Visualizing with VESTA to Plot Cross Sections of Electron Densities of Gold and Sulfur Bonding Atoms

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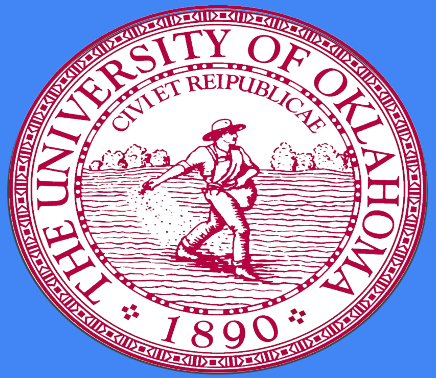
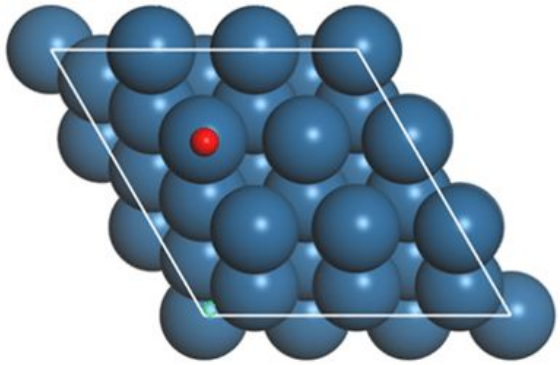
Experimental Condensed Matter Physics
University of Oklahoma REU Program 2020
July 31, 2020

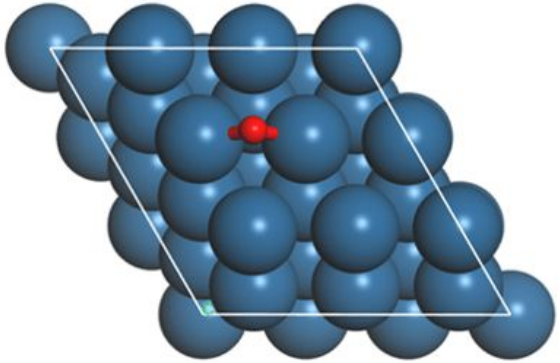


Motivation

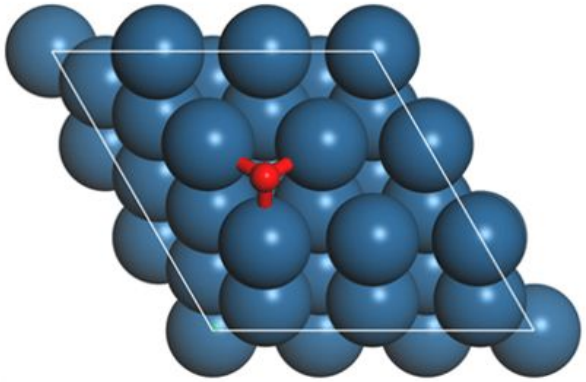
- Au-S bonding is not completely understood
  - Least understood part of SAMs (self-assembled monolayers)
- Applications for SAMs:
  - Electronics
  - Nanotechnology
  - Surface Modifications



