Los Alamos Computational Condensed Matter Summer School 2026

Flash Talks

Los Alamos NATIONAL LABORATORY

June 16, 2026

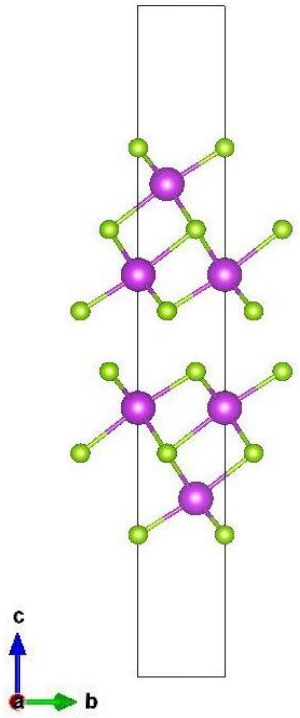
U.S. DEPARTMENT OF ENERGY

Development of ab initio Approaches to Study Photogalvanic Responses in Antiferromagnetic Topological Materials

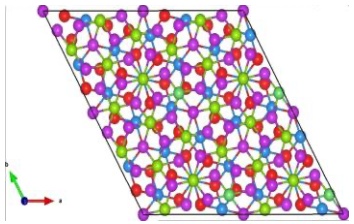
Alana Okullo · Advisor: Sugata Chowdhury · Institution: Howard University

- **First Principles study with three routes to unlock photogalvanic responses in centrosymmetric van der Waals bilayer Bi_2Se_3**

Bilayer Bi_2Se_3

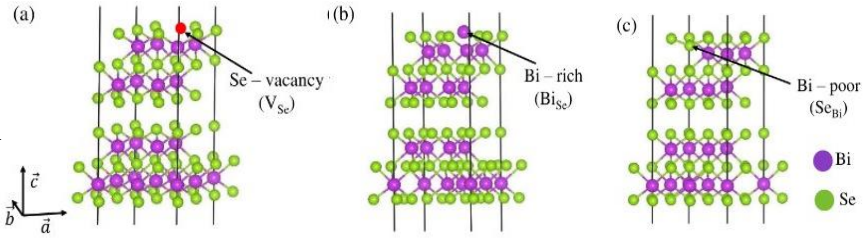


Twisted at hexagonal first commensurate angle 21.78°



Electric Field Application

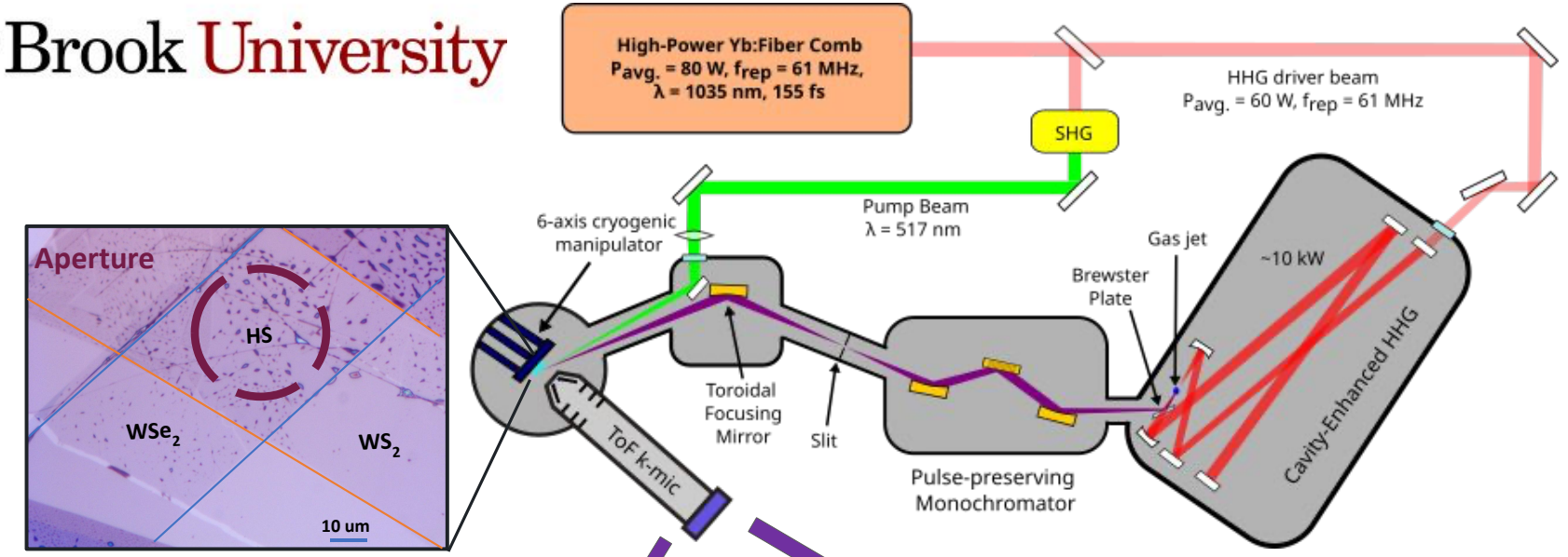
Defect Insertion

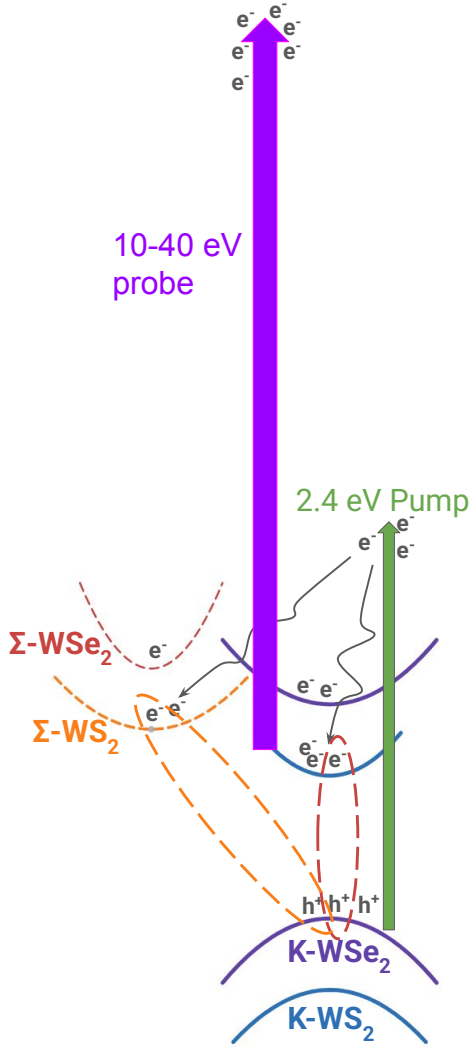


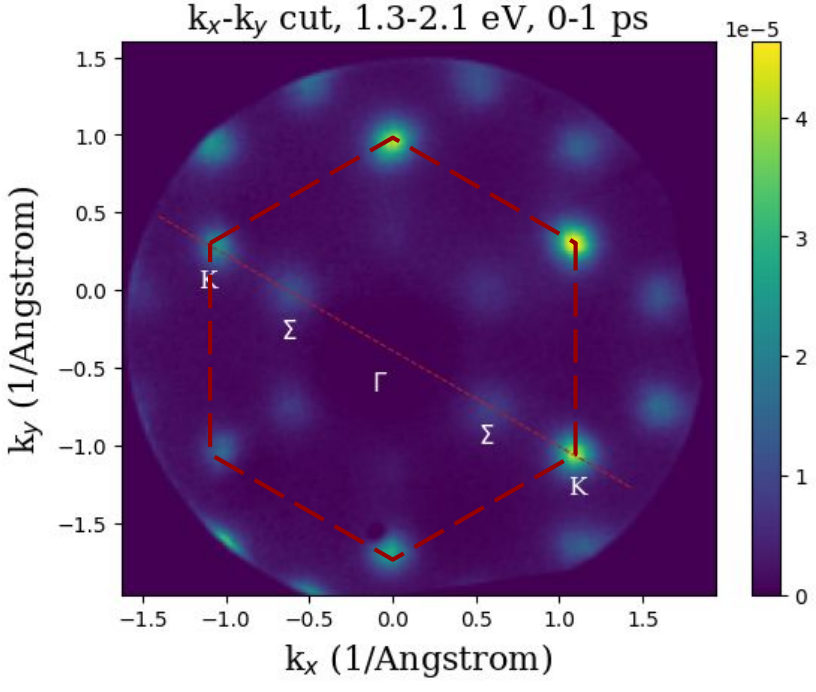
All three routes break inversion symmetry in bilayer Bi_2Se_3, and using first principles, we show that this enables significant photogalvanic currents

