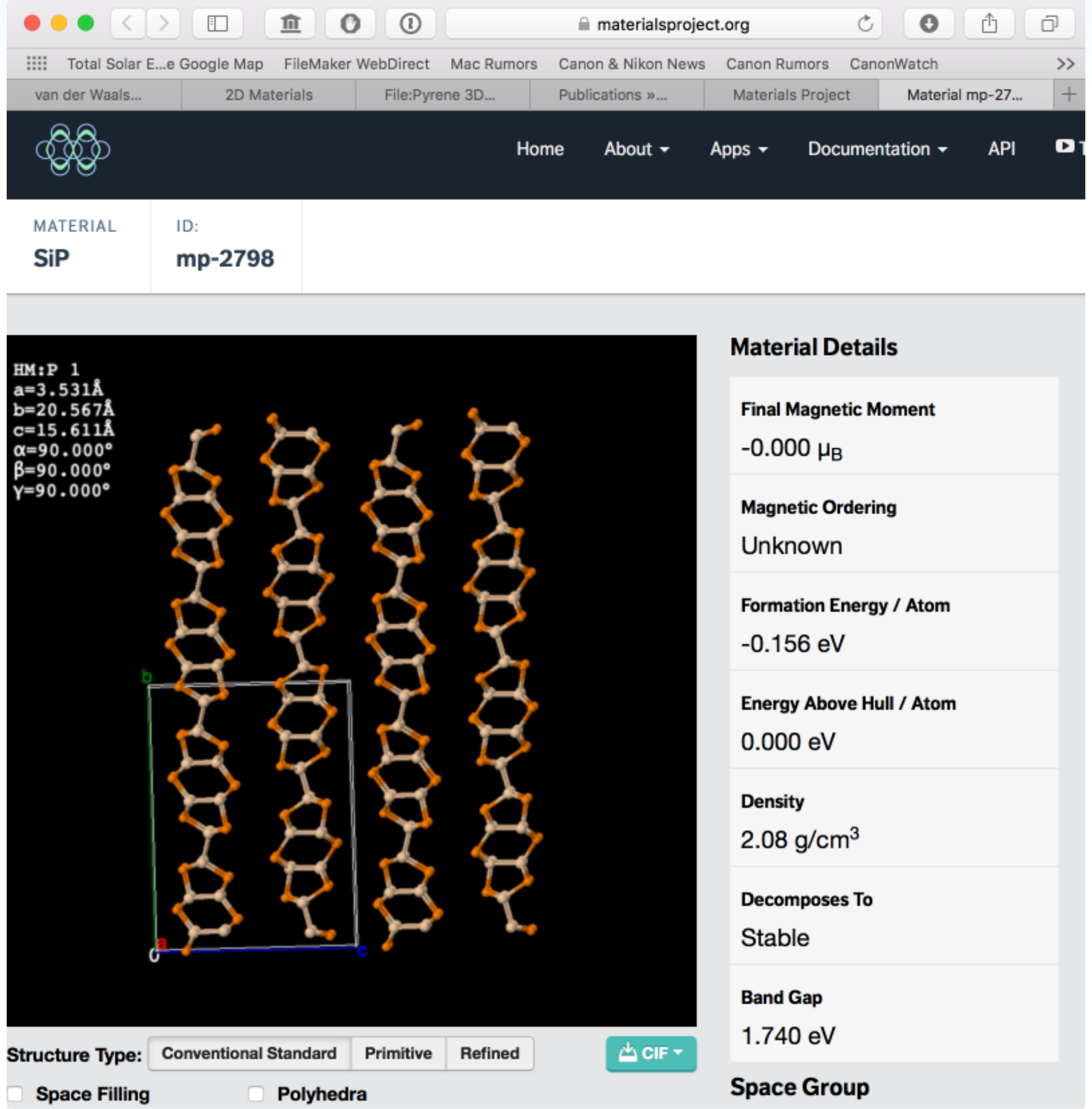

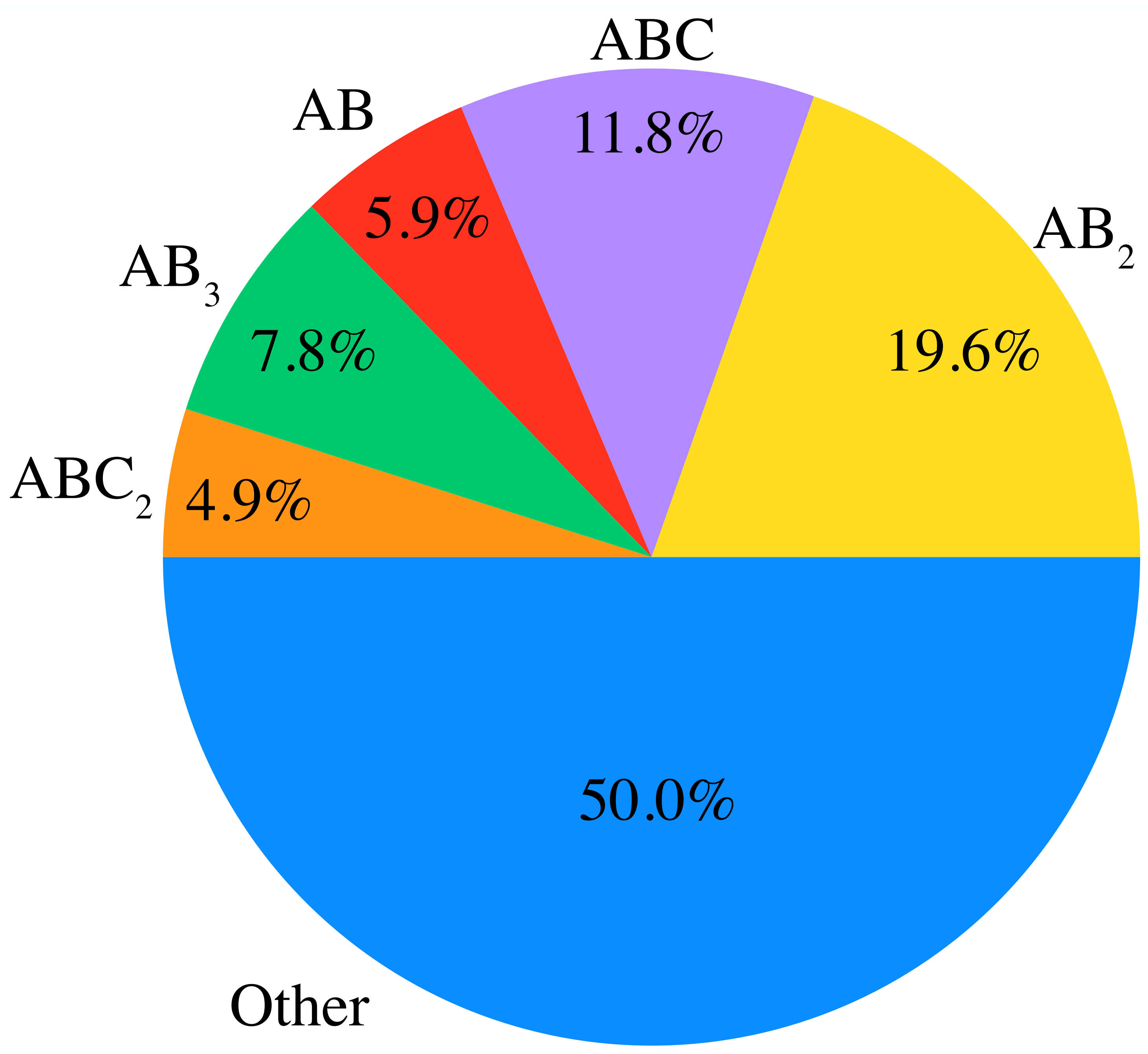

Identified 826 unique layered 3D bulk candidate materials for exfoliation.