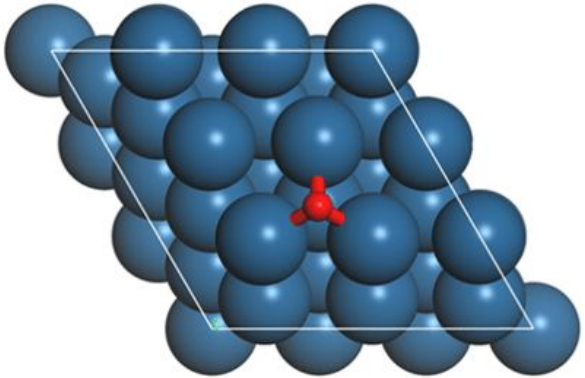
atop



bridge



hollow fcc



hollow hcp

Adsorption Sites on Au(111) Surface

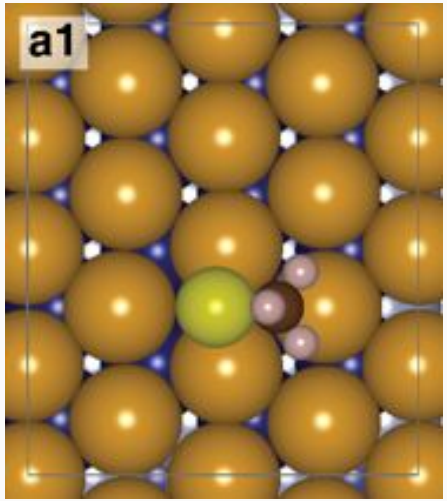
- Atop
- Bridge
- Hollow-fcc (face centered cubic)
- Hollow-hcp (hexagonal close packed)

Bridge Site: Top-Down View

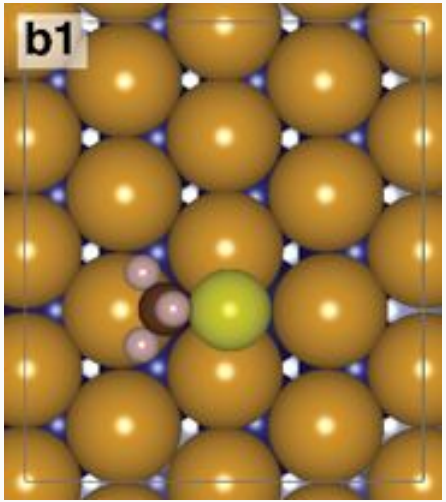
Bridge right = bridge-fcc
(face centered cubic)

Bridge left = bridge-hcp
(hexagonal close packed)

