Features of Atomically Dispersed Metal Catalysts on TiO_2

Sophia Jones, sophiajones1492@gmail.com
Sharada Lab
Oakwood School, Class of 2023
USC Viterbi Department of Chemical Engineering, SHINE 2023

Introduction

My Research

This summer my research focused on atomically dispersed metal catalysts on the surface of rutile TiO_2. 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, O_{ba}, O_{br}, Ti6c, O_{ba} vacancy, and O_{br} vacancy).

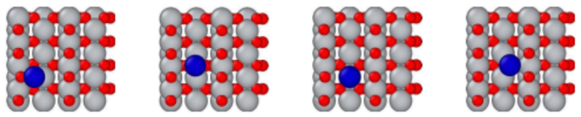

Figure 1: H1, H2, Ti5c, O_{ba} adsorption sites respectively from left to right. PC: Nicholas Humphrey [1]

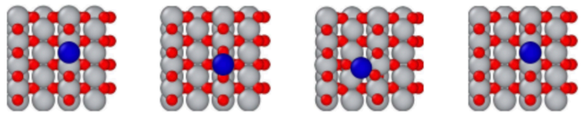

Figure 2: O_{br}, Ti6c, O_{ba} vacancy, O_{br} vacancy adsorption sites respectively from left to right. PC: Nicholas Humphrey [1]

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 CO_2 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

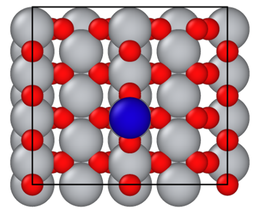

Figure 3: Pt adsorbed on Ti6c site visualized in OVITO. PC: Sophia Jones

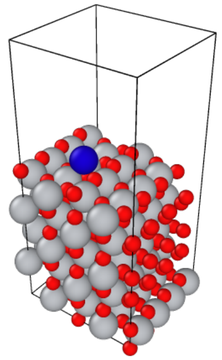

Figure 4: Pt adsorbed on O_{ba} site visualized in OVITO. PC: Sophia Jones

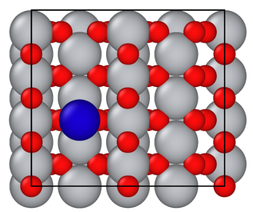

Figure 5: H2 adsorption site of Pt visualized in OVITO. PC: Sophia Jones

- 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)

$$BE = E_{Pt/TiO_x} - E_{TiO_x} - E_{Pt}$$

Figure 6: Formula to calculate binding energy. [2]

- 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

Results

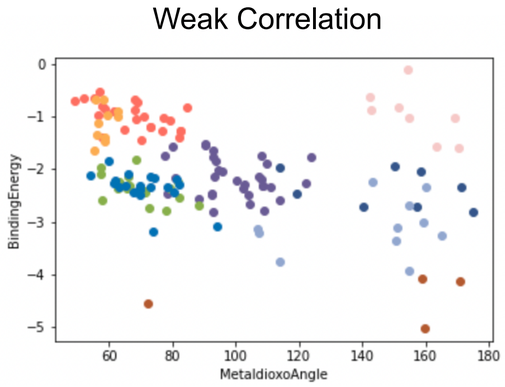

Figure 7: K-Means Clustered graph of binding energy, atomic number, and angle with eight clusters. PC: Sophia Jones

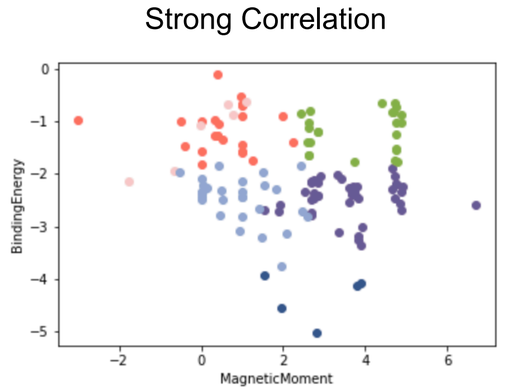

Figure 8: K-Means Clustered Graph of binding energy, magnetic moment, and surface type with six clusters. PC: Sophia Jones

How this Relates to Stem Coursework

My work with catalysis and density functional theory (DFT) will immensely benefit me in future Chemistry, Biology, and Physics courses both at the high school and collegiate level. In addition, my new exposure and experience in computer programming and data science will help me greatly in any future computer science courses or STEM professions.

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

Figure 9: Ti6c adsorption site with CO adsorbed on Co atom. PC: Sophia Jones

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 centor mentor Dr. Bonaparte-Saller as well as Dr. Mills and the rest of the SHINE team for all their support.

1. Humphrey, N., et al. (2020). J. Phys. Chem. C, 124(44), 24187-24195
2. Morgan, B. J.; Watson, G. W. A DFT+ U description of oxygen vacancies at the TiO2 rutile (1 1 0) surface. Surface Science 2007, 601, 5034–5041.