A condensed matter physics class and a Course-based Undergraduate Research Experience (CURE) with the MIT Atomic-Scale Modeling Toolkit

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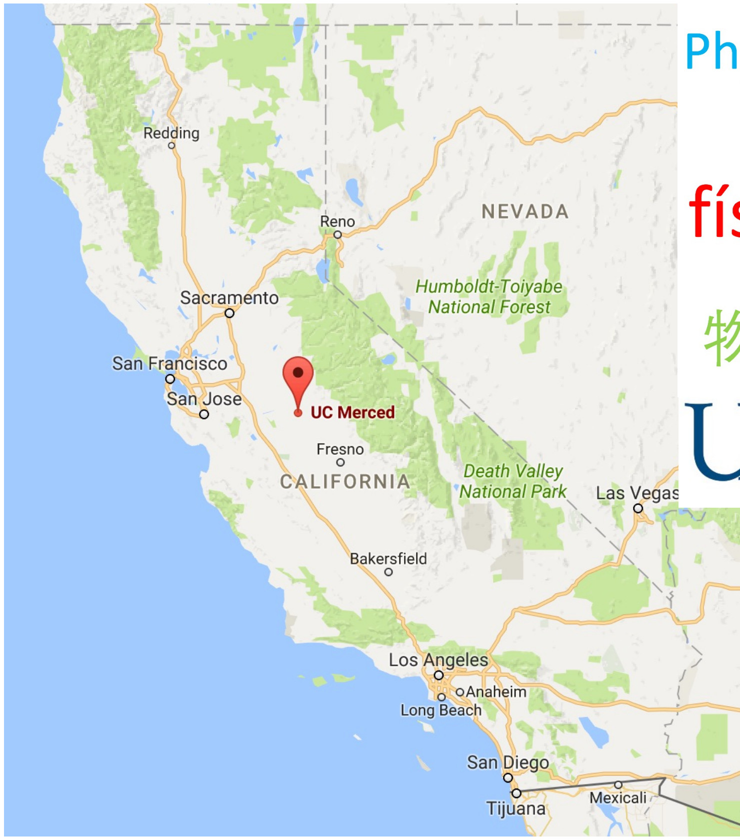
SAIL

Strubbe
Ab Initio
Laboratory

nanoHUB

UCMERCED

12 October 2022
nanoHUB webinar



Physik
भौतिक शास्त्र
physics
fizik
física
فیزیک
পদার্থবিজ্ঞান
物理学
φυσική
liknayan

UNIVERSITY OF CALIFORNIA
MERCED

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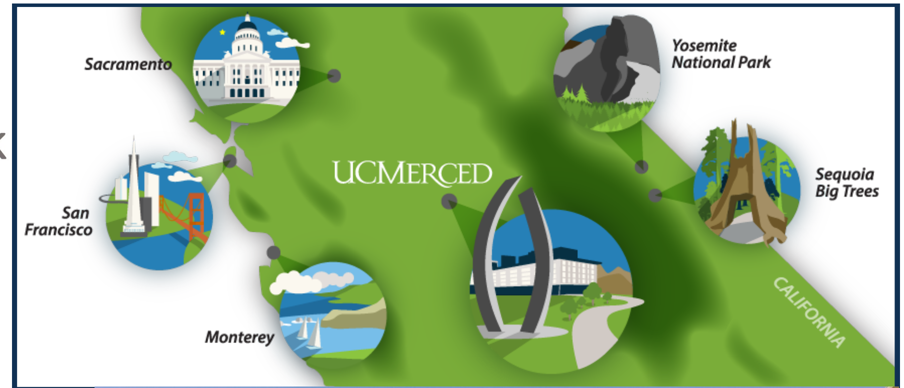
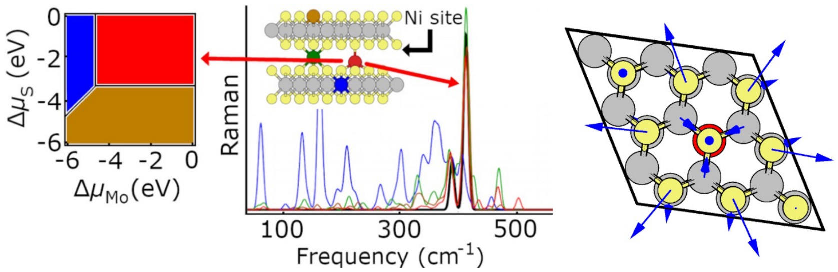


Founded 2005, 10th campus of the Univ. of California
First US research university of the 21st century
Fastest achievement of Carnegie R2 status
City of Merced population is about 80,000
Just finished “2020 Project,” doubling size of campus
9000 undergrads: 55% Hispanic/Latinx, 75% first-gen.