~25 meV
More
stable

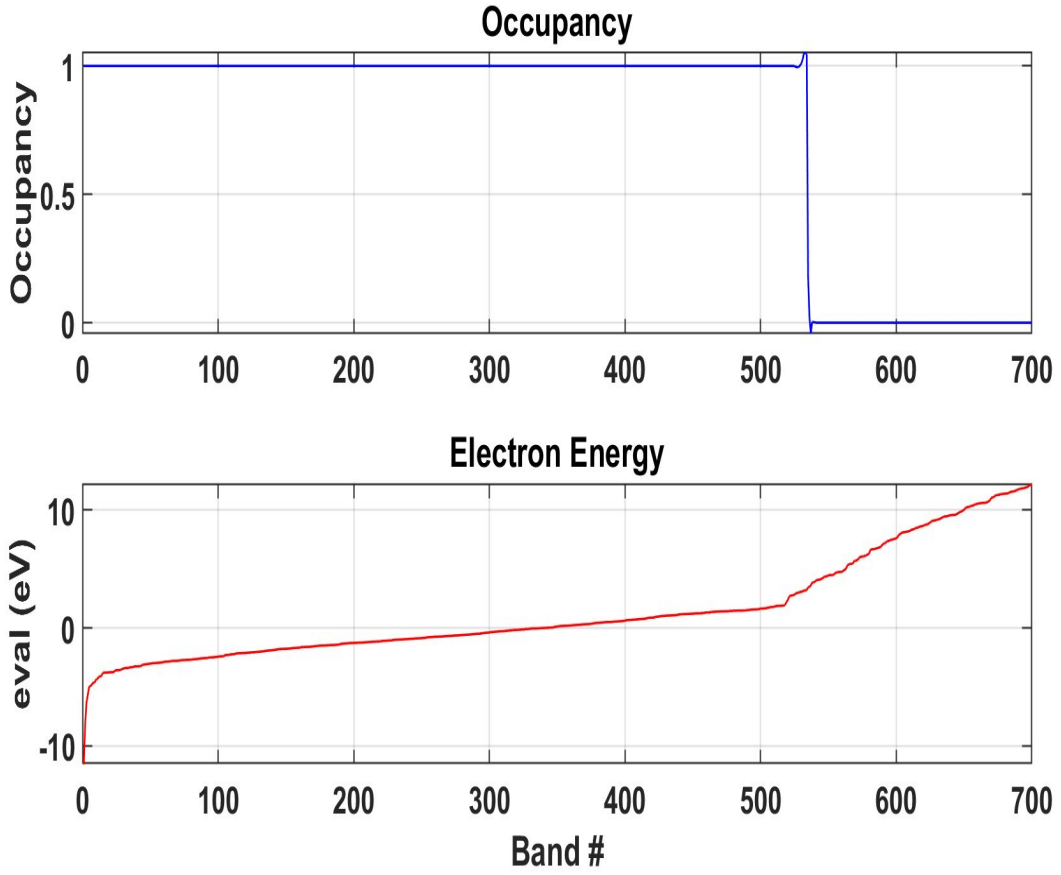


Problem:
What makes
them
different?



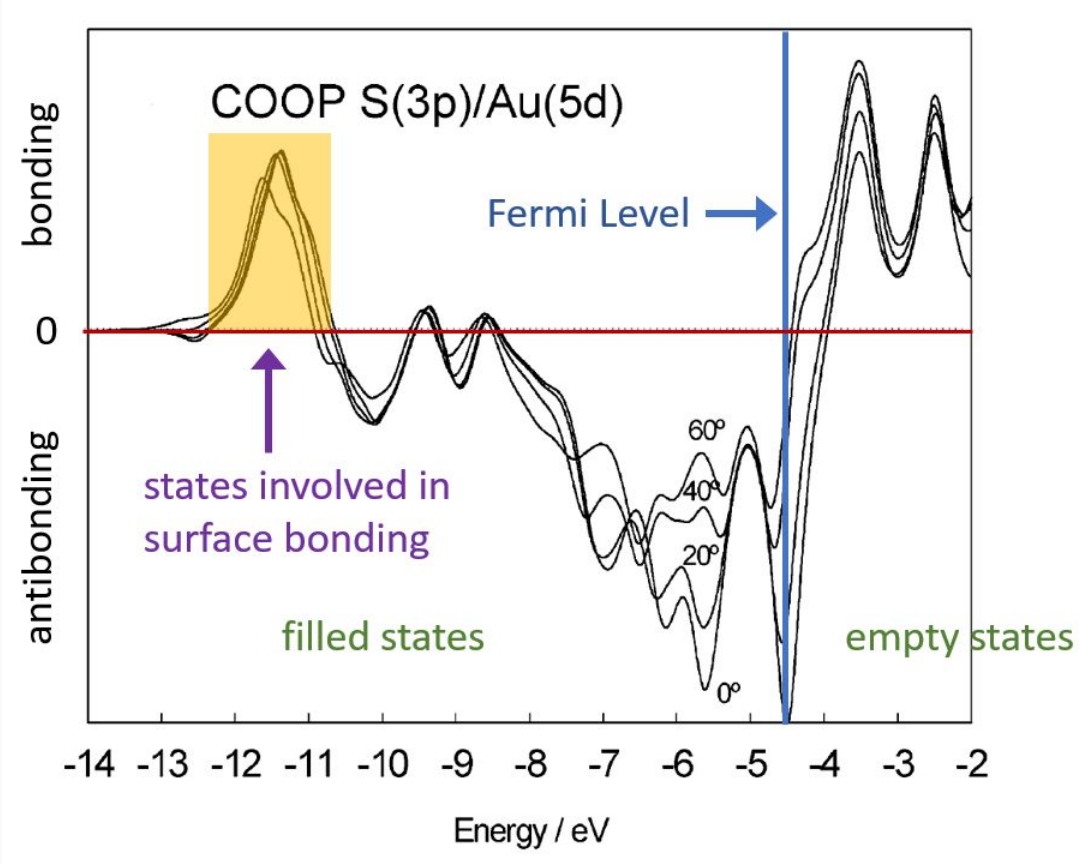
Terms:

- **Bands (orbitals)**: the range of energies that an electron may have within it
- **Occupancy**: filling orbitals with electrons
  - Filled → 1
  - Empty → 0



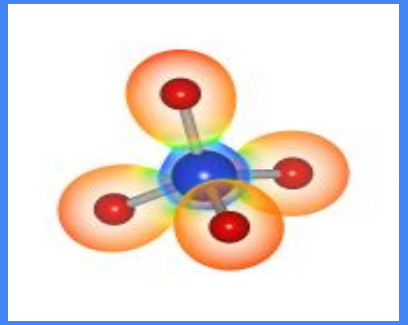
Determining Bands

- COOP (Crystal Orbital Overlap Population)
- -12.5 to -10.8 eV corresponds to our data as bands 7-47
- Below Fermi Level
  - Occupancy =1, filled state
- Above Fermi Level
  - Occupancy =0, empty state



F. P. Cometto, P. Paredes-Olivera, V. A. Macagno and E. M. Patrito, J. Phys. Chem. B 109(46), 21737 (2005)

Tools

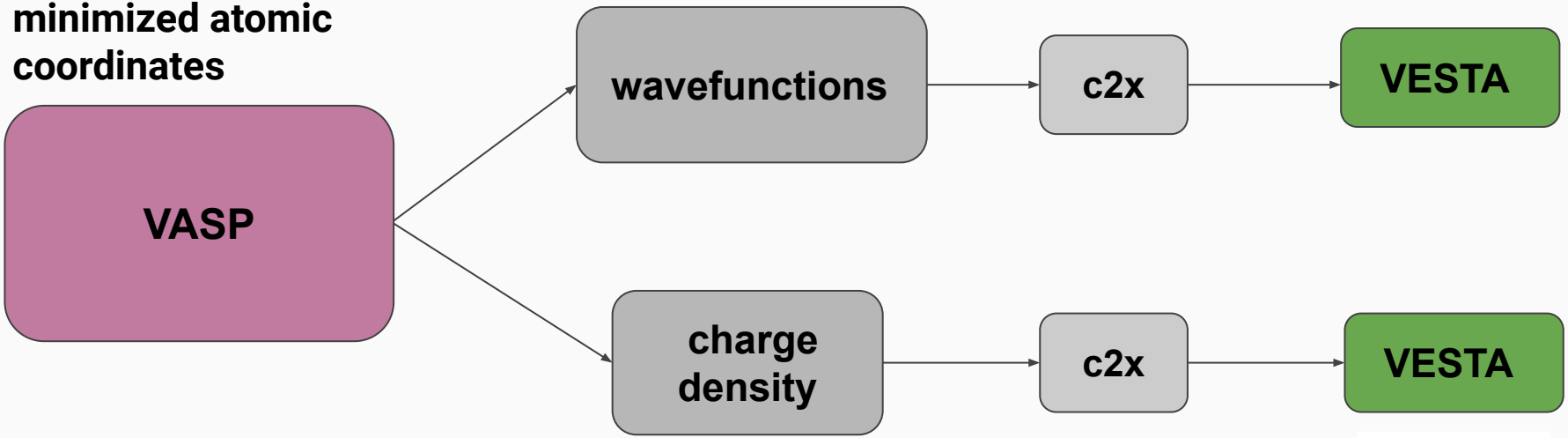


- VASP (**V**ienna **A**b initio **S**imulation **P**rogram) → density functional theory (DFT) program
- c2x → to convert dataset files to smaller files
- VESTA (**V**isualization for **E**lectronic and **ST**ructural **A**nalysis) → 3D visualization program for crystal structures and volumetric data

We were all learning!