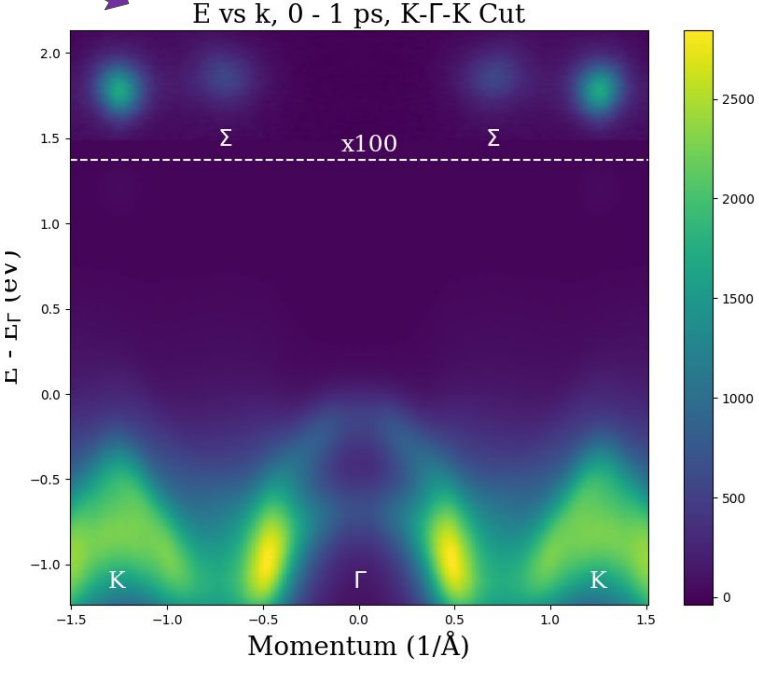
Future: moiré at smaller angles, magnetic photogalvanic response

Time-resolved XUV-μ-ARPES at Stony Brook University







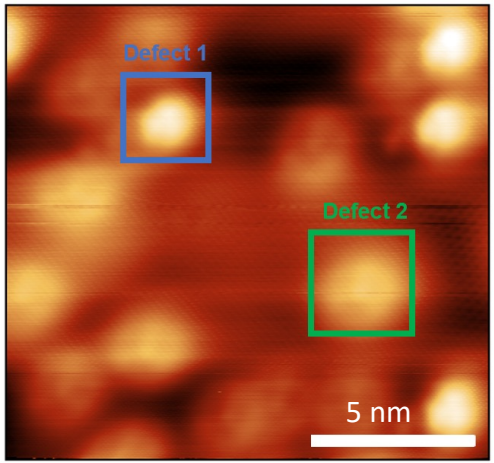


Visualization of p-type doping defects in MoS_2

STM/S and DFT investigation on point defects in MoS_2

Andrea Cabero del Hierro

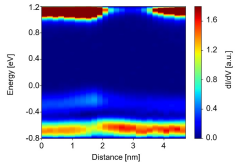
Experimental STM



Two distint defects observed in Nb-doped MoS_2

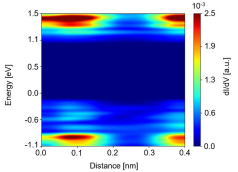
Defect 1 → Nb replaing Mo (1st layer)

Experimental STS



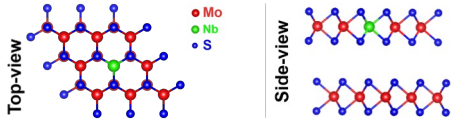
Experimental fingerprint of **Defect 1**

DFT Simulated STS



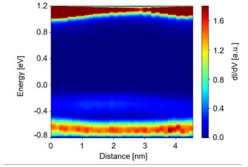
Simulation matches **Defect 1**

Atomic model (top and side view)



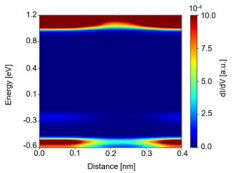
Defect 2 → Nb replaing Mo (2nd layer)

Experimental STS



Experimental fingerprint of **Defect 2**

DFT Simulated STS



Simulation matches **Defect 2**

Atomic model (top and side view)

Key conclusion:
STM images distinguish different point defects in Nb-doped MoS_2, while STS combined with DFT identifies the corresponding defect configurations.

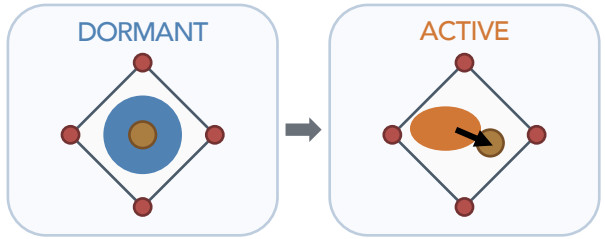
Impact:
Enables atomic-scale identification of p-type dopants in 2D materials.

Dormant lone pairs in Se(IV) vacancy-ordered halide double perovskites

Poster flash talk • LACCMSS

Anya S. Mulligan • UCSB Materials

In halide perovskites and related materials, *ns*² lone-pair electrons can drive local symmetry breaking and strong anharmonicity.

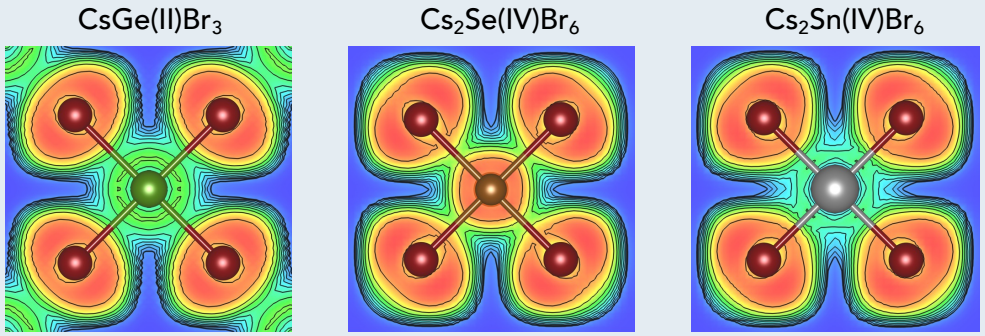


Question

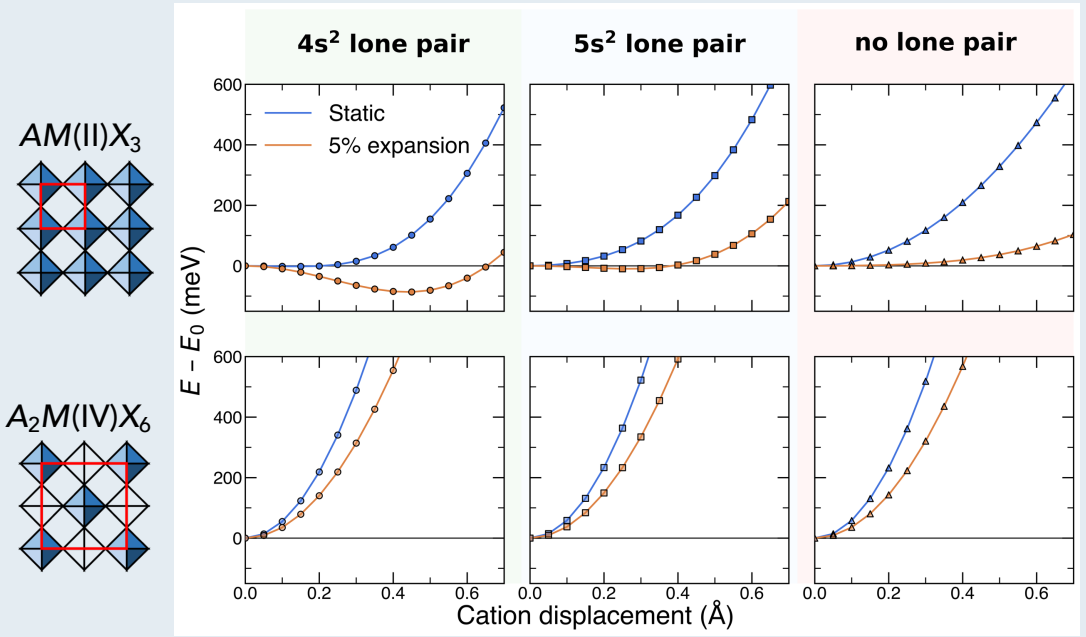
What determines lone pair activity?

- Characterized A_2SeX_6 vacancy-ordered double perovskites using XRD, Raman, ^{77}Se ssNMR, luminescence, and DFT.
- Observed no local or long-range symmetry breaking, even though Se(IV) hosts a 4s² lone pair.
- Framework connectivity controls lone-pair expression: isolated SeX_6 octahedra suppress the s–p mixing needed for off-centering.

Lone pairs, local structure, and why "0D" frameworks change the rules.



ELF: Se(IV) 4s² lone pair is localized and symmetric



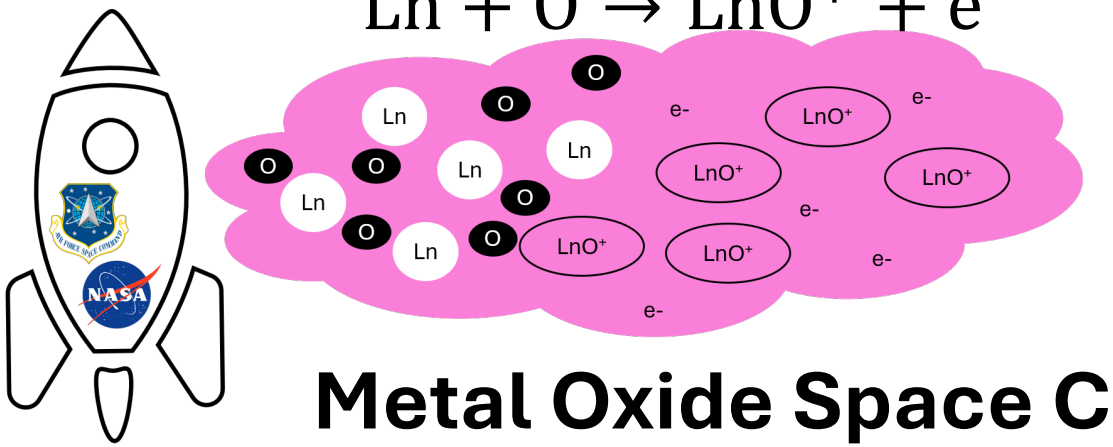
DFT off-centering: no double well in A_2SeX_6