Research in the Strubbe *Ab Initio* Laboratory (SAIL)

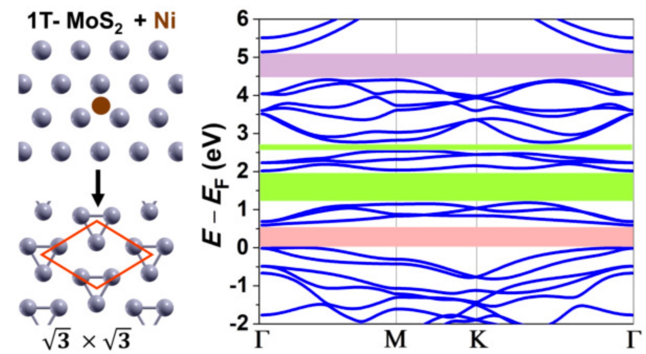
2D materials: doped Raman



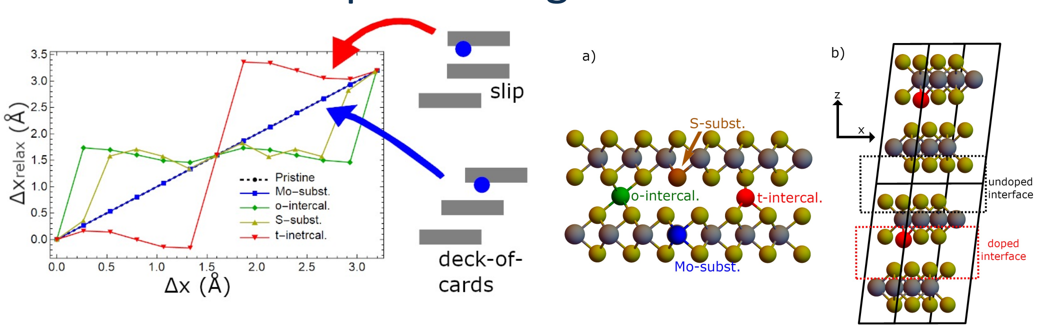
J. Phys. Chem. C 125, 13401 (2021)
J. Phys. Chem. C 10.1021/acs.jpcc.2c03999
Nanotechnology 34, 015706 (2023)

2D materials: reconstructed phases

arXiv:2107.07541 (2022)

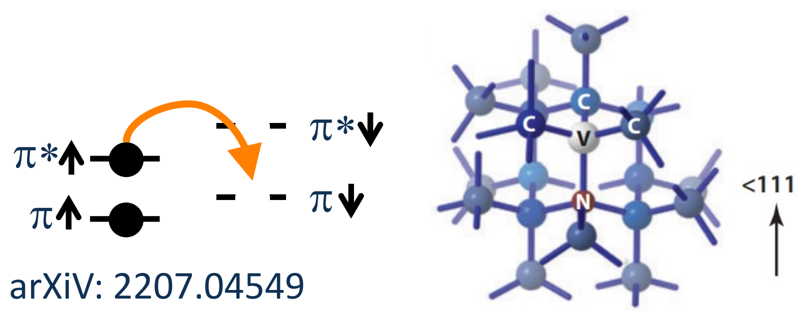


2D materials: doped sliding



arXiv: 2209.15629 (2022)

Quantum defects, spin-flip Bethe-Salpeter equation



arXiV: 2207.04549

The MIT Atomic-Scale Modeling Toolkit

https://nanohub.org/tools/ucb_compnano/

Begun for graduate Computational Nanoscience class at UC Berkeley in 2008, developed mainly by Elif Ertekin (now at UIUC) and Jeffrey Grossman (now at MIT).