Input: energy minimized atomic coordinates

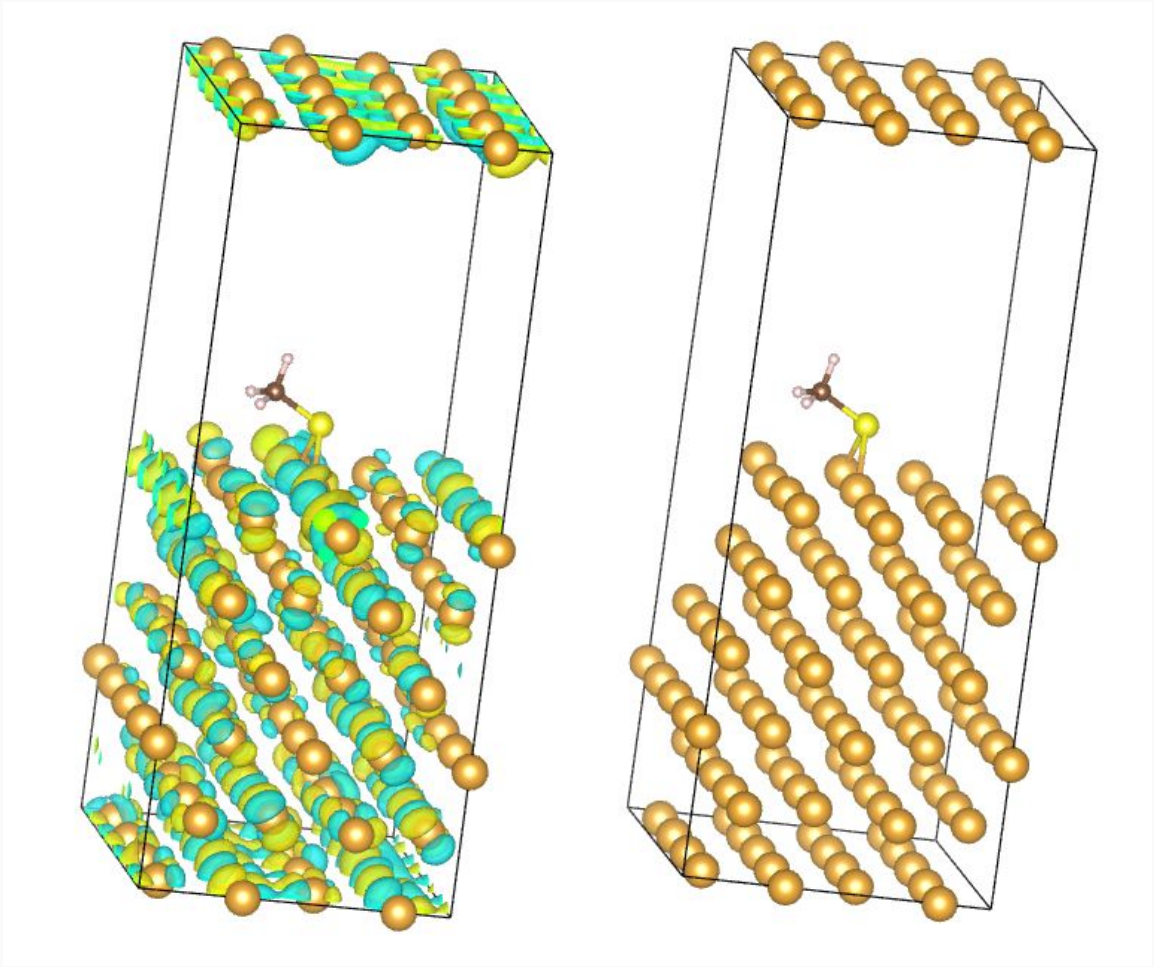
Output: electron density visualization



Input Data to Output Visualization

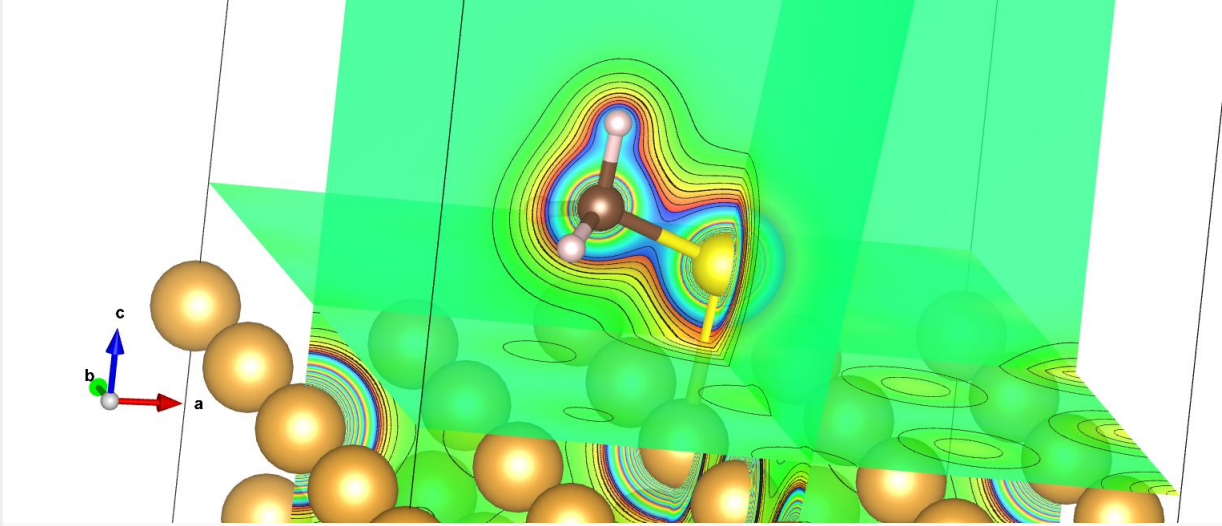
Unit Cells