Spectroscopy of the low-lying states of SmO^+, GdO^+, and DyO^+

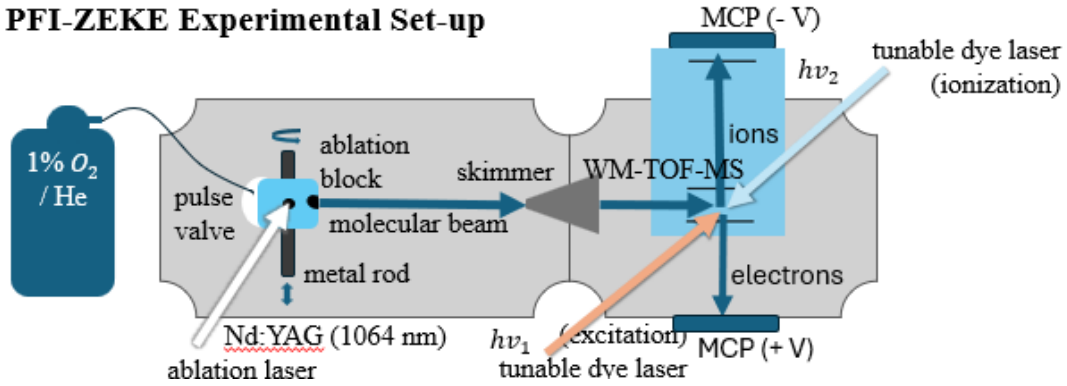
Caitlyn Armendariz-Dollar, Jiande Han, Michael Heaven

Emory University, GA

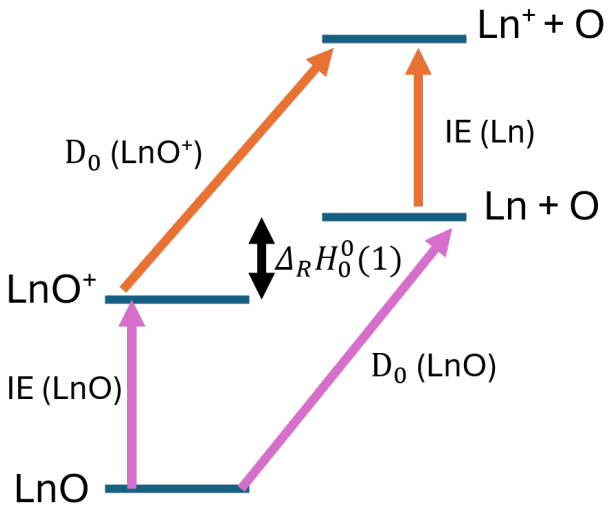
$$Ln + O \rightarrow LnO^+ + e^-$$



Metal Oxide Space Cloud



Thermochemical cycle



- Determination of electronic structure for LnO^+
- Determination of accurate ionization energy for LnO

Photoionization Spectroscopy of Transition Metal Fluorides MFs (M=Sr, Sc, Y)

Quynh Giao Lindsey [1], Jiande Han [1], Jiayue Lin [1], Aleksandra A. Kyuberis [2], Michael C. Heaven [1]

1. Department of Chemistry, Emory University, Atlanta GA 30322, USA - 2. Van Swinderen Institute for Particle Physics and Gravity, University of Groningen, Nijenborgh 4, 9747AG Groningen, the Netherlands

Motivation: Metal fluorides are promising molecules for laser cooling, precision measurements, and searches for symmetry-violating effects.

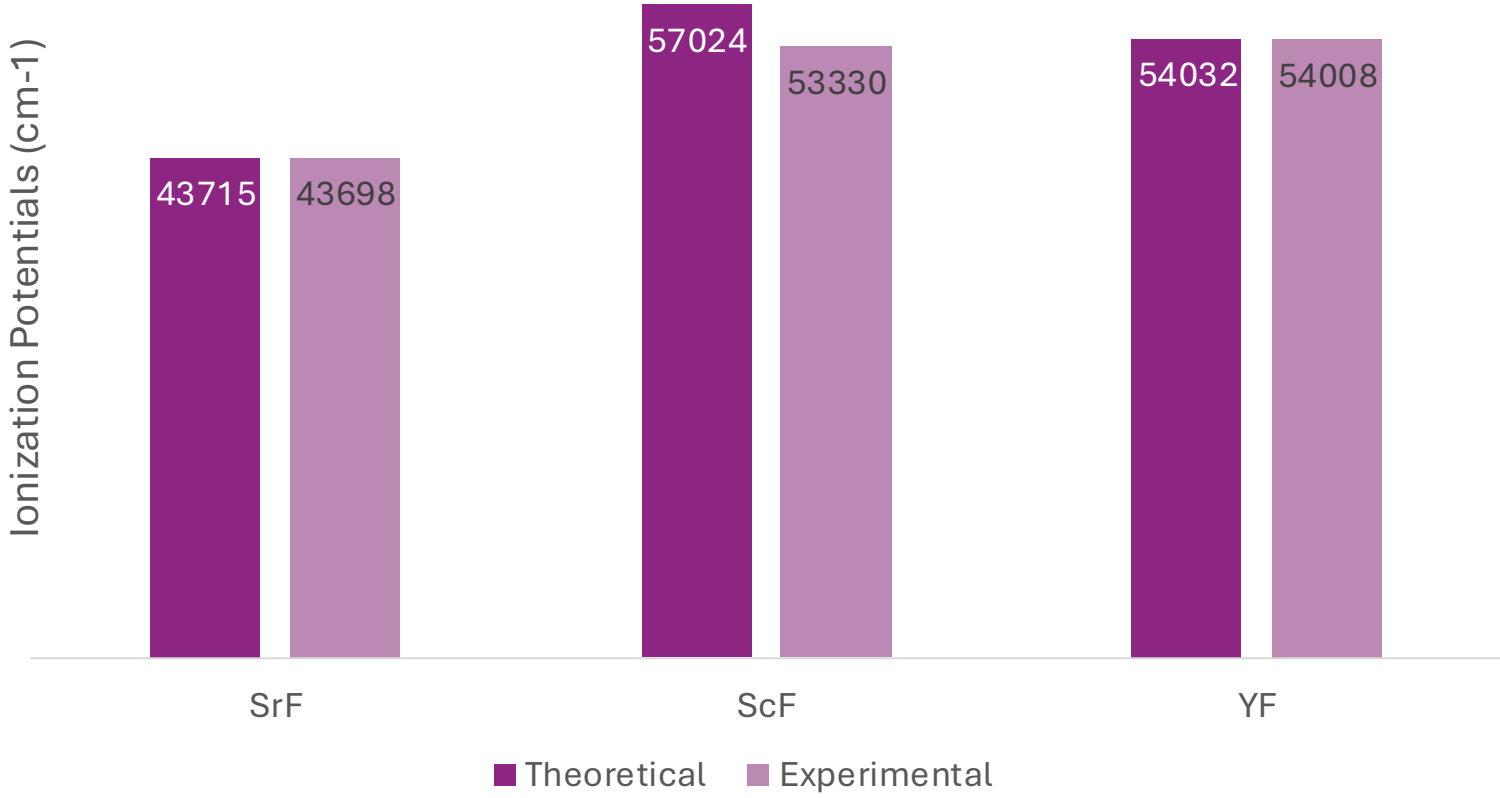
Objectives: We measured the ionization potentials of SrF, ScF, and YF and determined spectroscopic constants of their cations using high-resolution photoionization spectroscopy.

Methods:

1. Laser-induced fluorescence (LIF)
2. Resonance-enhanced two-photon ionization (RE2PI)
3. Pulsed-field ionization zero-kinetic energy (PFI-ZEKE)

Results:

1. Ionization potentials of SrF, ScF, and YF
2. Spectroscopic constants ($\omega_e, \omega_e x_e, B', B''$)
3. Vibrational energies of the cations SrF^+, ScF^+, and YF^+
4. First electronic transition of ScF^+ and YF^+



Stop by my poster to discuss the measured ionization potentials, vibrational constants, and electronic states of these metal fluoride cations.

Sameer Nabi

Los Alamos NATIONAL LABORATORY

RICE UNIVERSITY

MONTE CARLO SIMULATION OF HOT ELECTRON TRANSPORT

From carrier excitation to injection

Combine COMSOL electromagnetic fields with Monte Carlo transport to predict hot-electron injection in arbitrary nanostructures.

WHY?

Local field enhancement matters!

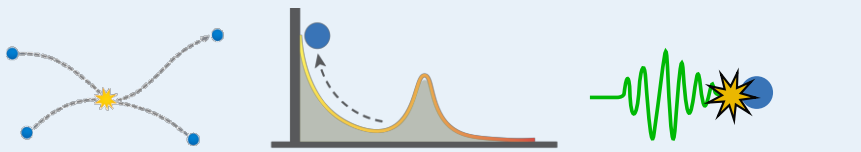
Geometry is key for efficient processes

DFT is impractical for large nanostructures

HOW?