I was TA and developer in 2009, and since then.

Rebranded for Introduction to Modeling and Simulation at MIT, Grossman and Markus Buehler.

Developed by me at UC Merced since 2016, for condensed matter physics classes.

Design philosophy: manage complexity of underlying code, less is more

Averages and Error Bars
Molecular Dynamics (Lennard-Jones)
Molecular Dynamics (Carbon Nanostructures and More)
Monte Carlo (Hard Sphere)
Monte Carlo (Ising Model)
Quantum Chemistry (GAMESS)
DFT for Solids and 2D Materials (Quantum Espresso)
Crystalline Structures and Densities (XCrySDen)
DFT for Solids, Surfaces, and Molecules (SIESTA)
Quantum Monte Carlo (QWalk)

"a technological and pedagogical *tour de force*" – student review

PHYS 141, PHYS 241, MBSE 245: Condensed Matter Physics

Introductory class on condensed matter physics for around 20 students: undergraduate physics majors, PhD students in physics, and PhD students in materials and biomaterials science and engineering

Topics: Drude model, free-electron model, bonding, phonons, crystal structure, X-ray diffraction, nearly free-electron model, Bloch's theorem, bandstructure, carrier statistics, semiconductor devices, magnetism in materials

Hands-on nanoHUB activities in every discussion section, done in groups
A few nanoHUB homework problems towards end of semester

Condensed Matter Physics Discussion Exercises

1: GAMESS; atomic energy levels and wavefunctions
2: GAMESS; covalent, ionic, and van der Waals bonding
3: Molecular dynamics; radial distribution function, solids, liquids
4: Quantum Espresso; vibrations in 1D chains
5: XCrySDen; visualization of 2D crystal structures
6: XCrySDen; visualization of 2D crystal structures
7: ”
8: XCrySDen: visualization of Brillouin zones
9: Quantum Espresso: vibrations in graphene and diamond
10: XCrySDen; visualization of paths through Brillouin zones
11: Quantum Espresso: bandstructures of 2D materials
12: Monte Carlo (Ising model): paramagnetism, ferromagnetism, and antiferromagnetism

Course Undergraduate Research Experience (CURE)

Bringing the excitement of research into the classroom!
Key aspects are: students learning and using research methods, having input into the project, generating new research data, and analyzing it to draw conclusions that are not known beforehand

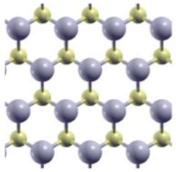
Many studies show:
Improves learning and motivation, promotes independent thinking, and increases retention of students in the major and STEM
Students apply knowledge, get a taste of research, feel like a scientist, have sense of belonging, go on to bigger research projects
Especially beneficial for minoritized/underrepresented students

D. Lopatto, *Science in Solution: The Impact of Undergraduate Research on Student Learning*, Research Corporation for Science Advancement (2009). https://www.researchgate.net/publication/229078320_Science_in_Solution

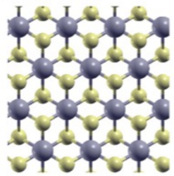
Rory Waterman and Jen Heemstra, eds. *Expanding the CURE Model: Course-Based Undergraduate Research Experience*, Research Corporation for Science Advancement (2018). https://rescorp.org/gdresources/publications/Expanding-the-CURE-Model.pdf