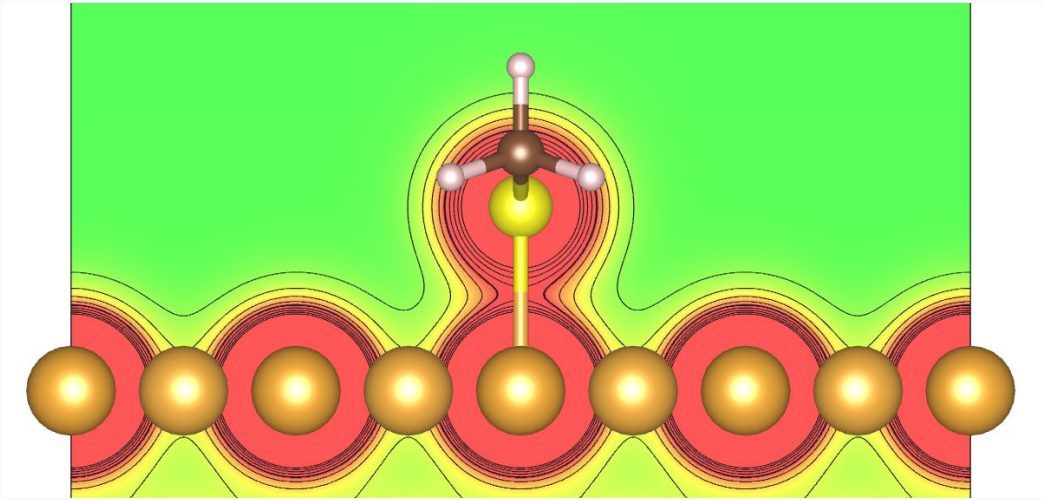
- VESTA: Bridge Right
- Isosurfaces → polarity
- Adsorbate Layer
- Periodic Gold Structure



Cross Sections

- Contours lines of the electron densities
- VESTA: Atop
  - 3 planes
  - 1 plane



