Analyzing Features of Atomically Dispersed Catalysts at Various CO Adsorption Sites on a rutile TiO_2 Surface

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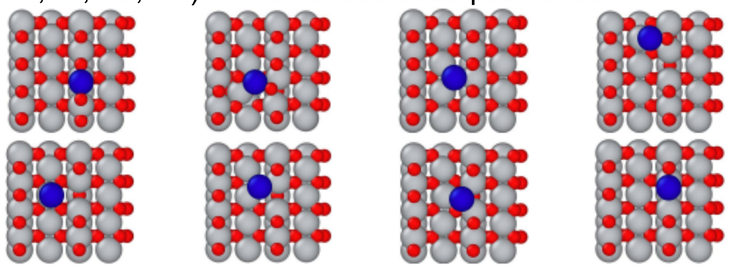
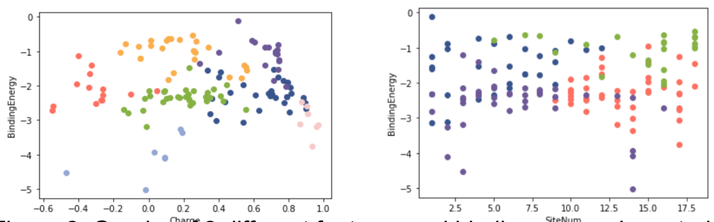
Introduction

The Sharada Lab places 9 different transition metals (Ag, Au, Co, Cu, Ir, Ni, Pt, Pd, Rh) on 18 various adsorption sites



(Figure 1: Pt Adsorption sites A1, A2, A3, A4, A5, A6, A7, A8 PC: Nicholas Humphrey, Selin Bac, and Shaama Mallikarjun Sharada)

on rutile TiO_2 Surface and analyzes their convergences to determine their efficiency in fuel catalysis reactions. I worked with both Selin Bac Bilgi and Nicholas Humphrey on refining the current data set and used machine learning to analyze the data's correlations. We were interested in the correlations between the BEs and other combinations of features as seen below.



(Figure 2: Graphs of 2 different features and binding energy I created to analyze for effect and correlation. PC: Chloé Andrieux-Amadeï)

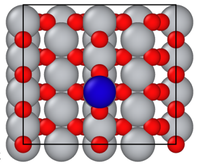
The features include Metal-Dioxo Angle, Coordination Number, Group, Atomic Number, Surface Type, Site, Magnetic Moment, and Charge.

Objective & Impact of Professor's Research

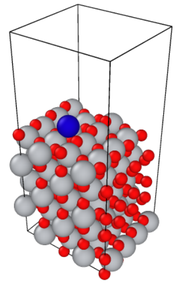
CO can be removed from the atmosphere by conversion into methane or into CO_2 and these reactions are not very efficient with their current use of Pt. Platinum is the leading metal used in catalysis reactions and it is pricey to use as the large quantity of metal inputted is mainly unused and lost in the reactions while creating many CO emissions. The Sharada Lab looks at making fuel catalysis more efficient by changing the type of metal used, decreasing the amount, maximizing the amount used in the reaction, and minimizing the CO emissions. They analyze 9 different single atom catalysts (Ag, Au, Co, Cu, Ir, Ni, Pt, Pd, Rh) on18 separate adsorption sites created by analyzing where the main metal moved to in the reactions.

Skills Learned

We began learning what each Pt adsorption site looked like, using OVITO to visualize the different sites throughout the metals and ensuring that every binding site shown was indeed a unique site to that metal.



(Figure 3: an image taken from OVITO of the Ti6c and Oba adsorption sites PC: Sophia Jones)



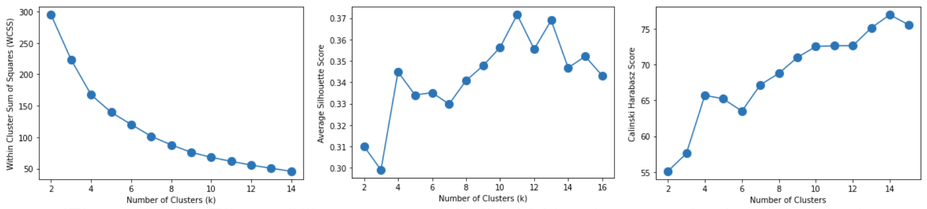
I used ASE and PANDAS in python to analyze the data to:

$$n_{O/Ti} = \sum_{j=1}^{N_{O/Ti}} S(|r_{O/Ti,j} - r_{Pt}|) \qquad S(r) = \frac{1}{\exp(\kappa(r - r_c)) + 1}$$

(Figure 4: The equations shown in the Sharada Lab's Publication that I worked at recreating in my python code. PC: Nicholas Humphrey, Selin Bac, and Shaama Mallikarjun Sharada)

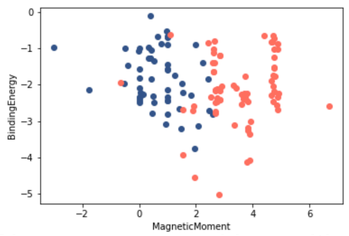
- produce coordination numbers (average distances with nearest titanium and nearest 2 oxygens)
- analyzing the surface as pristine or having an oxygen vacancy
- the platinum dioxo angle of the metal and the 2 nearest oxygens

I learned about machine learning and specifically k-means clustering, which uses an inputted number of cluster centers to group the data together in each for pairings that strongly affect each other.
Finding the optimal number of cluster centers (k) through:



(Figure 5: the Elbow, Silhouette, and Calinski-Harabasz methods respectively PC: Chloé Andrieux-Amadeï)

We graphed our work in accordance with binding energy and began analyzing if there were particular pairings that produced good clusters and therefore affected each other strongly and highly correlated.



(Figure 6: A graph yielded from the clusters of a grouping of 7 features, and graphed with the optimal number of clusters found previously. PC: Chloé Andrieux-Amadeï)

We are now working with HPC, DFT (Density Functional Theory), and geometry optimization to see what occurs on the cell when a CO is adsorbed onto the metal and submitted as a job. Those calculations will not converge in our SHINE time.

How This Relates to Your STEM Coursework

I'll be able to continue using the problem solving skills that I have learned in this course in future STEM courses and my new experience with research, learning patience when working with the unknown will lead me to be more understanding in future courses as I will have a different perspective on research I'll be learning about.

Next Steps and Advice for Future SHINE Students

My nexts steps involve passing on the work I did with geometry optimization using DFT and HPC so that the lab can submit those calculations and analyze the results produced. On the greater scale I will start looking at colleges through the lens of STEM and possibly STEM research to see where I could best further my experiences and education. My advice to further SHINE students would to be to go with the flow of your lab as the confusion in your work will disperse as you work more with your mentor and gain greater insight into their work.

Acknowledgements

I would like to thank Dr. Shaama Sharada for accepting me into her lab, Selin Bac Bilgi for mentoring me in python and data mining as well as Nicholas Humphrey for mentoring me in DFT and HPC. I would like to thank Sophia Jones for being an amazing lab mate and supporting me throughout this journey. I would like to thank Mary Bonaparte-Saller and Dr. Katie Mills for being strong mentors. I would like to also thank Julia Phillips, Tiffaney Hughes, and Austin Totty for writing me letters of recommendation and Simon Huss for sharing this program with me.