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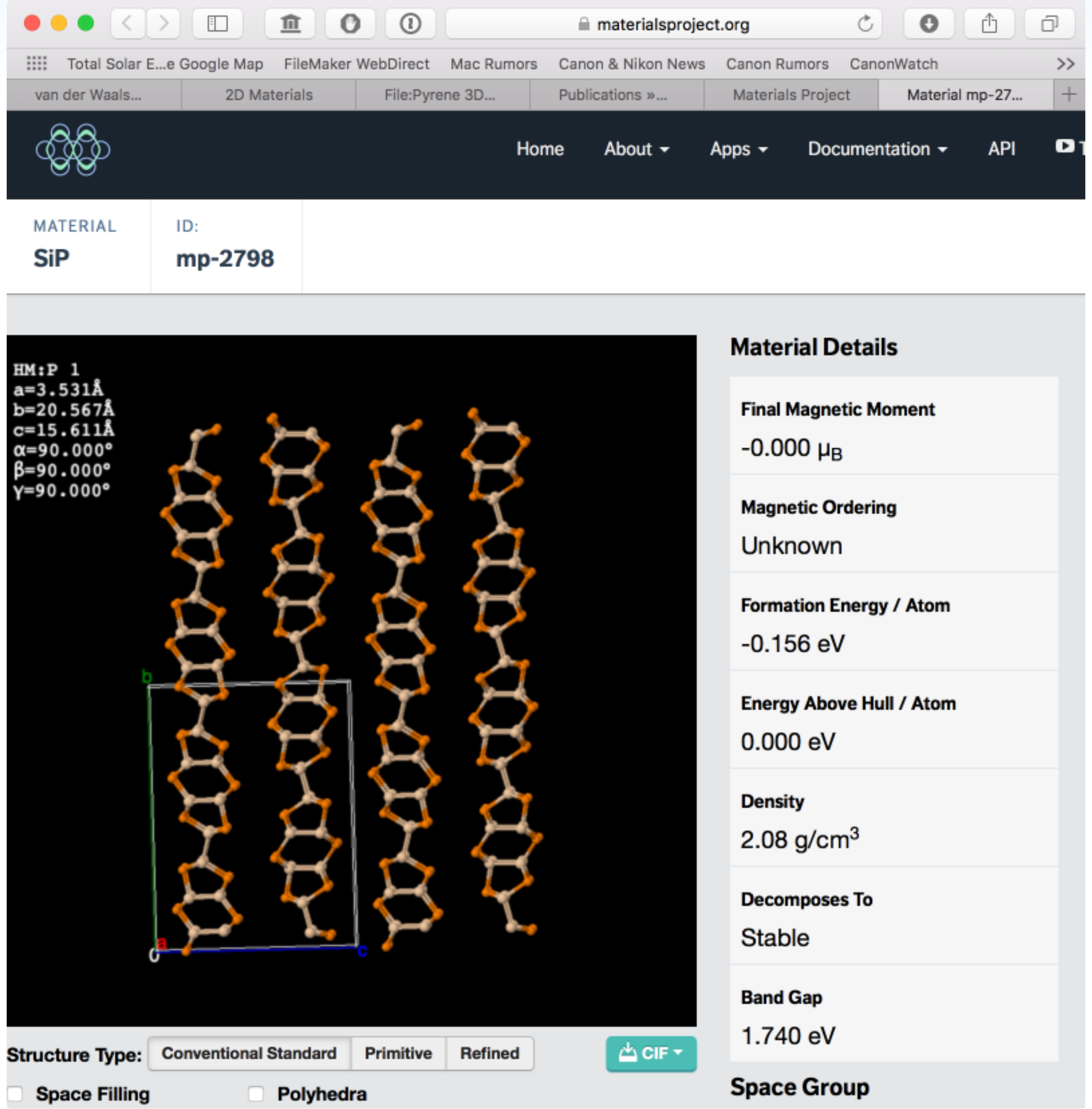
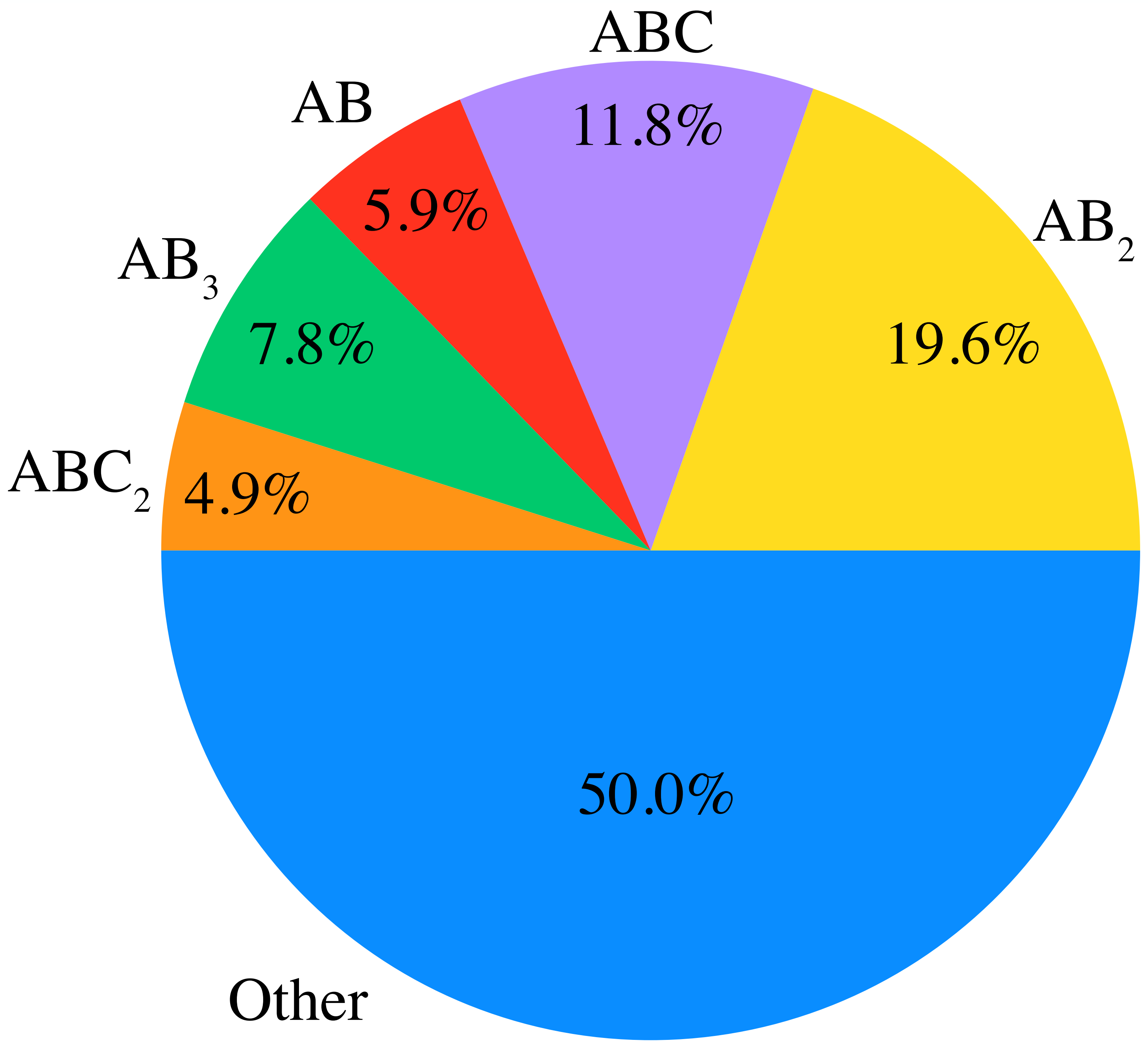
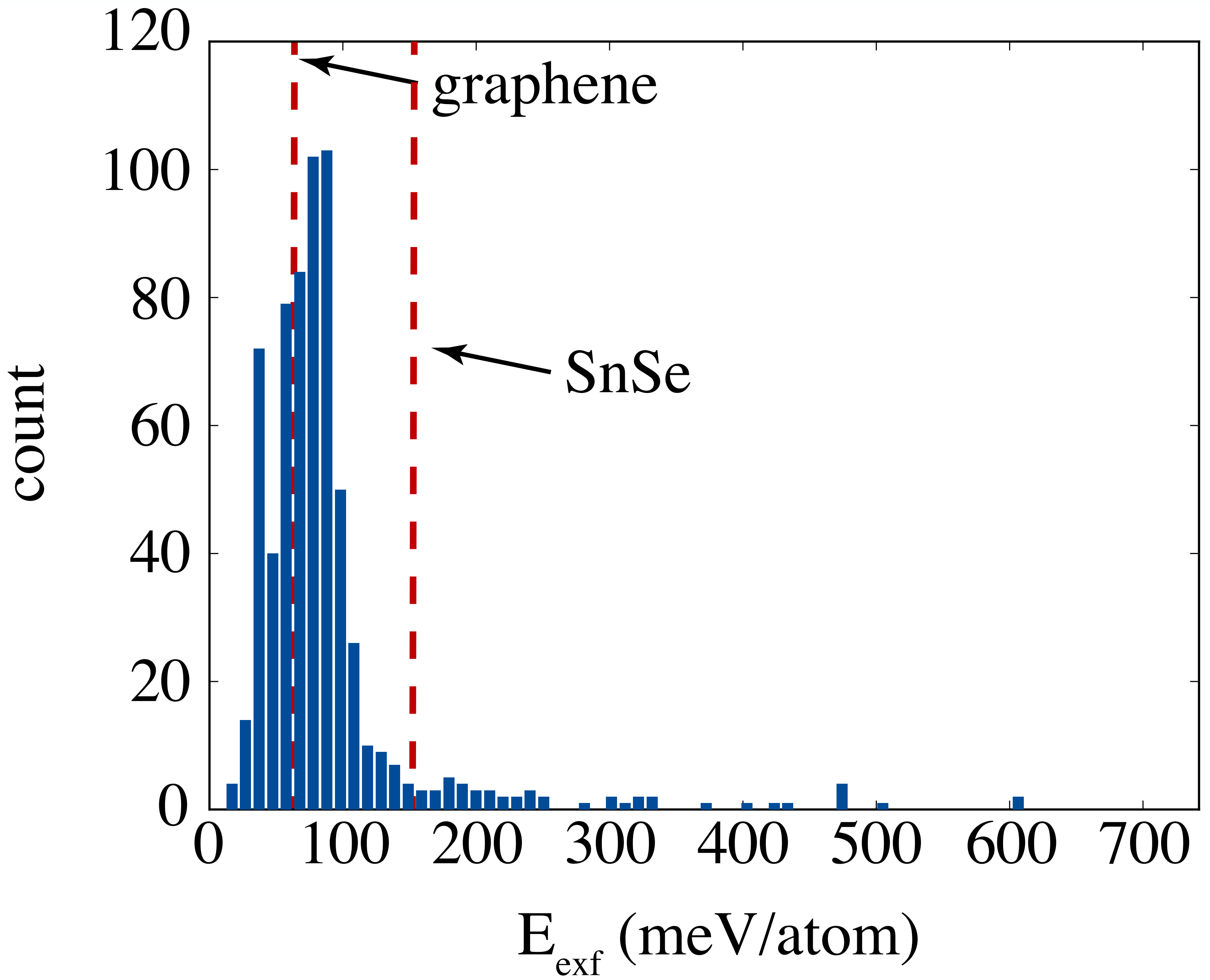
Datamining to Discover Layered Bulk Materials