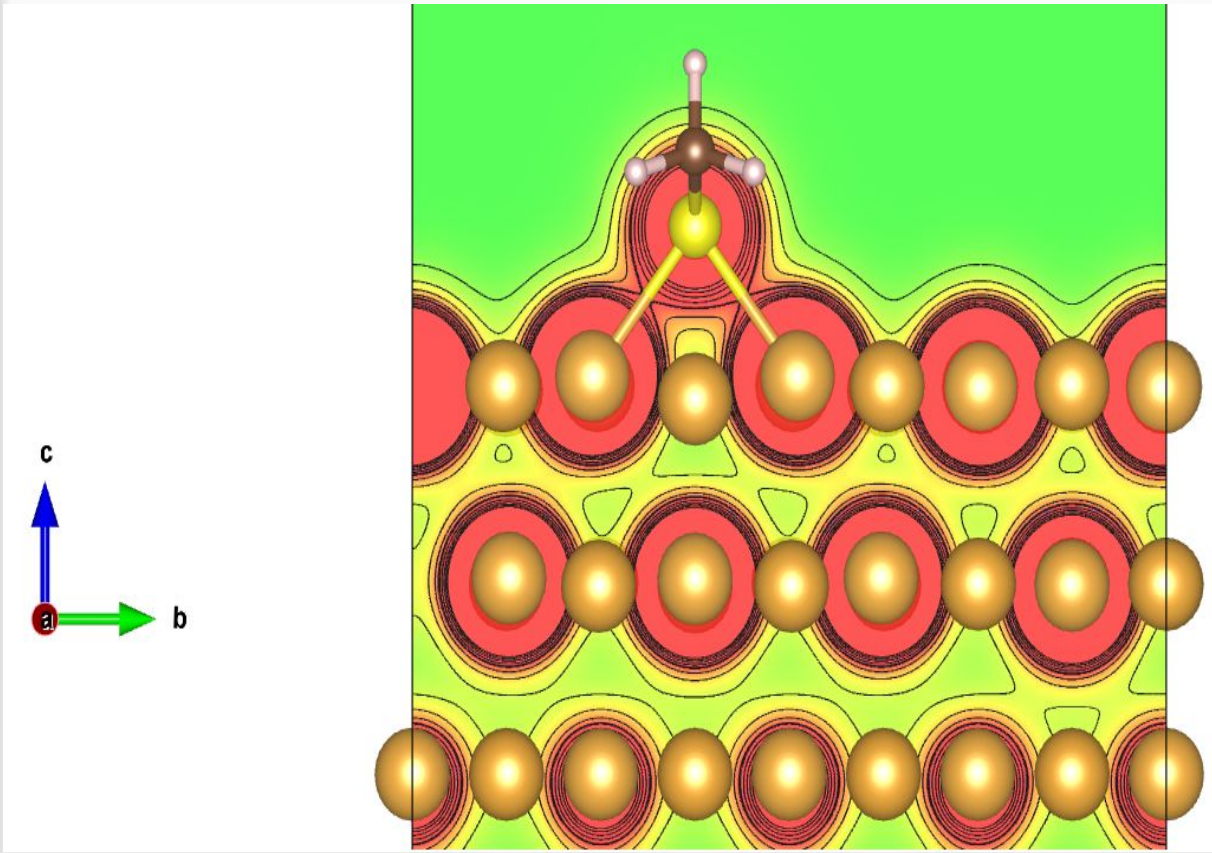


Observations

Initial plots → total charge densities

Study orbitals at different energy ranges where Au-S bonding is expected

Bridge Right



Charge Density Difference

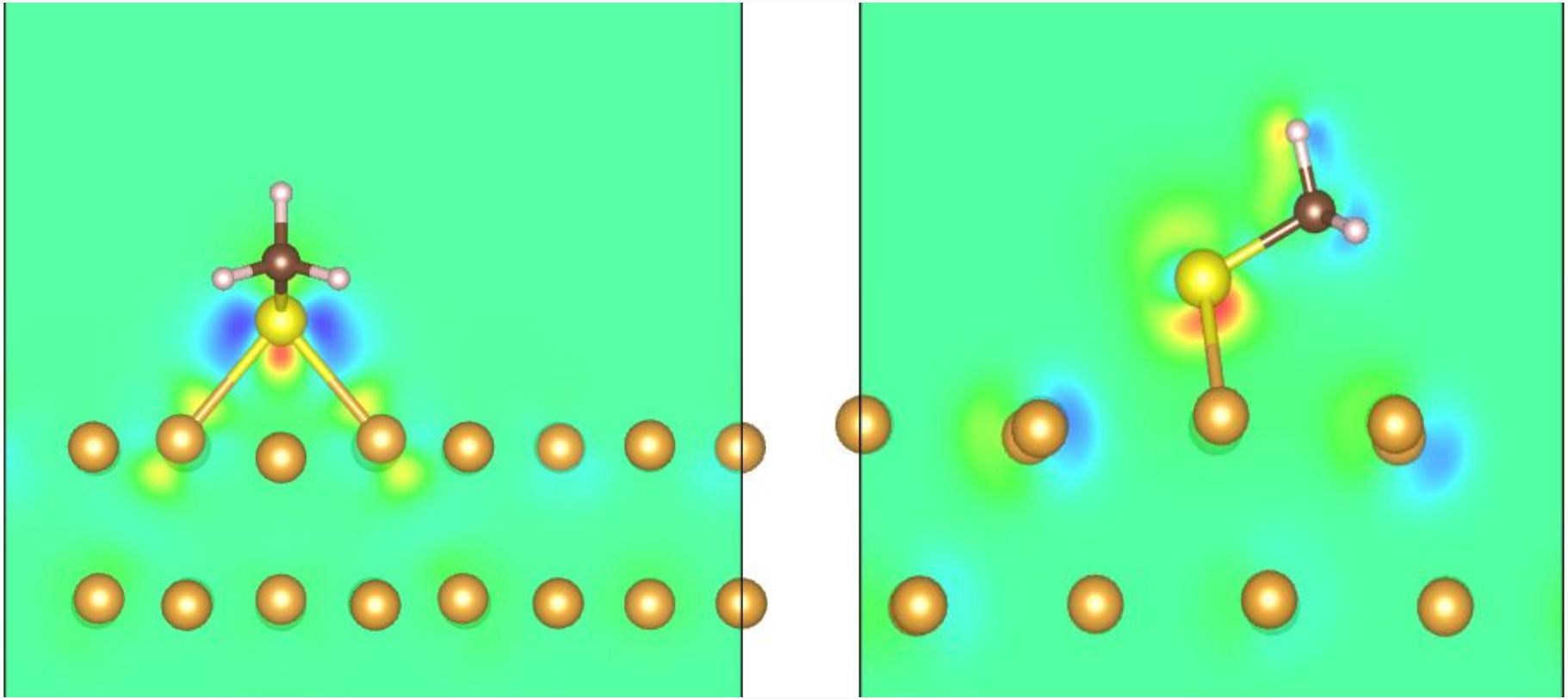
$$\Delta\rho = \rho_{AB} - \rho_{A} - \rho_{B}$$

AB → CH_3-S-Au(111)

A (Adsorbate) → CH_3-S

B (Substrate) → Au(111)

Charge Density Difference - Bridge Right



Conclusion and Future Work

- We learned how to use c2x and VESTA
- Plotted total charge densities
- Plotted charge density differences

Future work:

- Continue working with VESTA
- To plot more charge density differences → bands

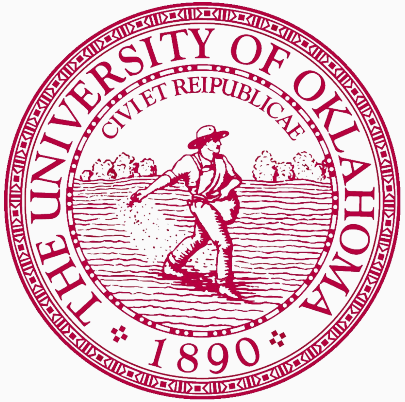
Acknowledgements

Thank you,

Dr. Bumm and his group,

Dr. Speyer and Dr. Ferry from Arizona State University,

Dr. Strauss and Dr. Abbott.



Questions?