The rise of 2D materials

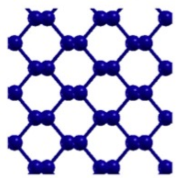
TMDCs-trigonal prismatic



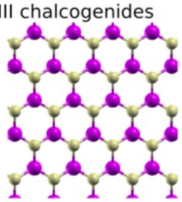
TMDCs-octahedral



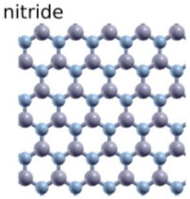
Phosphorene and IV-VI

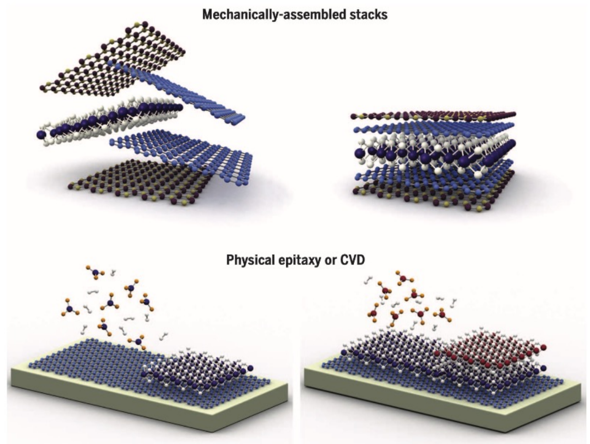


Group III chalcogenides



Boron nitride

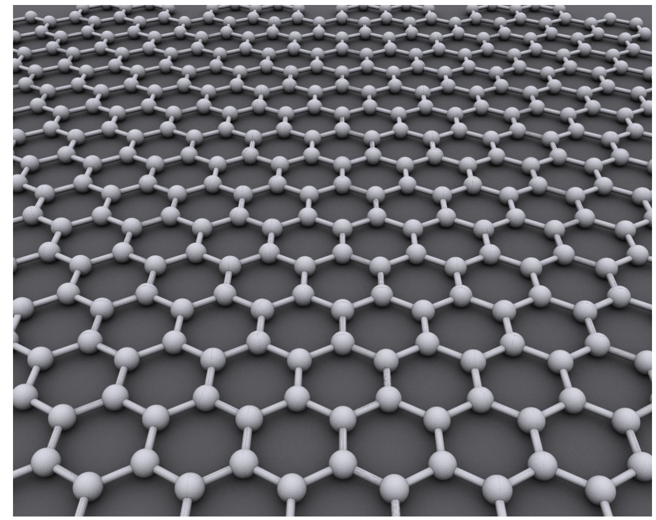