- Search MaterialsProject Database for layered 3D structures with van der Waals gap







Identified 826 unique layered 3D bulk candidate materials for exfoliation.

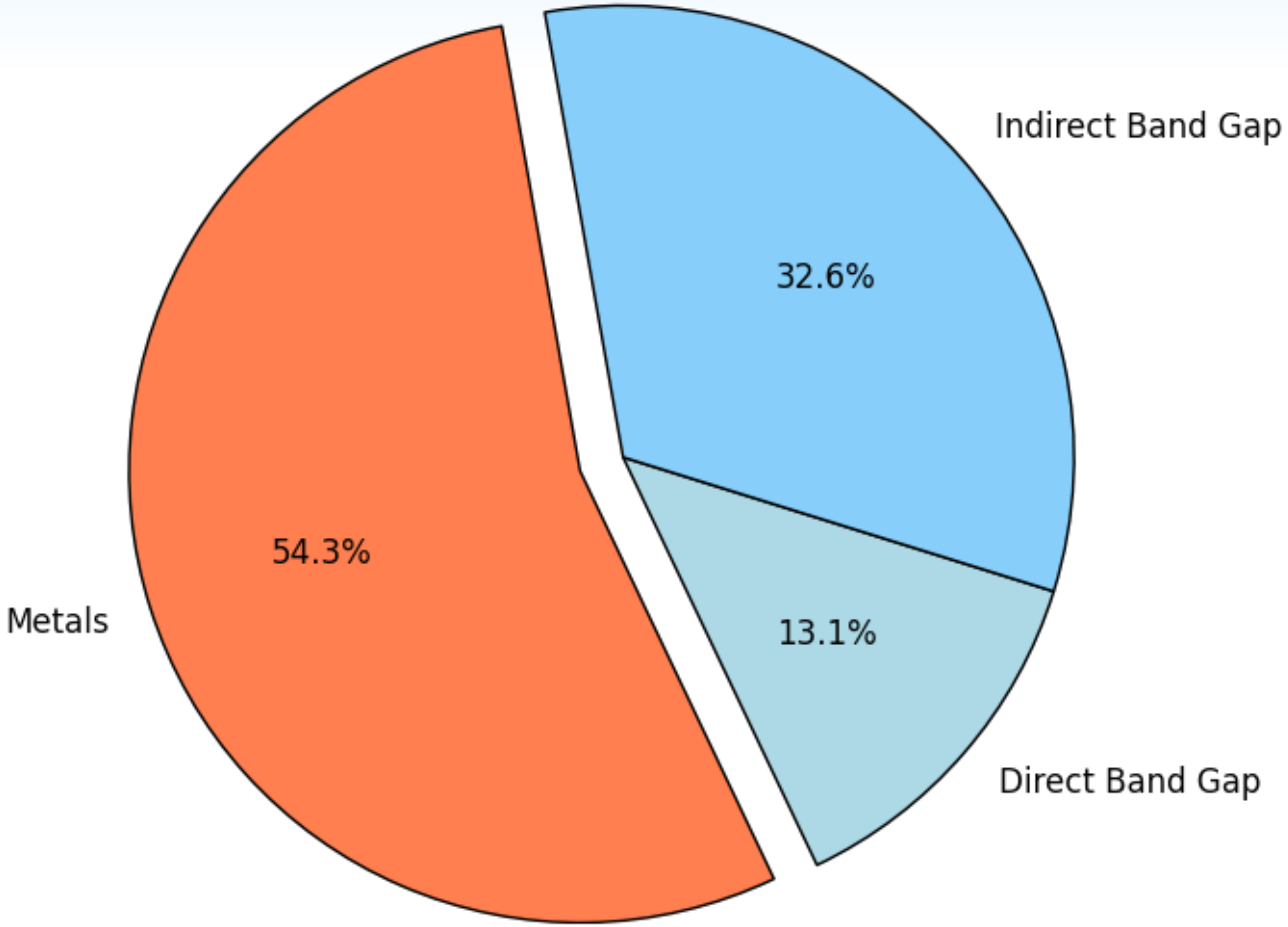
Identified 625 2D materials with energy below 150 meV/atom

UF FLAMES
Florida Laboratory for Advanced Materials Engineering Simulations

M. Ashton, J. Paul, S. Sinnott, RGH
submitted (2016)

Electronic Properties of 2D Materials

- Identify 2D materials with PBE bandgap between 0 and 3 eV
- Among the 625 stable monolayers, 282 are semiconductors (about 46%)
  - **201 materials with indirect gap**
  - **81 materials with direct gap**



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Effective Electron Masses of 2D Materials