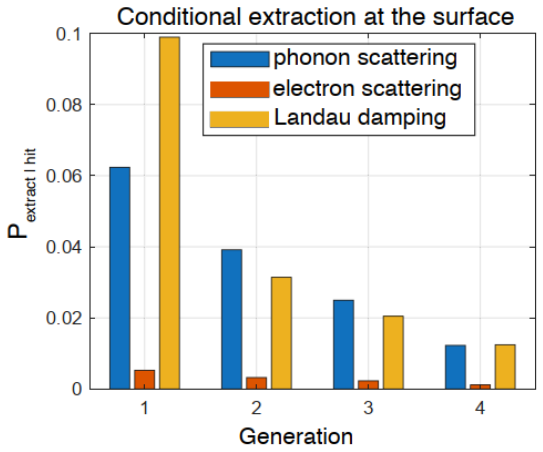
Couple COMSOL 3D EM simulations with an efficient Monte Carlo workflow

Key ingredients



e-e scattering | Landau damping | e-phonon scattering

RESULTS



Applications

Design efficient nanostructures

Understand microscopic mechanisms

TAKE HOME MESSAGE

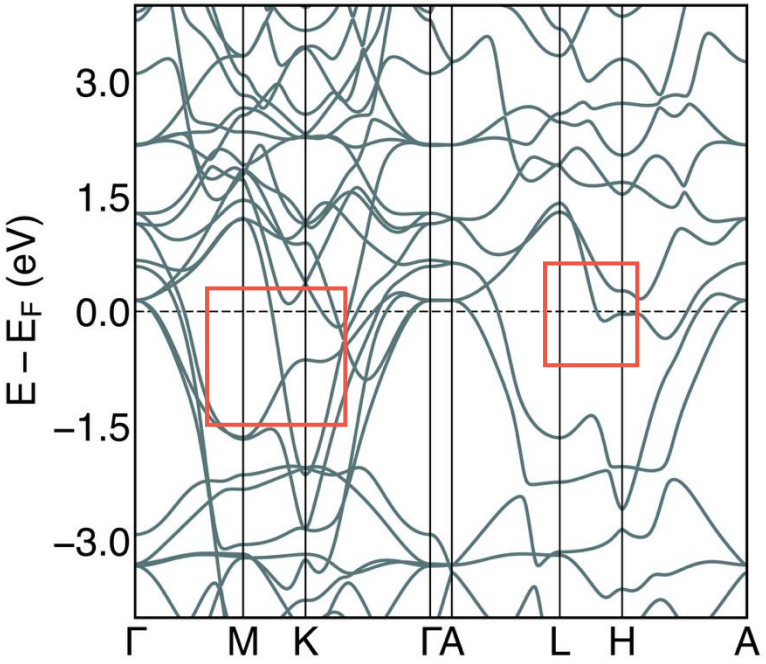
A predictive Monte Carlo tool to understand, engineer and exploit hot electrons in nanostructures for photochemistry and energy harvesting.

Giuseppe Giorgio — Rice University

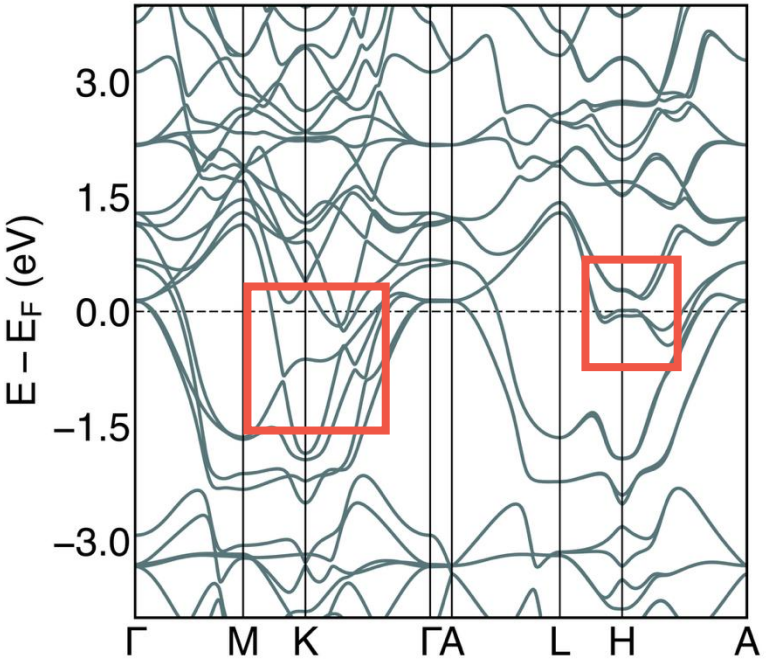
New materials for topological switching

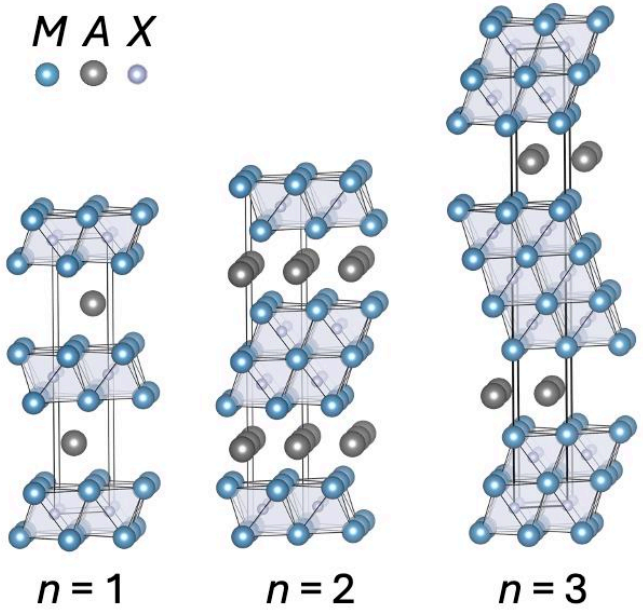
- Example: effects of spin–orbit coupling in M_2AX phases

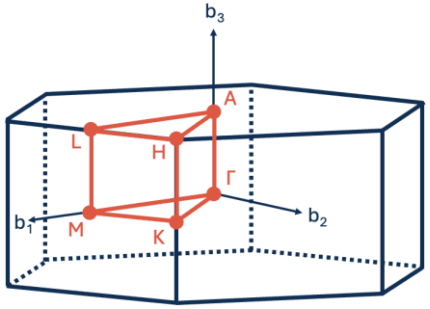
Ti_2PbC



Ti_2PbC with SOC







Hexagonal Brillouin zone

- Possible band crossings with linear dispersion
- Turning on spin–orbit coupling (SOC) lifts degeneracy

Electronic Structure, Vibrational Spectroscopy, and Many Body Effects in Hydrogen Bonded Clusters: Application to water

Long H. Nguyen[1] and Sotiris S. Xantheas[1,2]
[1] Department of Chemistry, University of Washington, Seattle, Washington 98195, United States
[2] Advanced Computing, Mathematics and Data Division, Pacific Northwest National Laboratory, 902 Battelle Boulevard, P.O. Box 999, MS J7-10, Richland, WA 99352, USA

Many Body Expansion (MBE)

A method of decomposing a property of a system containing *N* bodies (e.g. a cluster, liquid water) into components that depend only on 1-, 2-, 3- bodies, etc.

$$D_e = E_{tot}(N) - N \times E_{ref} = \sum_{i=1}^{N} E_{iB}$$

$$E_{1B} = \sum_{i} [E(i) - E_{ref}]$$

$$E_{2B} = \sum_{i<j} [E(ij) - E(i) - E(j)]$$

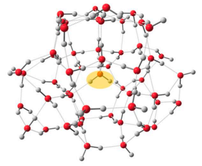
$$E_{3B} = \sum_{i<j} \sum_{j<k} [E(ijk) - E(ij) - E(ik) + E(i) + E(j) + E(k)]$$

Applications of MBE

- A successful framework for modeling intermolecular interactions classically
- Water-water interaction converges at the 4-Body term
- Captures pairwise additive hydrogen bonding (2-B term) and cooperative, non-additive many-body (3-B & beyond) effects
- Implemented in highly accurate *ab-initio* based, classical interaction potentials for water (TTM2-F, TTM3-F, TTM4-F, MB-pol, q-AQUA)

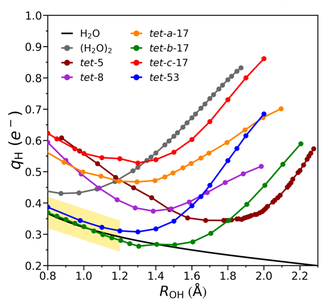
SS Xantheas, *JCP* **100**, 7523 (1994)
JP Heindel and SS Xantheas, *JCTC* **16**, 6843–6855 (2020)
JP Heindel and SS Xantheas, *JCTC* **17**, 2200 (2021)
KM Herman, JP Heindel and SS Xantheas, *PCCP* **23**, 11196 (2021)
JP Heindel and SS Xantheas, *JCTC* **17**, 7341 (2021)
KM Herman and SS Xantheas, *JPCL* **14**, 989 (2023)
JP Heindel, KM Herman and SS Xantheas, *Annu. Rev. Phys. Chem.* **74**, 337 (2023)
D Tzeli and SS Xantheas, *Adv. Quant. Chem.* **92**, 95 (2025)

New environment-dependent 1-B water model



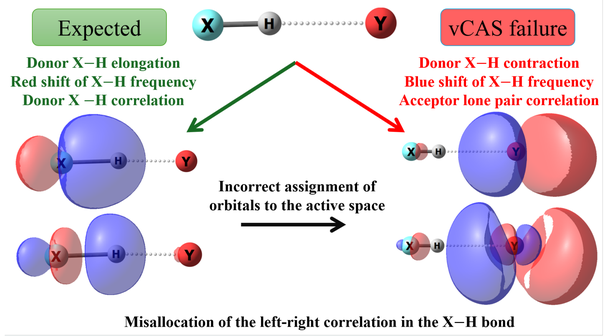
- Construct hierarchical models with tetrahedral coordination mimicking the 1st, 2nd and 3rd solvation shells of a water
- Perform Discreet Variable Representation (DVR) and VPT2 calculations of the anharmonic vibrational frequencies of the solvated monomer at MP2 and CCSD(T) levels of theory
- The fundamentals converge by the second solvation shell and lie within the bands of liquid water (the bending mode ν_2 blue shifts, while the O–H stretching modes ν_1 and ν_3 red shift)

