**Introduction**

This summer my research focused on atomically dispersed metal catalysts on the surface of rutile TiO₂. I looked at combinations of nine transition metals (Au, Ag, Co, Cu, Ir, Ni, Pd, Pt, and Rh) across eighteen different adsorption sites (A1-A10, H1, H2, Ti5c, O₂w, O₅w, Ti6c, O₅w vacancy, and O₆w vacancy). We collected data on the different electronic and chemical properties of the binding sites (magnetic moment, atomic number of the metal, metal coordination number, adsorption site, charge, surface type, metal-dioxygen angle, and element group).

We investigated the potential relationships between the binding energy of each adsorption site and the remaining eight characteristics listed above using an unsupervised form of machine learning called K-means clustering with the hopes of developing trends that can be utilized to predict the proper catalyst combinations.

**Objective & Impact of Professor’s Research**

The Sharada Lab aims to use their research on atomically dispersed catalysts to create more effective catalysts in converting CO into CO₂ in order to reduce overall CO emissions in catalytic converters. In addition, atomically dispersed catalysts utilize smaller amounts of precious metals, therefore reducing the cost of the catalytic reactions and providing incentive for their use.

**Methods**

- Density Functional Theory to model geometries of adsorption sites
- Used the ASE package in Python to collect data and OVITO to visualize adsorption sites

**Results**

- Determined and removed any duplicate sites from data set
- Determined binding energy, coordination number, periodic group, and surface type for each combination of metal and site (lab partner, Chloe, and I did the calculations together)

\[
BE = E_{Pt/\text{TiO}_2} - E_{\text{TiO}_2} - E_{Pt}
\]

**Next Steps**

- Continue analyzing K-Means Clustering data to find relationships between different features
- Use VASP and HPC (high performance computing) to run geometry optimizations for adsorption sites with CO adsorbed on the metal atom
- Manipulated the feature data using Pandas library and imported into spreadsheets
- Analyzed the data using unsupervised machine learning approach: K-Means Clustering
  - Optimized cluster number using three statistical approaches: elbow method, silhouette score, and Calinski-Harabasz score
  - With optimized cluster numbers, used K-means method to cluster various combinations of features and graphed the data in the respective clusters

**Acknowledgements**

I would like to sincerely thank Professor Sharada for allowing me this incredible opportunity to participate in her lab. I would also like to thank my amazing PhD mentors Selin Bac and Nicholas Humphrey for all of their help and guidance throughout this research journey. I would like to thank Chloe Amadei for being a great lab mate. Finally, I want to thank my mentor mentor Dr. Bonaparte-Saller as well as Dr. Mills and the rest of the SHINE team for all their support.