Preliminary results for effective masses obtained with PBE functional

Effective Electron Masses of 2D Materials

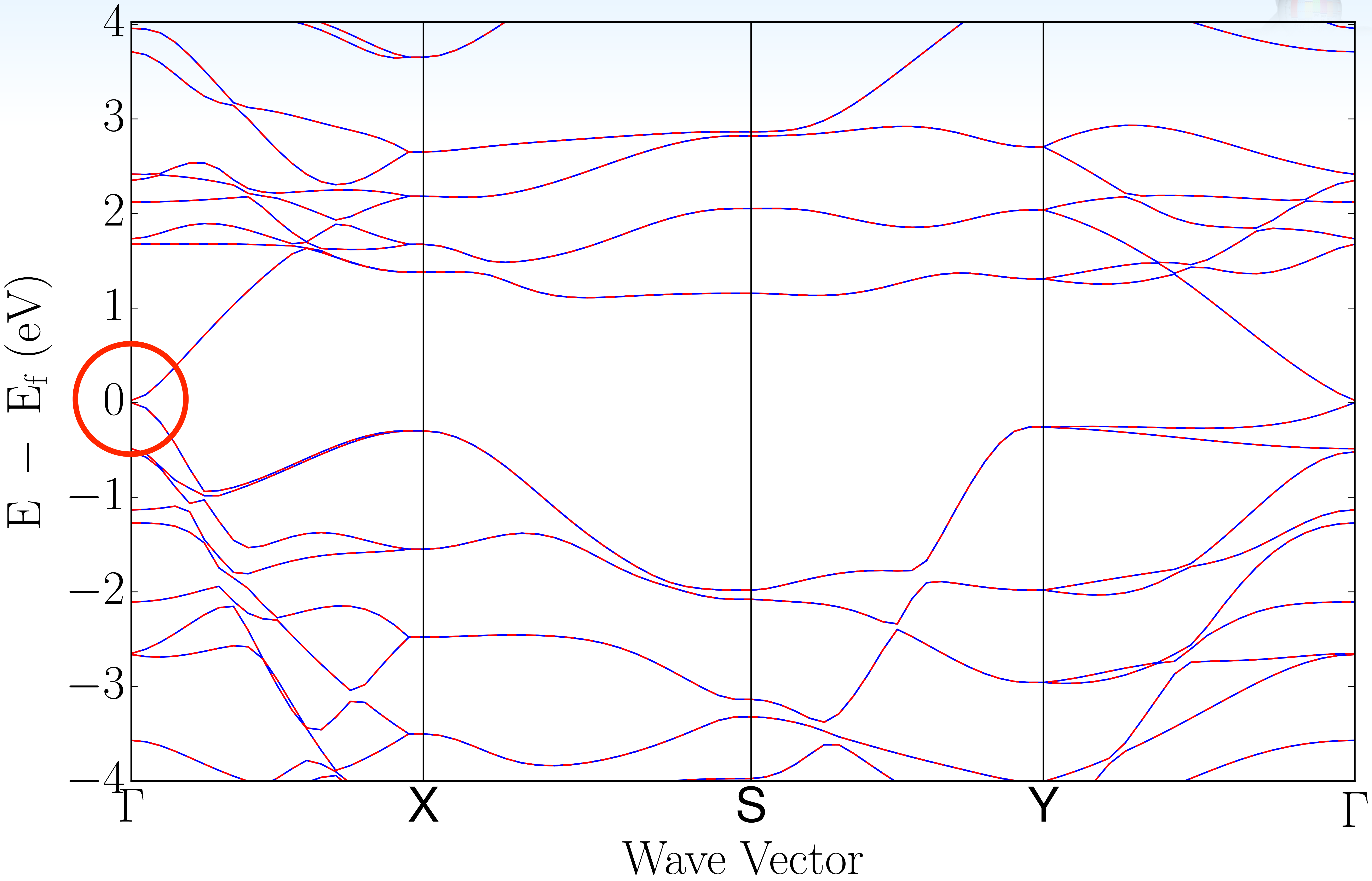
Preliminary results for effective masses obtained with PBE functional

Small effective masses for 2D group-IV monochalcogenides

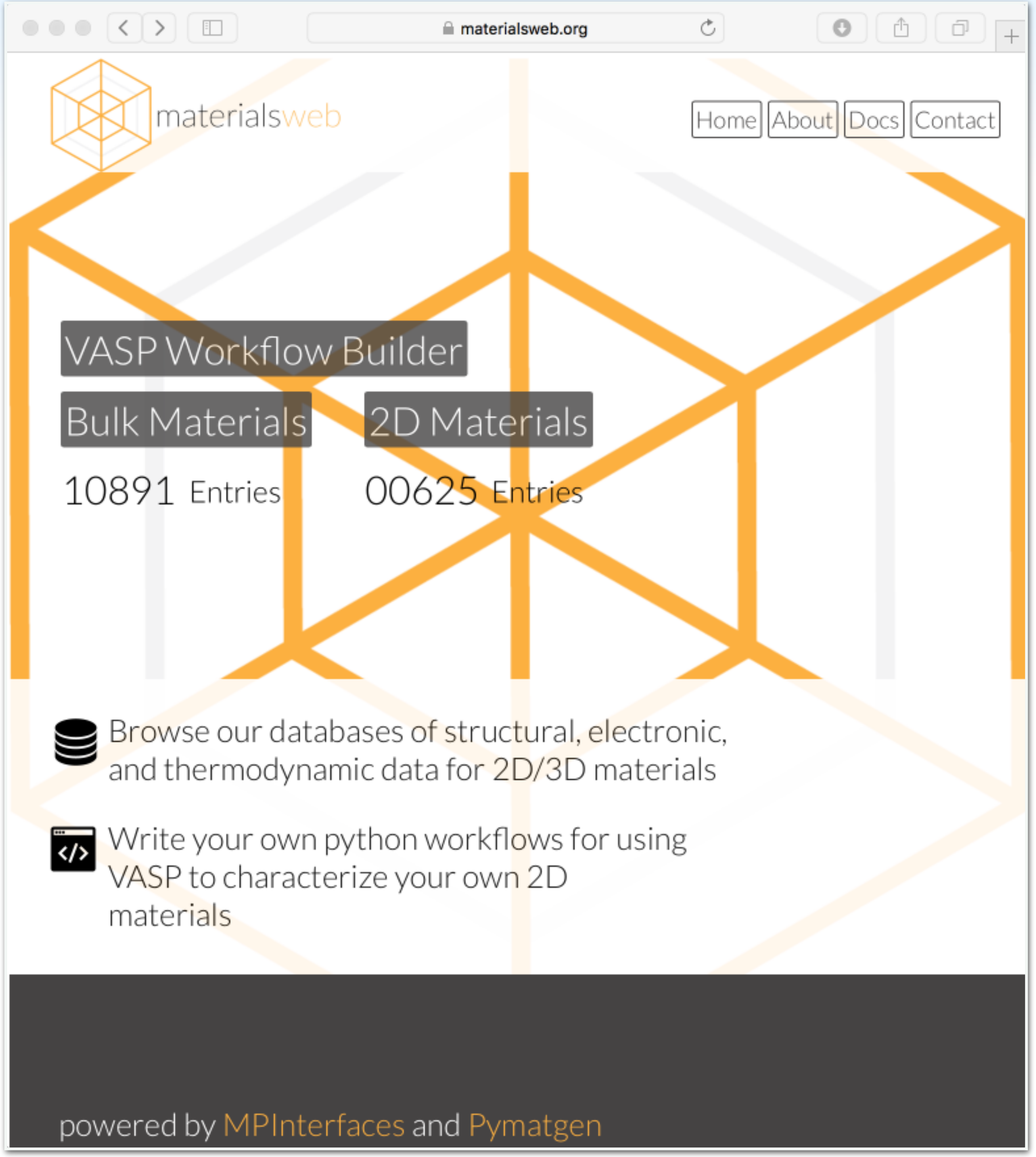
Exotic Electronic Properties of 2D Materials

2D materials with zero gap

- Graphene
- TiNI
- Nb3IrS8
- HfSiTe
- ZrBr
- InBi
- SrSbSe2F
- NiP2
- YIC
- ZrGeTe
- YBrC
- ZrTe5
- HfTe5