- The 1-B water potential dis-sociates to the correct OH^- + H^+ asymptote upon elongation of the OH bond (the commonly used gas phase Partridge – Schwenke potential dissociates to H• + OH•



LH Nguyen, GD Santis, and SS Xantheas, *JCP* under review

Failure of CASSCF to describe the hallmark of Hydrogen bonding



Problem

- Hydrogen bond formation produces a clear structural signature: the donor X–H bond weakens and elongates accompanied by a red shift of the X–H stretching frequency relative to the isolated monomer
- Valence CASSCF instead predicts a X–H bond contraction and a blue shift of the X–H frequency

Reason

- In the lowest energy solution of vCASSCF, one of the weakly occupied orbitals in the dimer is used to correlate the electrons in the acceptor lone pair rather than those in the donor bonding orbitals (missing left-right correlation)
- For hydrogen bonding the donor X–H bond needs left–right correlation between the bonding and antibonding orbitals

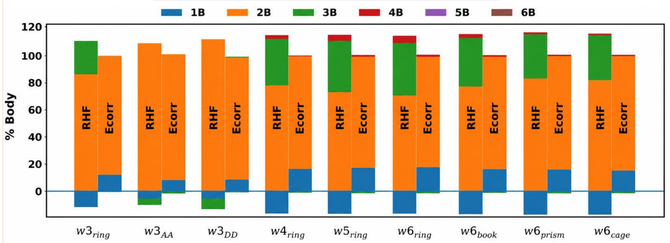
Main Takeaways

- vCASSCF & additional methods describing dynamical correlation (MRCI, CASPT2) should not be used as a black box methods for modeling HB
- The lowest energy vCASSCF wavefunction can still describe the wrong chemical correlation
- Orbitals in the active space must be chosen appropriately

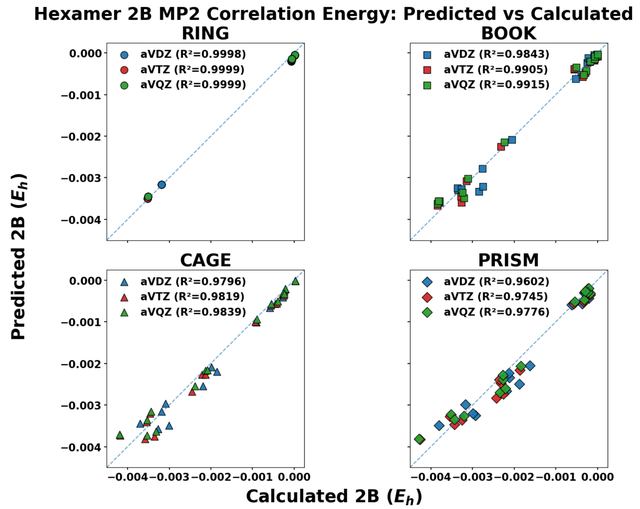
LH Nguyen, TH Dunning, Jr., and SS Xantheas, *JCTC* under revision

MBE of the HF and MP2 contributions to the cluster binding energy

$$D_e^{\mathrm{MP2}} = D_e^{\mathrm{RHF}} + D_e^{\mathrm{corr}}$$



- The HF binding energy converges at the 3-B term
- The correlation energy component of the MP2 binding energy **converges at the 2-Body term**
- Facilitates the use of pre-computed grids for the **monomer** and **dimer** to estimate the correlation contributing to the MP2 binding energy of **a cluster of arbitrary size and geometry**



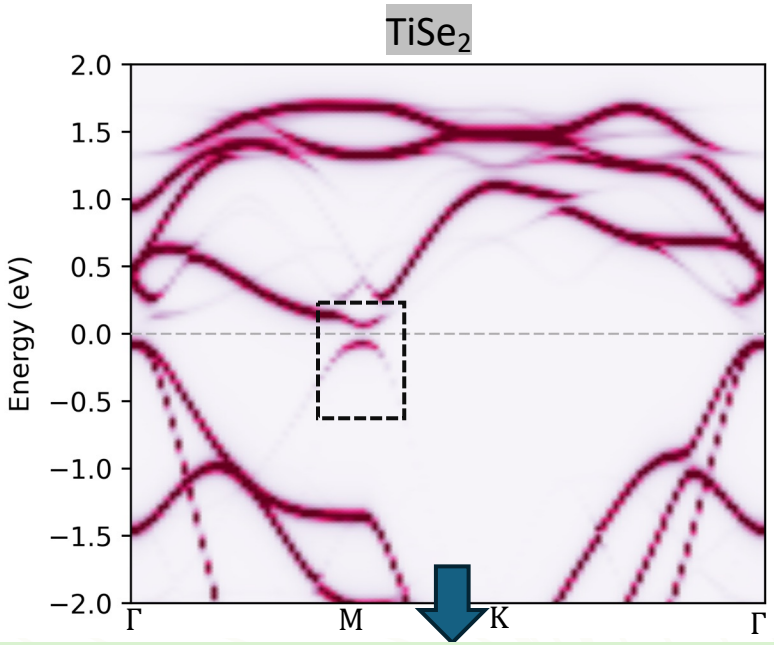
Predicted vs calculated 2-B MP2 correlation energies for water hexamers indicating that the dimer grid captures the dominant 2-B contribution to the MP2 correlation energy quite well

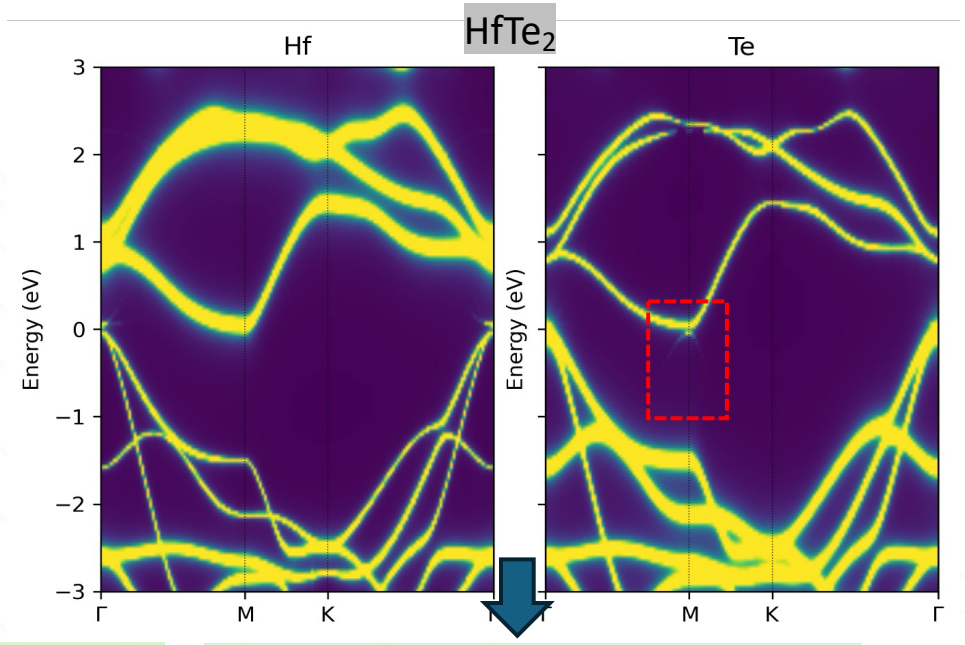
LH Nguyen, A. B. Hale, and SS Xantheas (in preparation)

Samuel Archer

How do we know an excitonic insulators when we see one?

Revisiting band backfolding and symmetry breaking in monolayer $TiSe_2$ and $HfTe_2$ at the meta-GGA DFT level





Initially proposed as excitonic insulator (in the bulk form)

New excitonic insulator candidate

Experiment:

Backfolded bands
With(out) lattice distortions

Excitonic phase!

Our calculation:

Backfolding reproduced without excitonic effects!

Question:

What is the true signature of excitonic condensation?