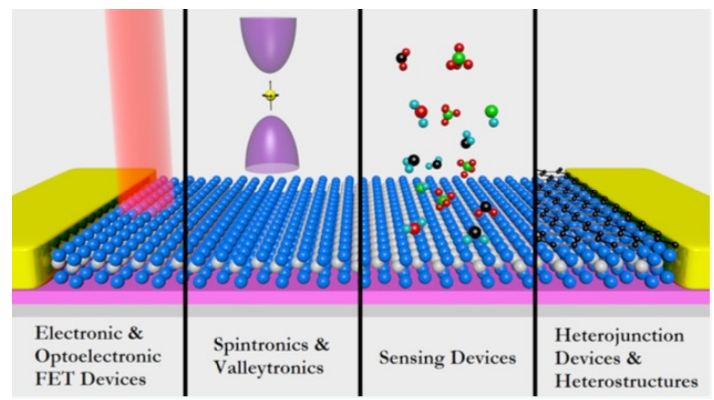


K. S. Novoselov, A. Geim, *et al.*, *Science* 353, 461 (2016)

Strong covalent bonds in-plane
Weak Van der Waals interlayer interactions

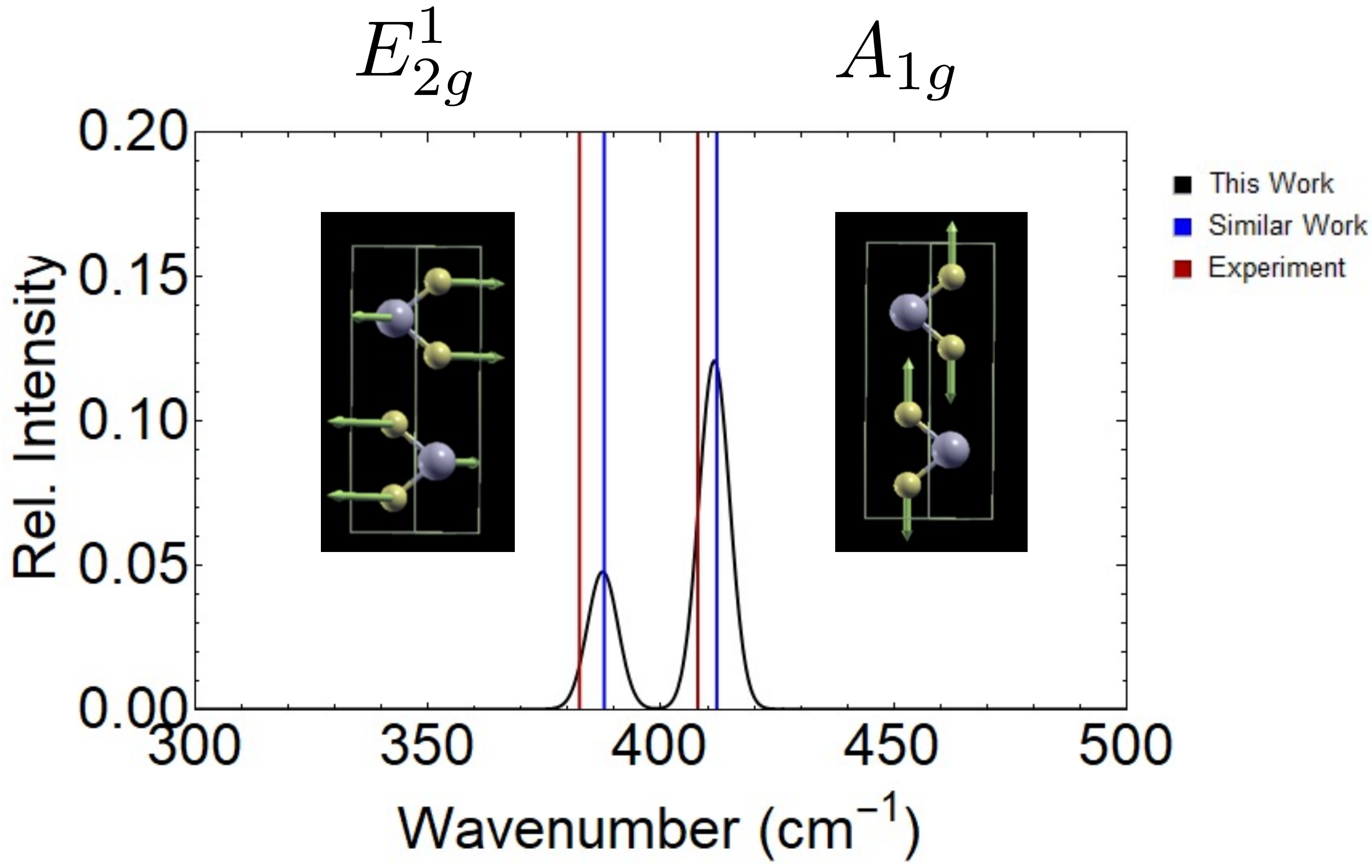
Electronic and optical properties, monolayers and few layers, heterojunctions, qubits or quantum emitters, topological effects