Website: https://materialsweb.org



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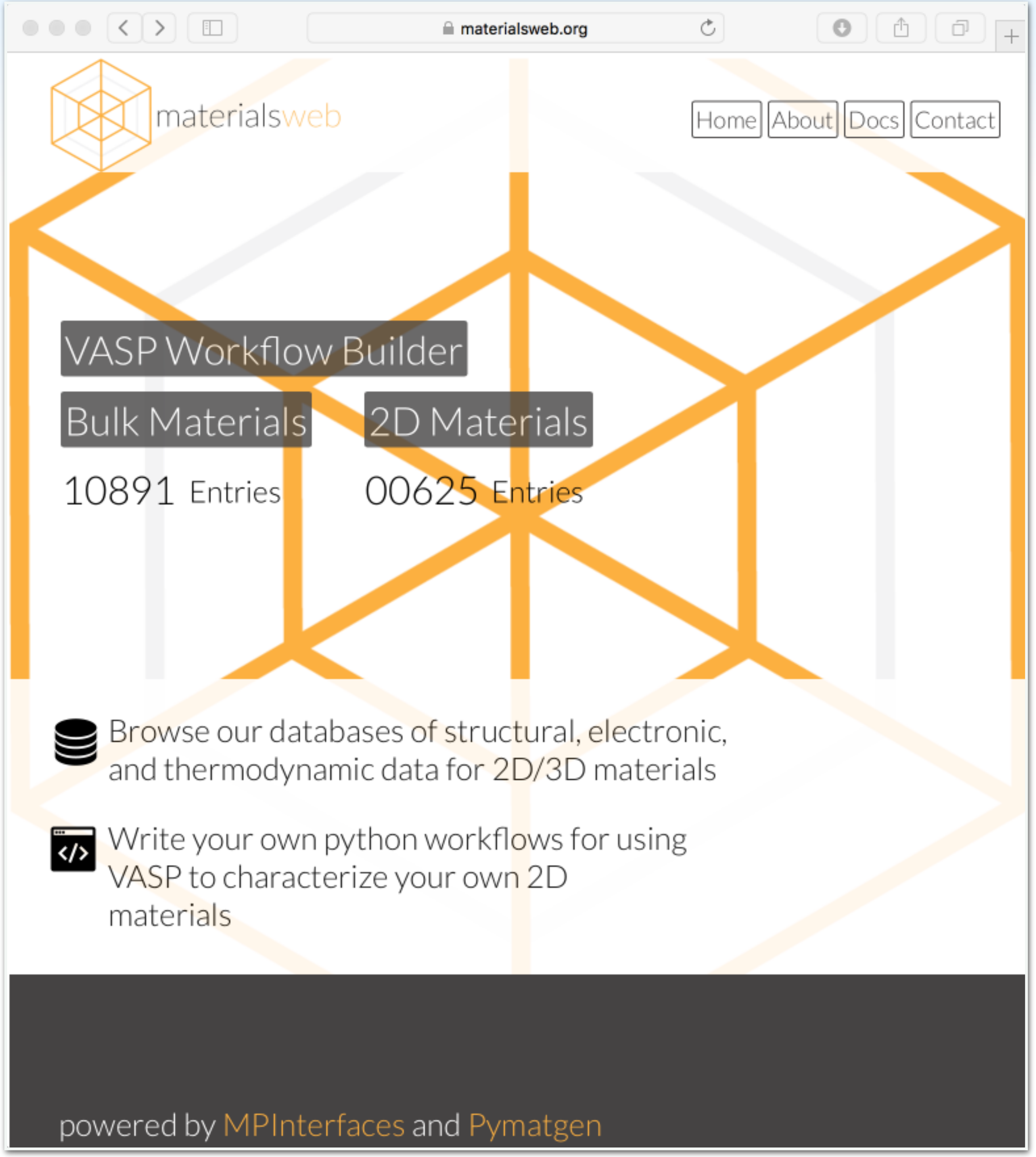