RPA

Hybrid

Meta-GGA
τ

GGA
Δn

LSDA
n

Terahertz Dynamics at the Actinide Frontier: Linking Low-Frequency Vibrations, Electronic Structure, and Bonding in Molecular Uranium Complexes:

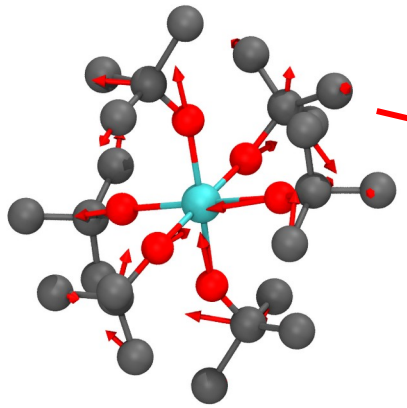
Michele Pittalis, Michael T. Ruggiero

University of Rochester

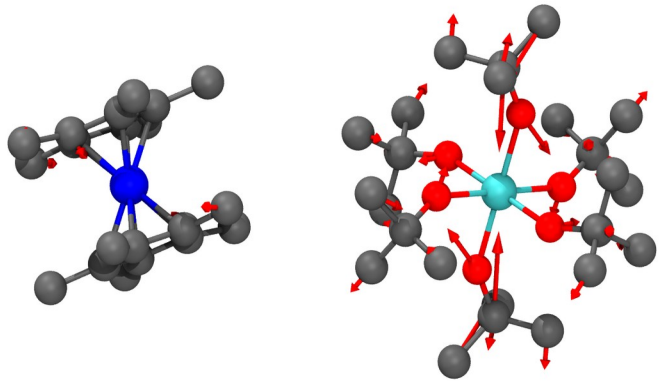
Probing Actinides: Low-frequency Raman spectroscopy serves as a powerful probe for understanding actinide-ligand bonding in molecular uranium complexes

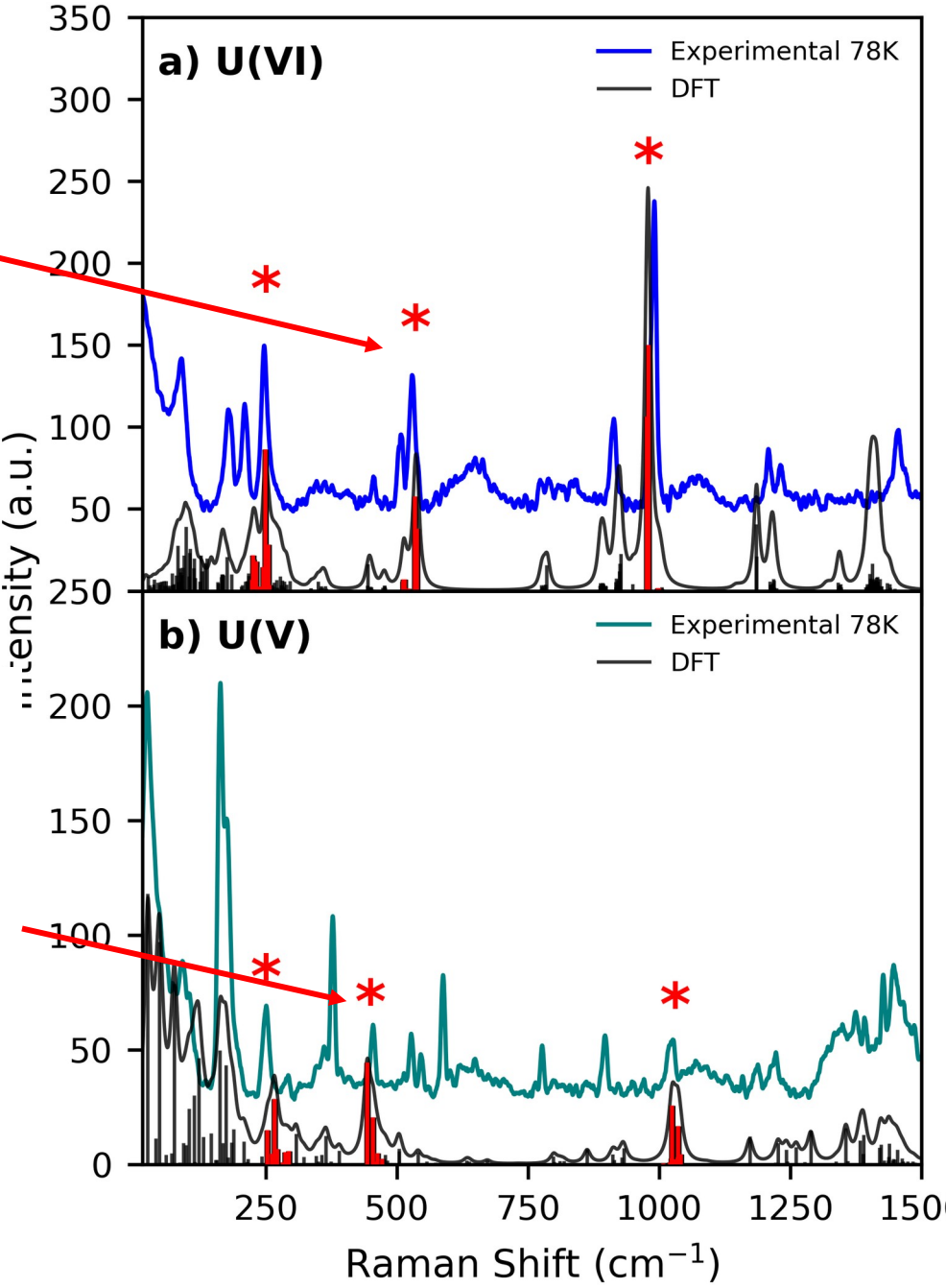
Challenge in Raman Spectra: The vibrational spectra in the solid state are highly complex. Uranium-ligand vibrational modes modes heavily mix with the motions of the organic ligands.

Our Approach: To interpret this complex data, we employ Local Mode Analysis (LMA), to successfully isolates the intrinsic U-O stretching force constants so we can extract direct, quantitative information about the local bonds.



U O C Co





Magnetic Anisotropy in Single-Crystal $CuCrS_2$

From magnetic transitions to entropy change

Ovijit Das

Jacob Pfund · Michael A. Susner · Menka Jain

University of Connecticut, Storrs · Wright-Patterson AFB

THE TAKEAWAY

CVT-grown single crystals reveal strong, axis-dependent magnetism — anisotropy invisible in powders.

Background

$CuCrS_2$ is a layered triangular-lattice chalcogenide with frustrated Cr^{3+} spins and unconventional AFM order. Near 37.5 K a magneto-structural transition couples magnetic ordering with lattice distortion — yet its anisotropy is largely unstudied.

Approach

Growth Chemical vapor transport in a 2/3-zone furnace.

Structure XRD (00ℓ peaks) + Raman (257, 314 cm^{-1}); Rietveld a=b=3.51 Å, c=18.49 Å.

Magnetism ZFC/FC χ, M–H loops & heat capacity, measured in-plane (ab) and out-of-plane (c).

Key Findings

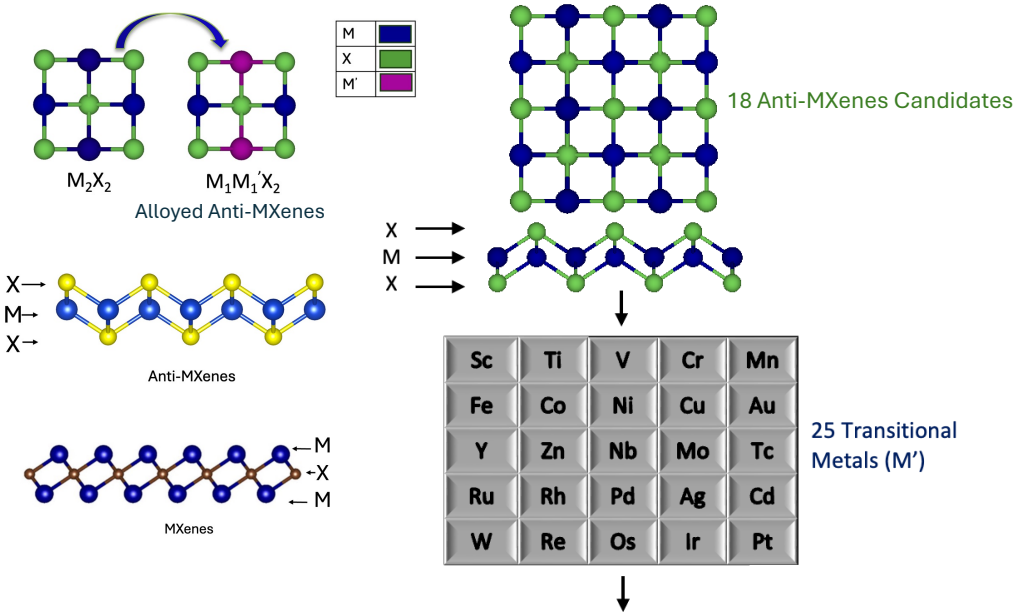
- Noncollinear AFM ordering confirmed at $T_n \approx 37.5$ K.
- Strong anisotropy: susceptibility much lower along c than in-plane.
- S-shaped M–H at low T; linear paramagnetism above Tc.
- Secondary $CuCr_2S_4$ phase identified near 378 K from c-axis data.