R. Ganatra *et al.*, *Nano Lett.* 8, 4074 (2014)

Raman Spectrum of Pristine MoS_2

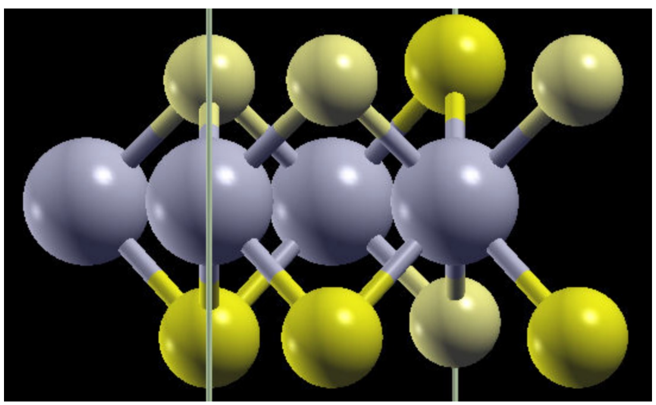


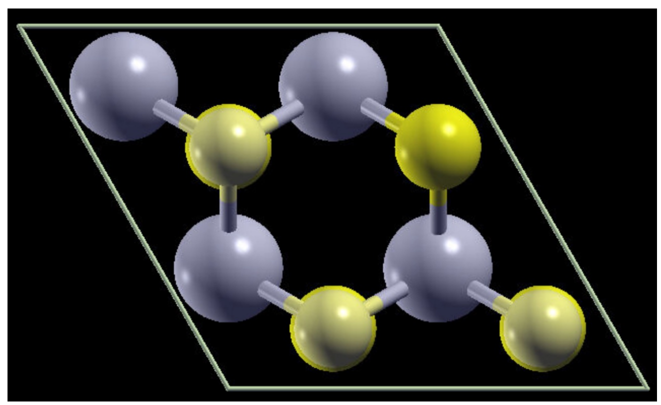
A. Molina-Sánchez and L. Wirtz, *Phys Rev. B* 84, 155413 (2011). [Theory]
C. Lee *et al.*, *ACS Nano* 4, 2695 (2010). [Exp't]

Calculation by
Enrique Guerrero

CURE on Raman spectra of $MoS_2Se_{2(1-x)}$ monolayer alloys

Final project, with presentations and papers.
Lecture on 2D materials' unique physics and applications.
Each student assigned one of 22 symmetry-unique structures in a 2x2 supercell with 8 S atoms
HW: calculate relaxed structure and Raman spectrum of pristine MoS_2 and $MoSe_2$
HW: calculate relaxed structure of assigned structure
Presentation: relaxed structure, choice of property (e.g. density of states, elastic tensor, etc.)
Submit data to spreadsheet and output repository: structure, bandgap, phonon data, etc.
Final paper: analyze full class data set, find most stable structure, identify trends.
Quantum ESPRESSO tool. Needed to use parallel run functionality to enable calculations.





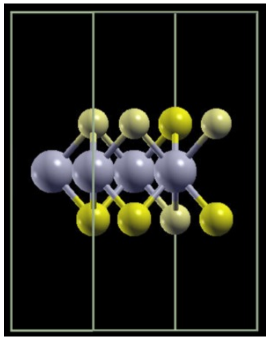
Final project structures

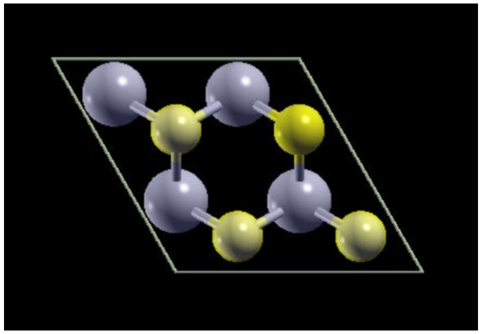
1. x=1. All S.
2. x=7/8. Replace S #1.
3. x=3/4. Replace S #1 and #2 (vertically offset).
4. x=3/4. Replace S #1 and #3 (horizontally offset).
5. x=3/4. Replace S #1 and #4 (vertically and horizontally offset).
6. x=5/8. Replace S #1, #3, #5 (same plane).
7. x=5/8. Replace S #1, #2, #3 (2 stacked).
8. x=5/8. Replace S #1, #3, #8 (both planes, none stacked).
9. x=1/2. Replace S #1, #3, #5, #7 (same plane, Janus).
10. x=1/2. Replace S #1, #2, #3, #4 (horizontal stripes, stacked).
11. x=1/2. Replace S #1, #3, #6, #8 (horizontal stripes, non-stacked).
12. x=1/2. Replace S #1, #2, #3, #6 (perpendicular stripes, stacked).
13. x=1/2. Replace S #1, #2, #3, #5 (3 in one plane, 1 in other, stacked).
14. **x=1/2. Replace S #1, #3, #5, #8 (3 in one plane, 1 in other, non-stacked).**
15. x=3/8. Inverse of #8.
16. x=3/8. Inverse of #7.
17. x=3/8. Inverse of #6.
18. x=1/4. Inverse of #5.
19. x=1/4. Inverse of #4.
20. x=1/4. Inverse of #3.
21. x=1/8. Inverse of #2.
22. x=0. All Se.

Before substitution: all 8 S sites are equivalent by symmetry. And, any pair of S atoms in the same plane are equivalent.