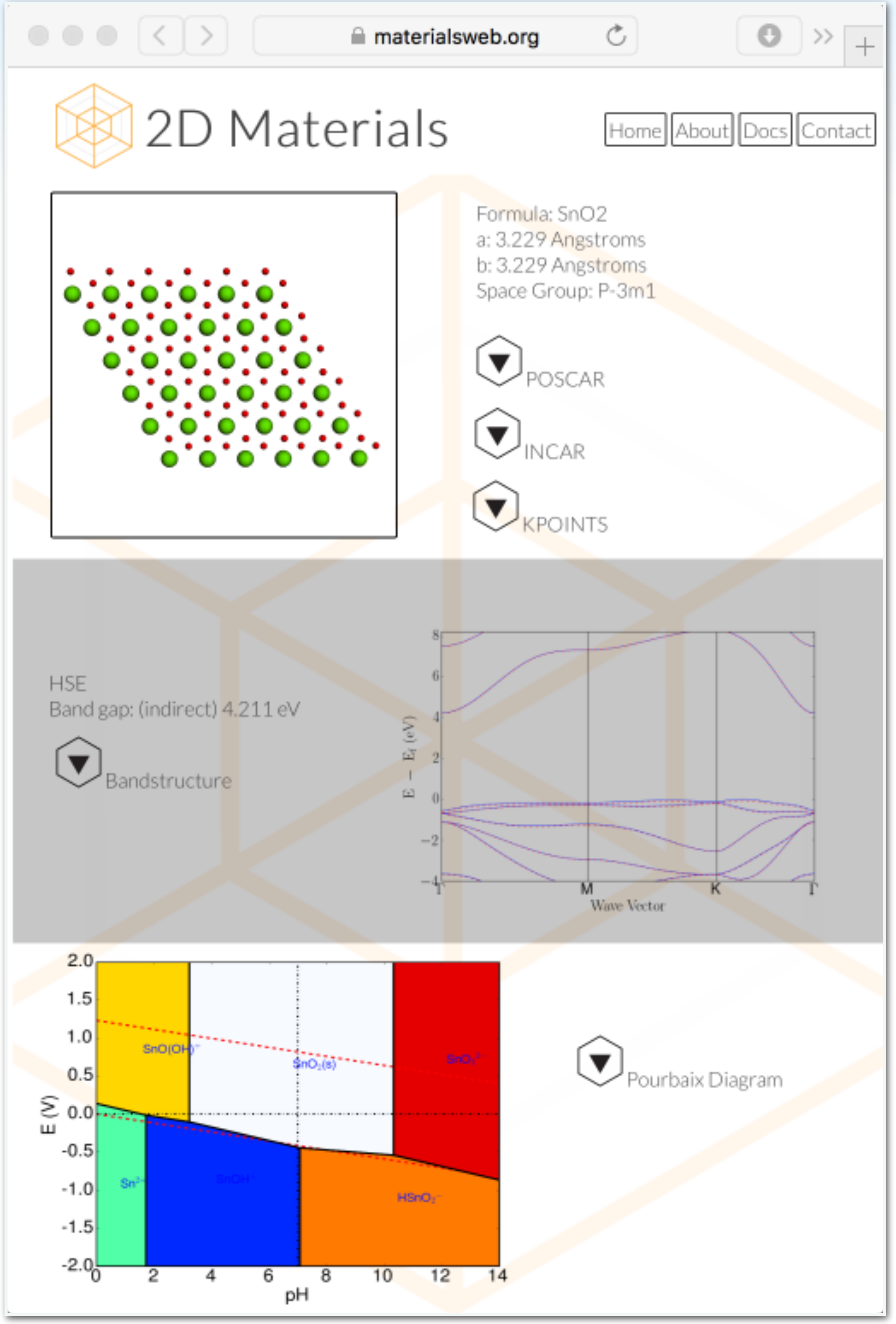

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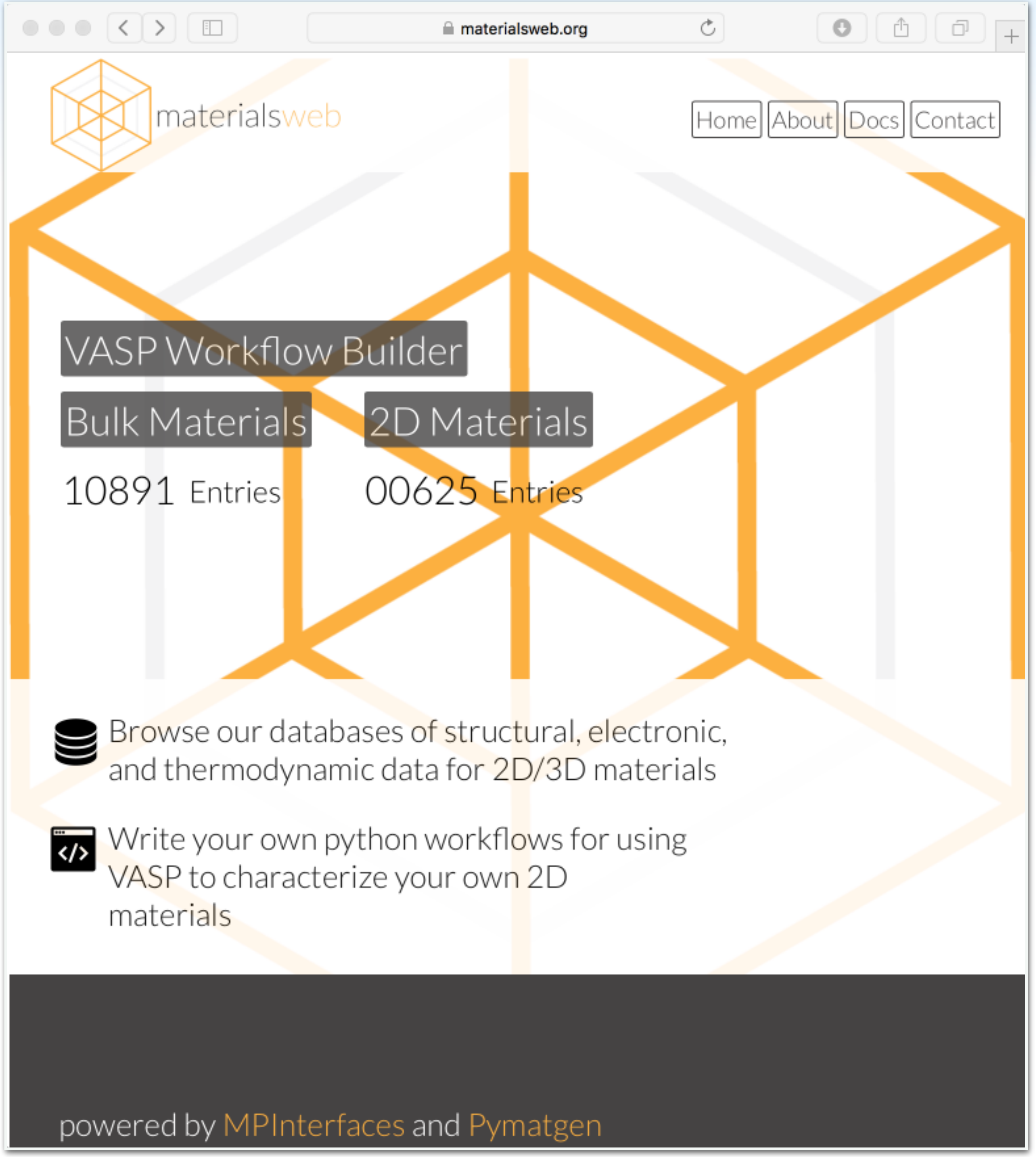
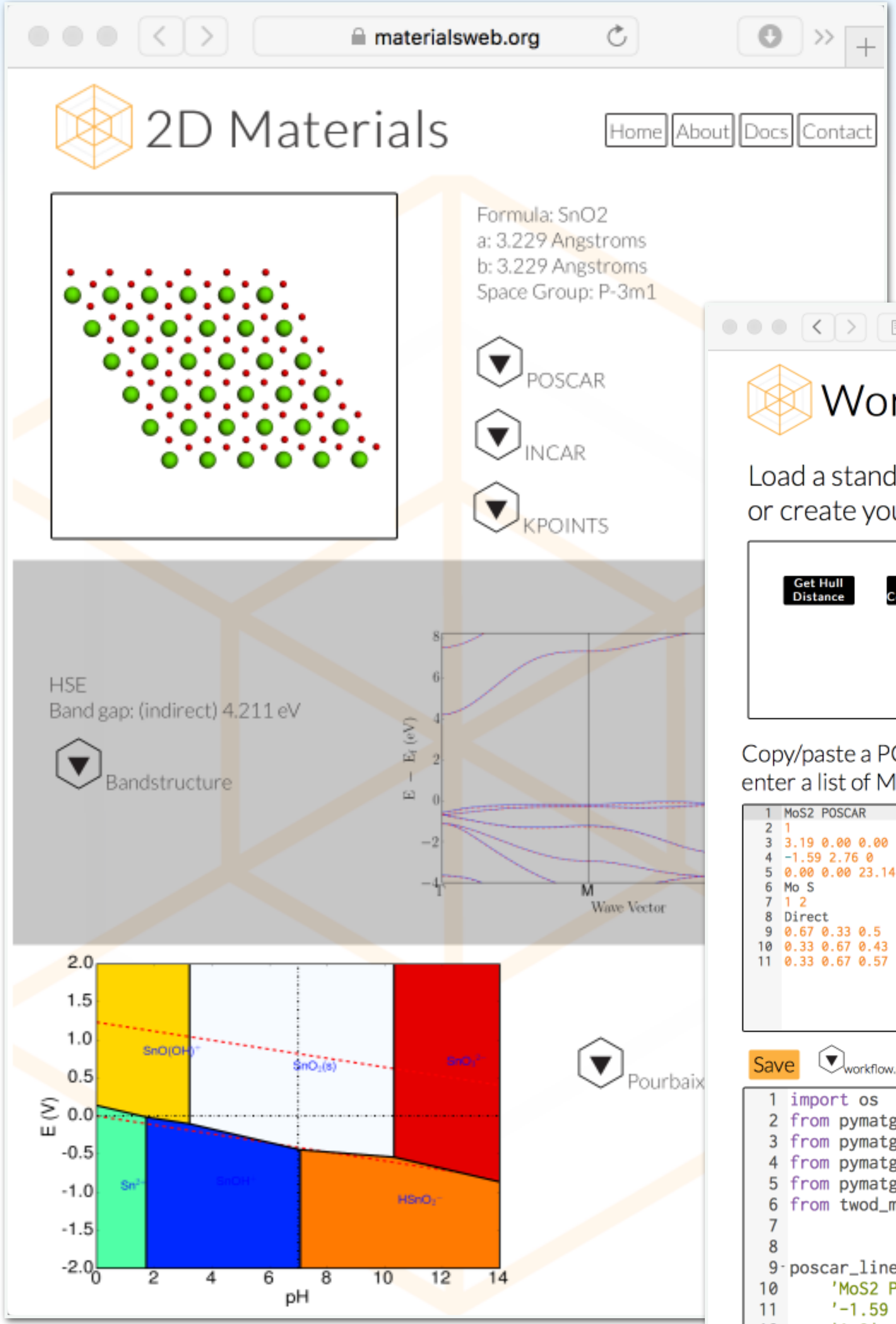
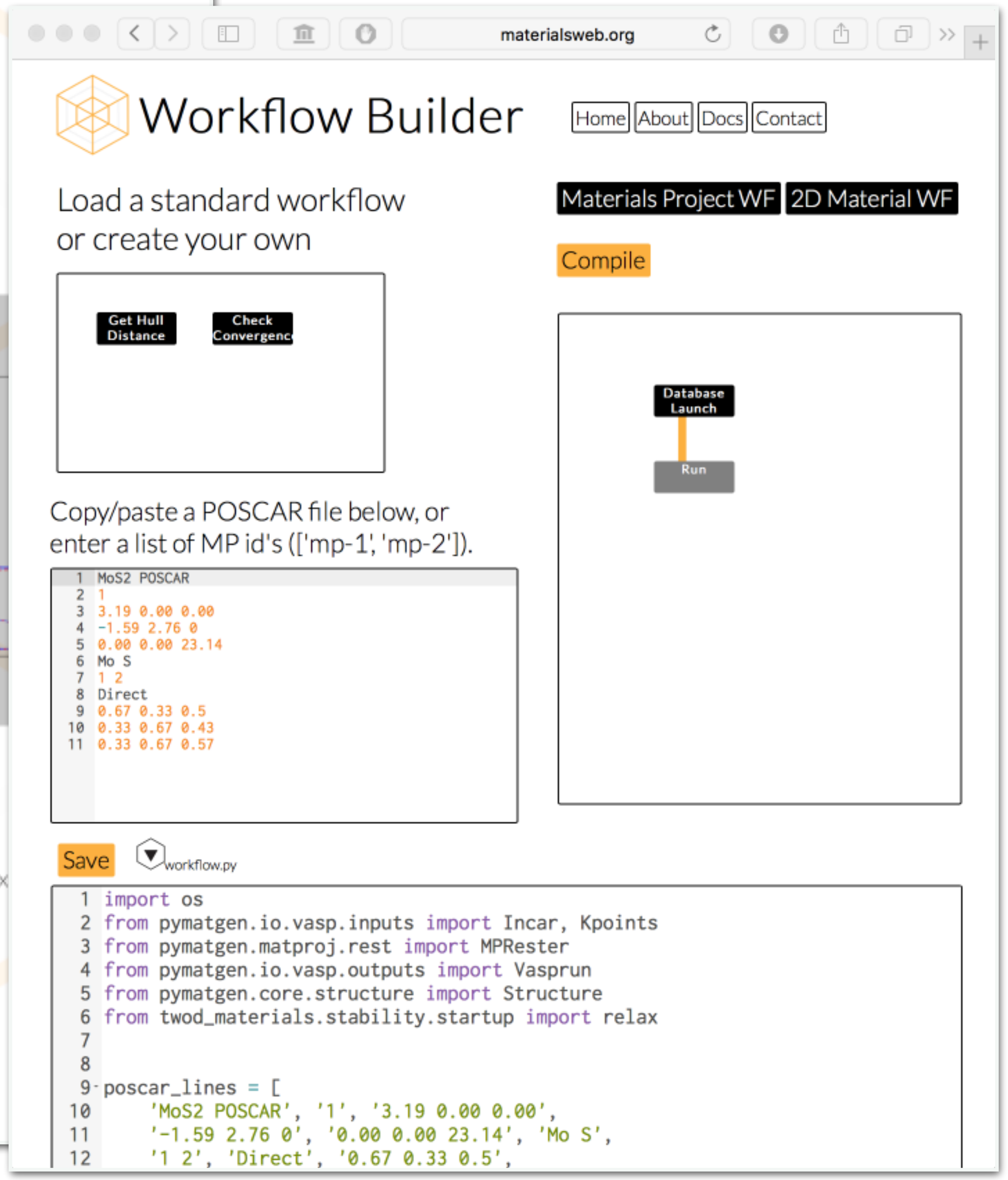