Funding: AFRL (GF4GGA21207H002) · NSF (5677710)

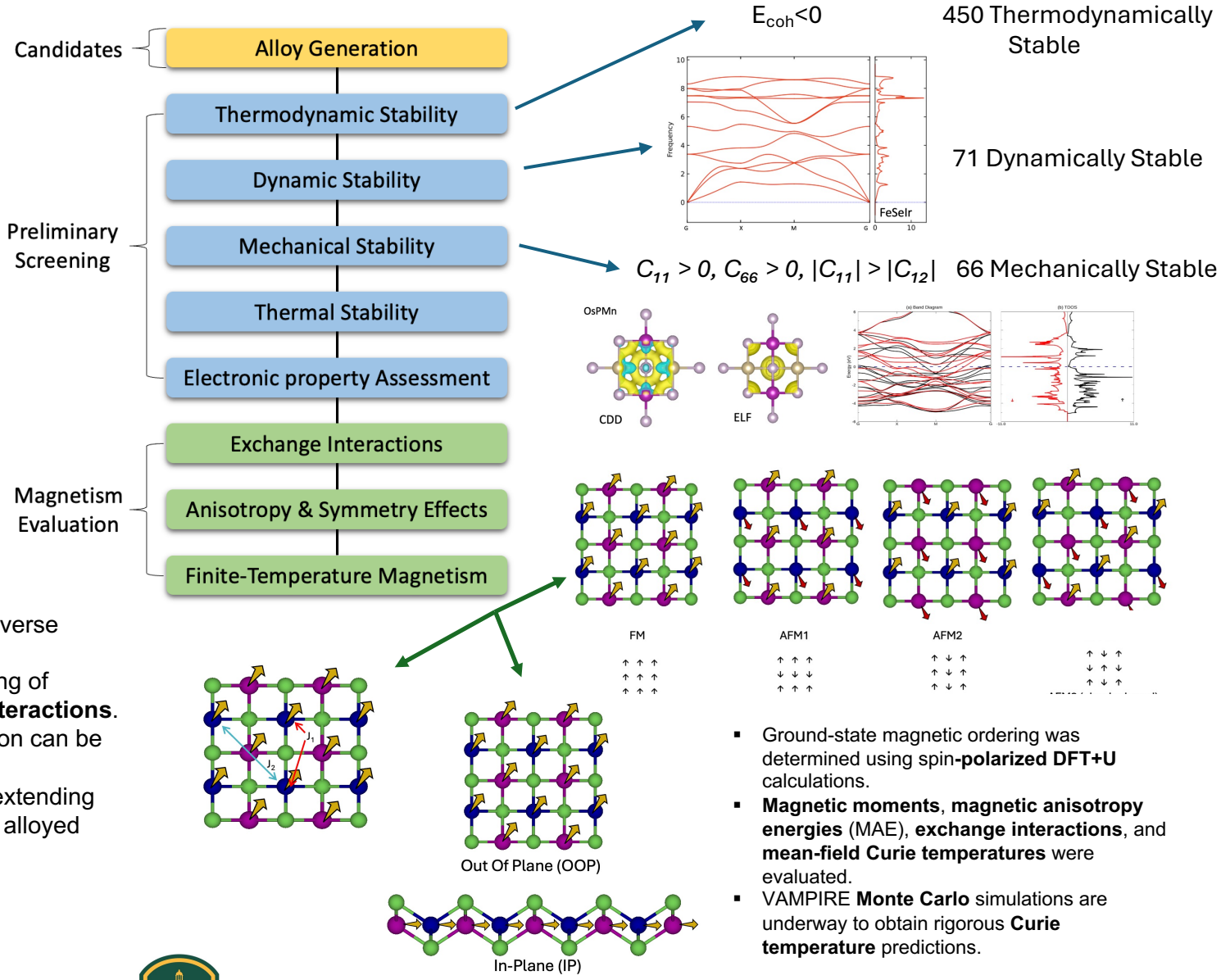
High-Throughput First-Principles Screening of Alloyed Anti-MXenes for Energy and Spintronic Applications

Puja Rijal

Advisor: Dr. Kevin Shuford



~ 450 Alloyed Anti-MXene Candidates



- High-throughput screening identified **66 stable alloyed anti-MXenes** with diverse structural, electronic, and magnetic characteristics.
- Alloying expands the anti-MXene design space and enables systematic tuning of **stability, conductivity, magnetic ordering, anisotropy, and exchange interactions**.
- Composition-dependent trends demonstrate how secondary-metal substitution can be used to **engineer emergent properties** within a single material family.
- Future work will explore **catalytic** and **energy-storage applicat**ions, while extending **magnetic characterization** through Monte Carlo simulations and additional alloyed systems.

- Ground-state magnetic ordering was determined using spin-**polarized DFT+U** calculations.
- **Magnetic moments**, **magnetic anisotropy energies** (MAE), **exchange interactions**, and **mean-field Curie temperatures** were evaluated.
- VAMPIRE **Monte Carlo** simulations are underway to obtain rigorous **Curie temperature** predictions.

Understand & Discover

J. Gu, Z. Zhao, J. Huang, B.G. Sumpter, and Z. Chen, ACS Nano, 15, 6233-6242 (2021)
D. Torelli and T. Olsen, 2D Materials, 6, 045018 (2019)

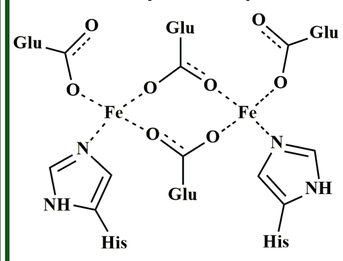
Investigation of the Catalytic Promiscuity of the Dye-Decolorizing Peroxidase Enzyme

Victoria C. Munoz* and Dr. Rajeev Prabhakar
Department of Chemistry, University of Miami, FL, USA

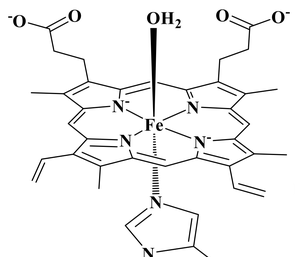
Abstract: A computational mechanistic investigation is being performed to examine the catalytic promiscuity of dye-decolorizing peroxidase (DyP), a heme-containing metalloenzyme that functions both as a peroxidase and hydrolase. Molecular dynamics (MD) simulations, molecular docking, quantum mechanics/molecular mechanics (QM/MM) optimization, and density functional theory (DFT) calculations are used to analyze hydrolytic and oxidative cleavage of the P–C bond of the substrate 2-amino-1-hydroxyethylphosphonic acid. This work examines how the iron–porphyrin center, oxidation number, spin state, ligand environment, and noncovalent interactions influence DyP reactivity, with the goal of guiding the design of its synthetic analogues.

Catalytic Promiscuity of DyP

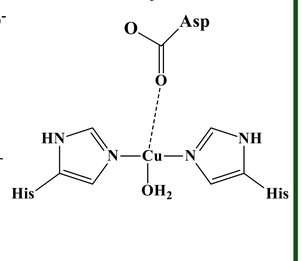
Examples of promiscuous mono- and dinuclear catalysts



Fe(II)-Fe(II) site



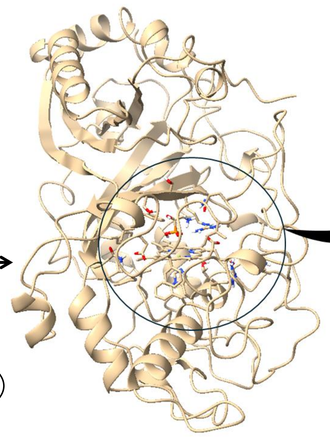
Fe(II)-porphyrin (Por) site

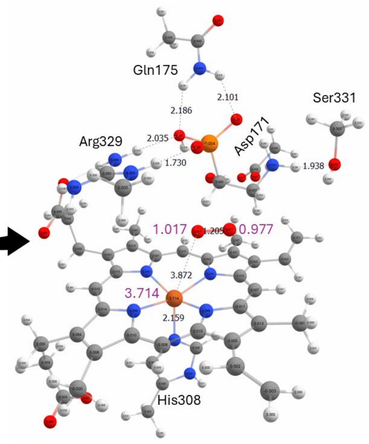


Cu(II)-N_2O site

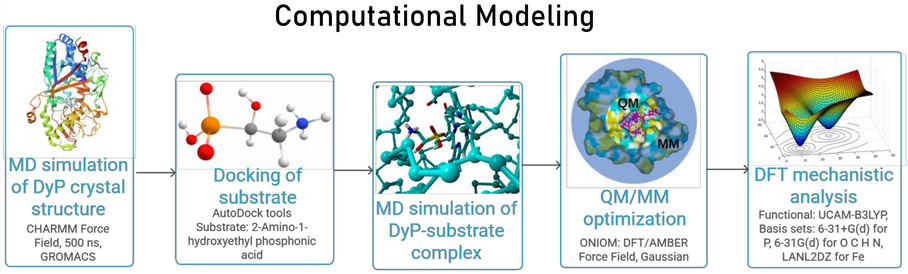
- Why DyP?
- Catalytically promiscuous
- Redox active
- Biomimetic complex