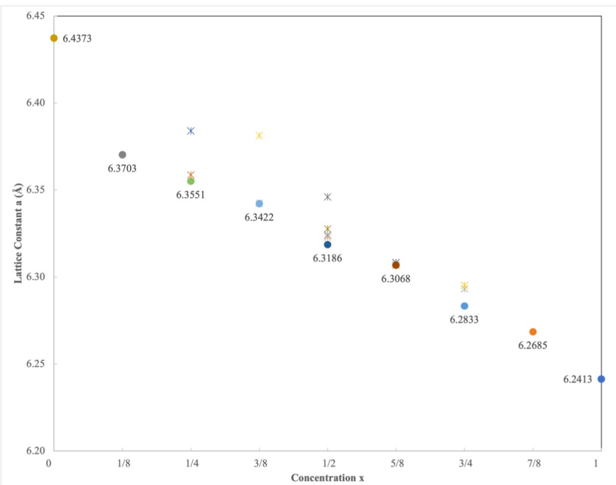
#14 is equivalent by symmetry to 7 other structures: pick any site in top plane to replace, and then replace the 3 sites in the bottom plane that are not beneath it; or flip any of those upside down.

Bonus (unclaimed) for showing I missed or duplicated a structure.



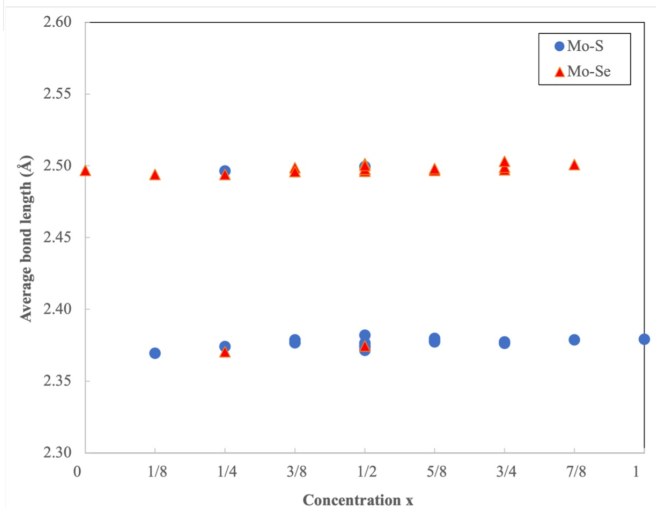


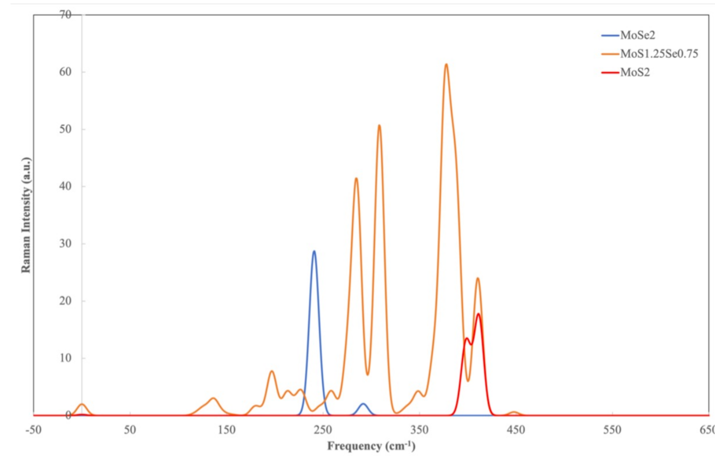
CURE on Raman spectra of $MoS_2Se_{2(1-x)}$ monolayer alloys



Lattice constant

Bond lengths





Raman spectra

(Note anomaly)

Sign up for Part 2! Wednesday, October 26

Interactive modeling of materials with density functional theory using the Quantum ESPRESSO interface within the MIT Atomic Scale Modeling Toolkit

Dr. Enrique Guerrero, UC Merced

Online resources

https://nanohub.org/resources/ucb_compnano/supportingdocs

2022-10-12_nanoHUB_webinar_slides.pdf (these slides)

2022-10-12_nanoHUB_webinar_exercises.pdf (handout for examples)

Acknowledgments regarding CURE

Participation by all the students in my class

Tool development by Dr. Enrique Guerrero

Discussions with Marcos García-Ojeda (UC Merced) and Anubhav Jain (LBNL)

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RESEARCH CORPORATION
for SCIENCE ADVANCEMENT