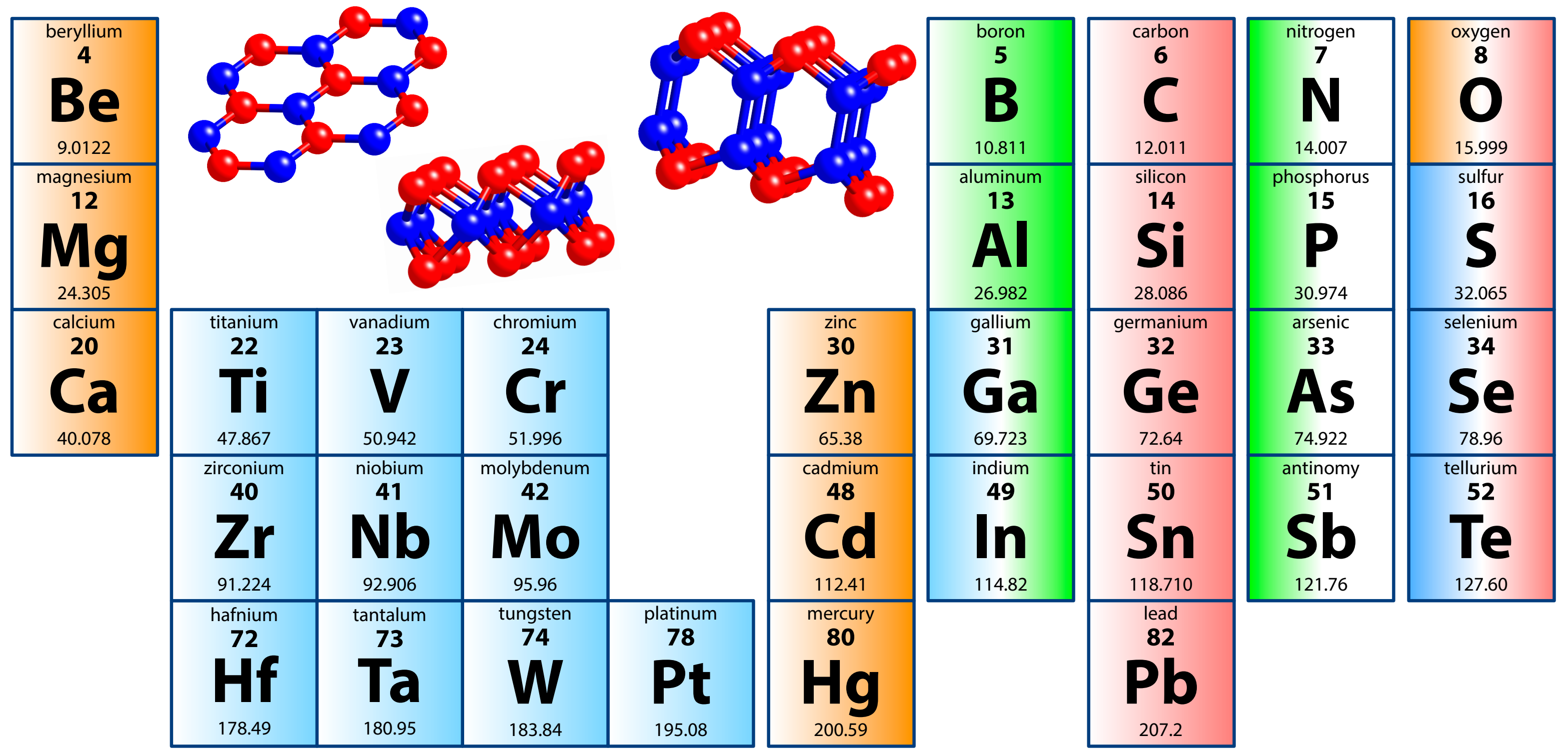


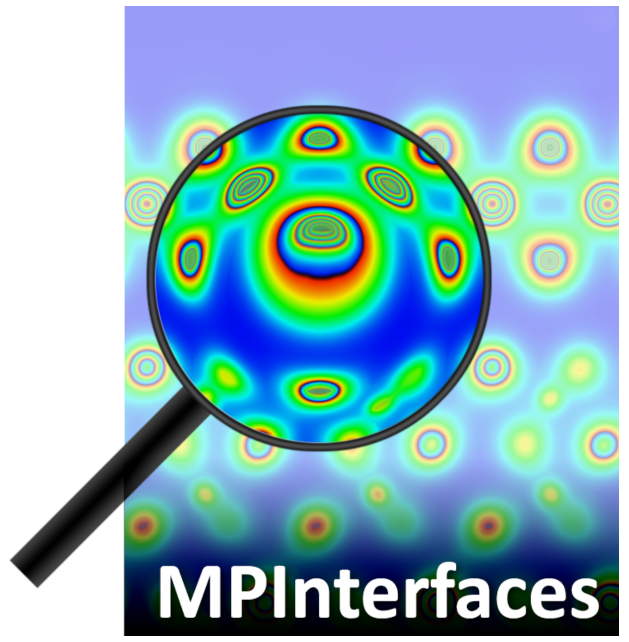
2D Materials Design for Production of Cold Electrons