Natural enzymes → Multiple shortcomings



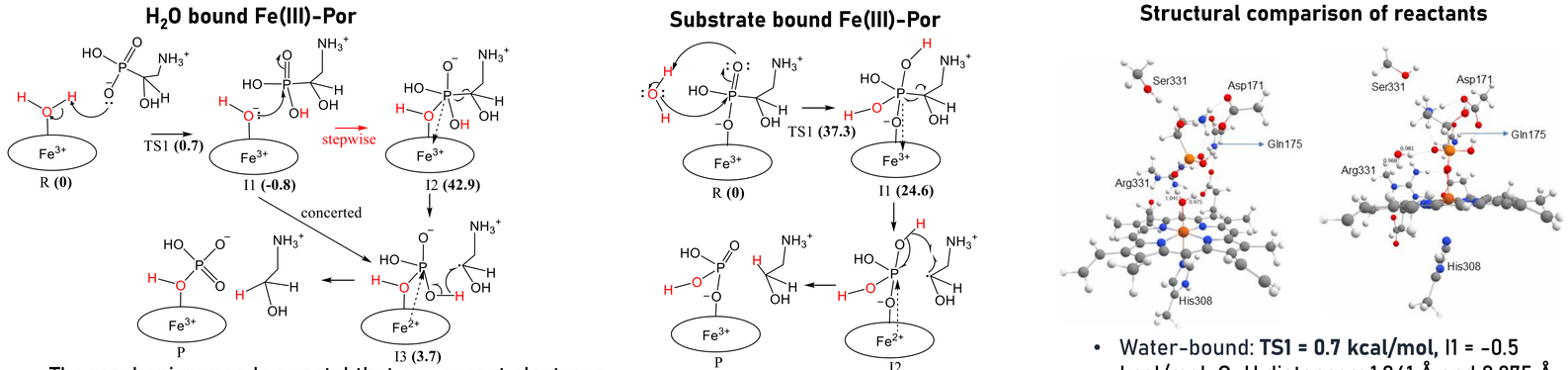


Computational Modeling



Presenting Metal-Mediated Homolytic Cleavage of P–C Bond: Hydrolysis

Compared H_2O bound to metal and substrate bound to metal pathways

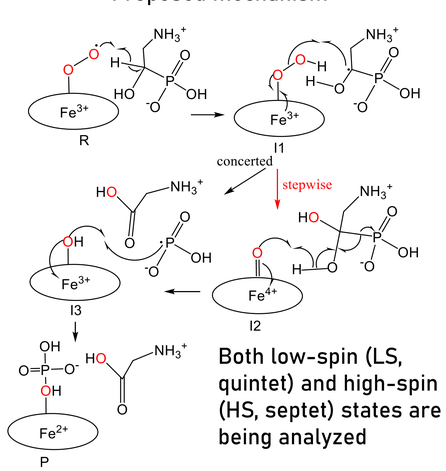


- The mechanism needs a metal that can accept electrons.
- Homolytic cleavage occurs unlike typical hydrolysis reactions.
- **Water-bound pathway is energetically favored.** Fe(III)-bound water is significantly activated.
- The concerted pathway is more favorable, since I2 (42.9 kcal/mol) >>> I3 (3.7 kcal/mol).

- Water-bound: **TS1 = 0.7 kcal/mol,** I1 = -0.5 kcal/mol, O–H distances: 1.041 Å and 0.975 Å
- Substrate-bound: **TS1 = 37.3 kcal/mol,** I1 = 24.6 kcal/mol, O–H distances: 0.981 Å and 0.968 Å

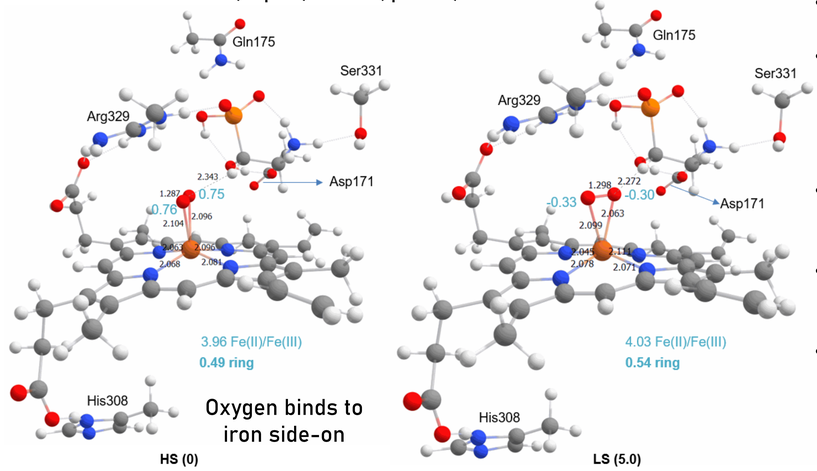
P–C Bond Cleavage: Oxidation

Proposed mechanism



Both low-spin (LS, quintet) and high-spin (HS, septet) states are being analyzed

HS (septet) vs LS (quintet) reactants



Oxygen binds to iron side-on

- **HS:** TS1 = 34.7 kcal/mol, I1= 24.2 kcal/mol
- **LS:** TS1 = 30.3 kcal/mol, I1= 9.0 kcal/mol
  HS: Reactant O–O species has more oxygen character than superoxide character.
- HS/LS: The ring/porphyrin ring is getting partially oxidized.
- Both HS and LS first steps of the oxidation pathway are high in energy.
- Currently both HS and LS pathways are plausible.

Conclusions and Future Work

- Both oxidation and hydrolysis occur via homolytic cleavage.
- Radical from the substrate may be stabilized by active-site residues.
- The Fe(III)-bound water concerted pathway is significantly more favorable than the stepwise.
- Complete the reaction mechanisms.
- Design versatile DyP-inspired metal-containing catalysts.

- Sugano, Y.; Yoshida, T.; Tsuge, H. Dye-Decolorizing Peroxidase (DyP) Complex with Ascorbic Acid (PDB ID: 3VXI). RCSB Protein Data Bank 2012. https://doi.org/10.2210/pdb3VXI/pdb
- EJAtlas, *Textile Industries and Pollution in Tehuacan, Mexico*, accessed 2026.

Jenna Bologa

Stacking-Driven Structural and Magnetic Tuning in $V_{1/3}NbS_2$ and $Mn_{1/3}NbS_2$

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University of California Merced, Merced, CA 95343, USA

AB and ABC stacking is only ~1–5 meV/f.u. apart; suggesting accessible structural and/or magnetic switching

Same atoms, different stacking → different magnetic textures

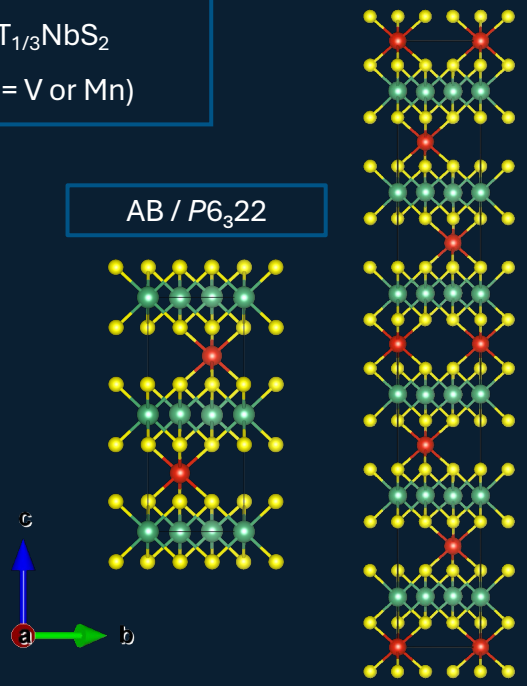
Chemical Formula:

$T_{1/3}NbS_2$

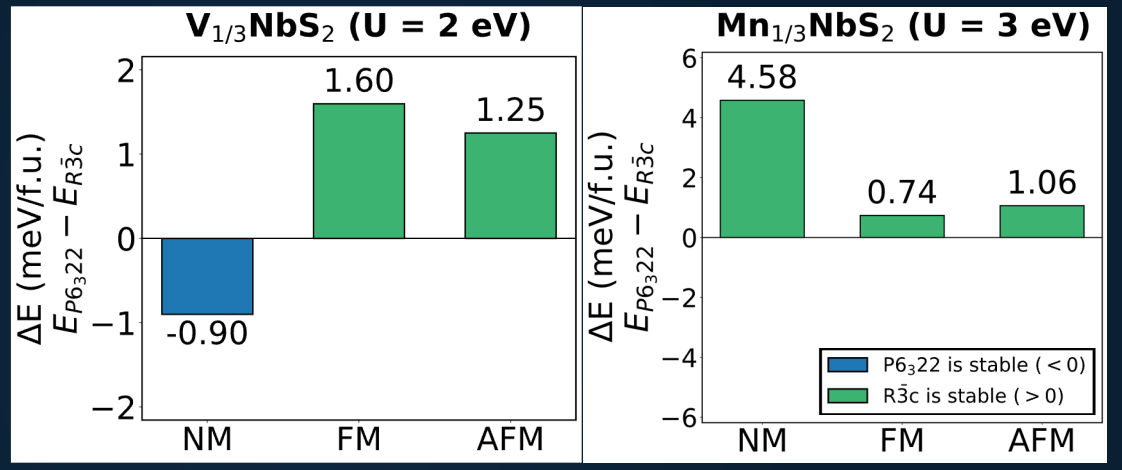
(T = V or Mn)

ABC / $R\bar{3}c$

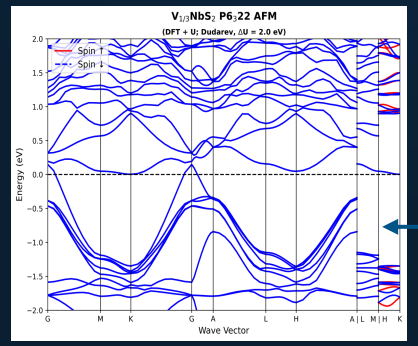
AB / $P6_322$



Low energy separation → switchable candidate

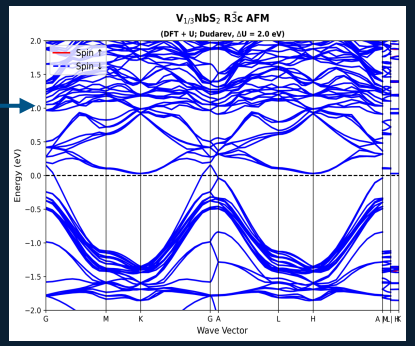


Same formula → different electronic fingerprints



V-based ABC phase: possible topological material[1]

V-based AB phase shows altermagnetic band character



How we test this:

- ✓ Compare NM/FM/AFM stability using DFT+U and vdW corrections
- ✓ Benchmark lattice parameters and magnetic moments against experiment
- ✓ Test pressure-driven structural and magnetic changes

[1]S. S. Fender et al., J. Am. Chem. Soc. **147**, 32315 (2025).