Richard G. Hennig, Joshua Paul, Michael Ashton, University of Florida

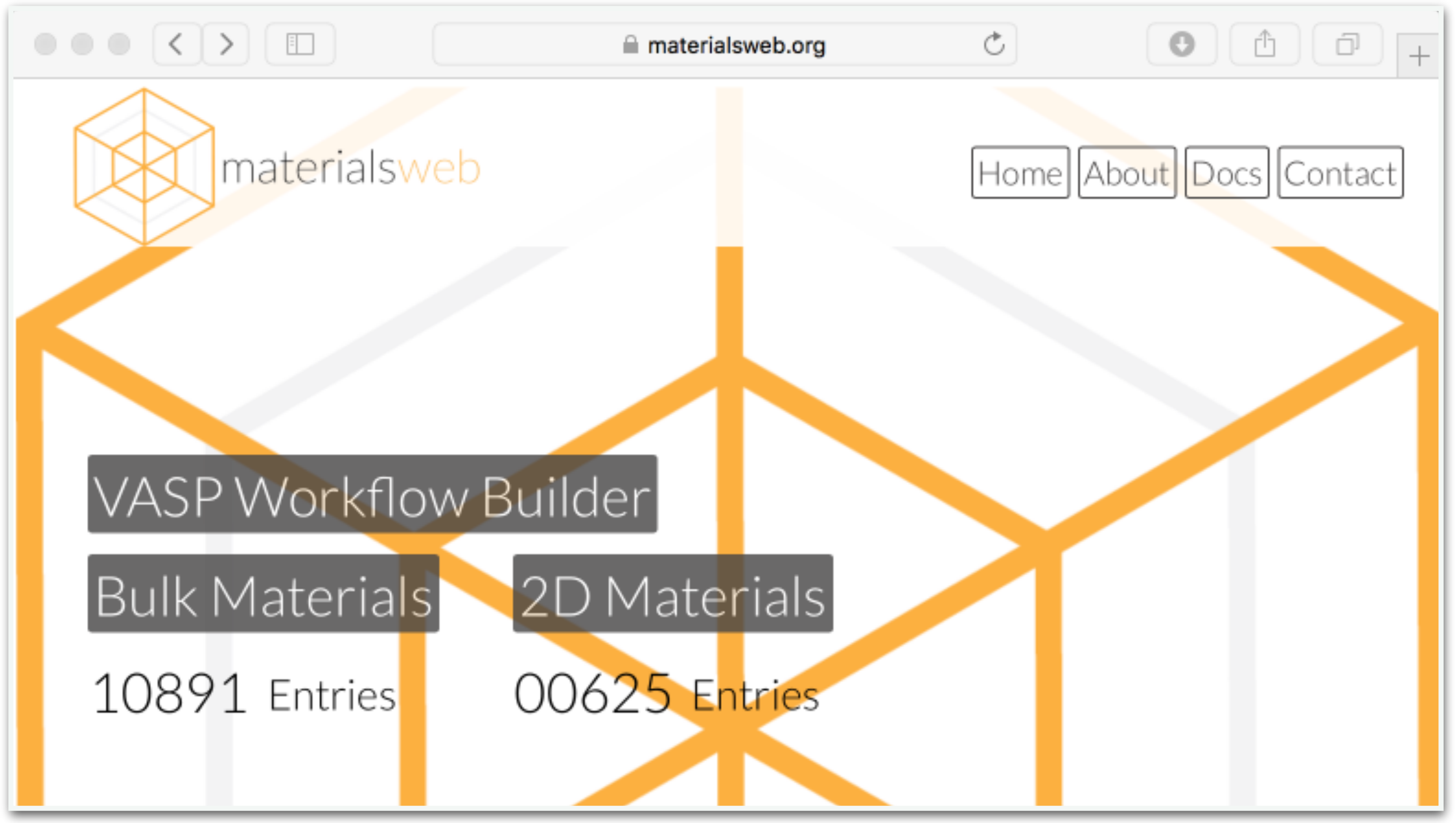
MPInterfaces

High throughput framework for 2D materials



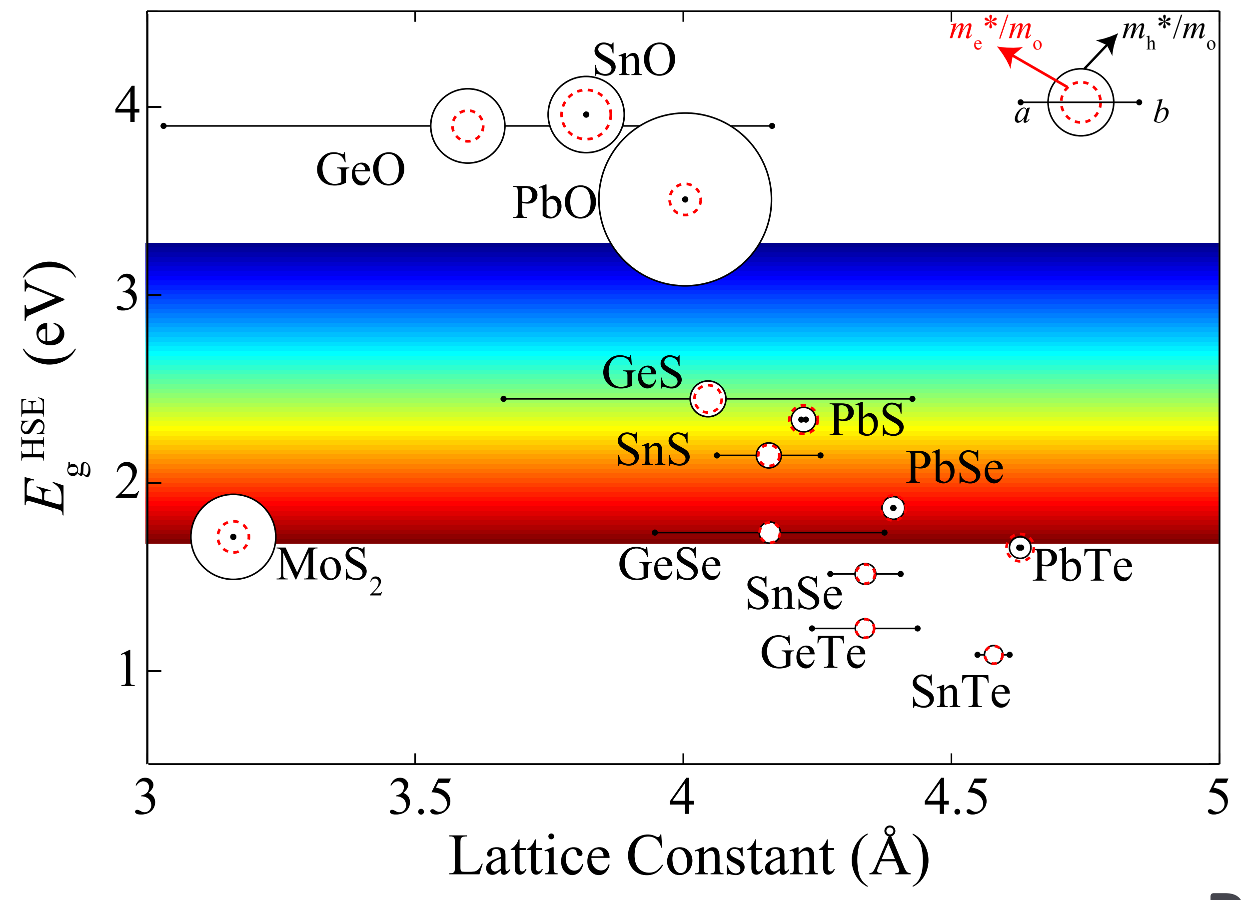


Data available at http://materialsweb.org



Screen 2D materials for photocathodes

- Formation from layered bulk materials
- Semiconductors with small effective masses
- Promising family of group-IV monochalcogenides



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