Exploring Characteristics of Adsorption Sites for Atomically Dispersed M_1/TiO_2 (M = Ag, Au, Co, Cu, Ir, Ni, Pd, Pt, Rh) Catalysts

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Introduction

Lab Overview

The Sharada lab works with dynamic and static computational methods to model a variety of atomically dispersed catalysts. This research utilizes quantum chemistry to visualize and collect data on heterogeneous catalysis on an atomic level.

Purpose of my lab work

I worked with my mentor Selin Bac Bilgi to visualize nine precious metals as atomically dispersed catalysts on rutile TiO_2 and look at different relationships between the viable binding sites found with each catalyst. We were interested in identifying possible relationships between binding energy and other characteristics of binding sites.

Objective & Impact of Professor's Research

Impact

The Sharada lab is hoping to use the knowledge they gain regarding catalysis to aid in purer hydrogen production for fuel purposes and help reduce CO emissions with the hope of more efficient catalytic converters.

Objective of research

- Using molecular dynamics methods to identify new binding sites for atomically dispersed metal catalysts on rutile TiO_2
- Discovering correlations between binding energy and other site dependent electronic and chemical properties

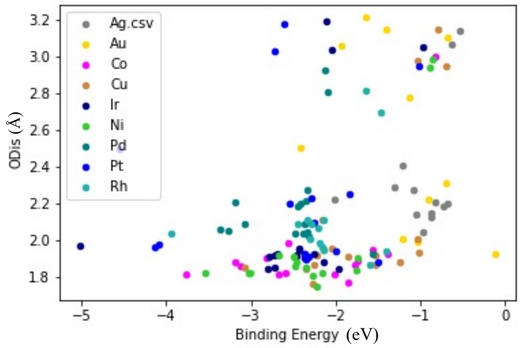


Figure 1 : Graph generated in python showing the relationship between binding energy and closest Oxygen distance to each catalyst PC: Justine Ludden

Methods/Skills Learned

- Static Density Functional Theory to visualize atomic structure and determine binding sites with two types of O and Ti atoms

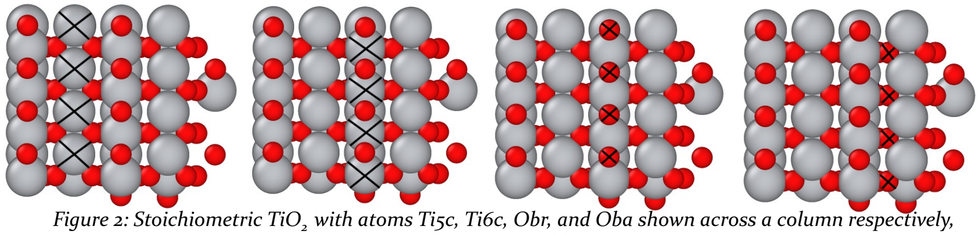


Figure 2: Stoichiometric TiO_2 with atoms Ti5c, Ti6c, Obr, and Oba shown across a column respectively, PC: Justine Ludden

- Platform's OVITO and ASE utilized to open these visualizations and determine any duplicates

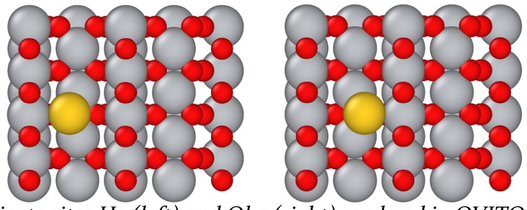


Figure 3: Duplicate sites H2 (left) and Oba (right) rendered in OVITO for catalyst Au, PC: Justine Ludden

- Collected closest neighboring Oxygen and Titanium distances from single atom catalyst using python and functions of ASE
- Calculated cutoff radius for coordination number using the average of the nearest-neighbor O and Ti distances for the six non-oxygen-vacancy sites for each precious metal catalyst

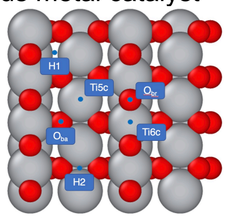


Figure 4 : The six non vacancy sites visualized on a single cell of TiO_2 PC: Selin Bac Bilgi [1]

$$n_{O/Ti} = \sum_{j=1}^{N_{O/Ti}} S(|r_{O/Ti,j} - r_{Pt}|)$$

$$S(r) = \frac{1}{\exp(\kappa(r - r_c)) + 1}$$

Figure 5: Equations used to calculate the O and Ti Coordination number for each site, PC: Selin Bac Bilgi [1]

- Calculated coordination numbers for Oxygen and Titanium
- Used binding energy, magnetic moment and Bader charge collected to graph with Pandas and matplotlib in python

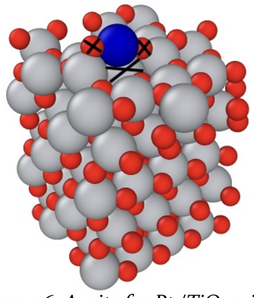


Figure 6: A1 site for Pt_1/TiO_2 with coordination points marked PC: Justine Ludden

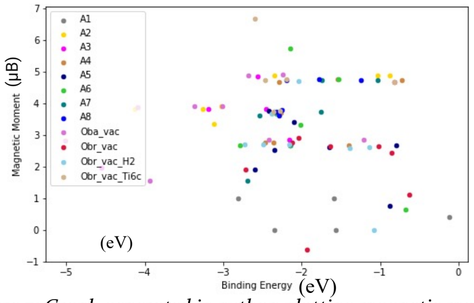


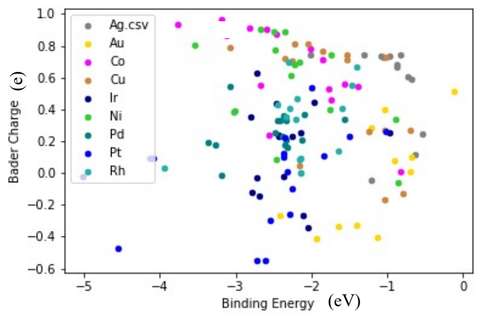
Figure 7: Graph generated in python plotting magnetic moment against binding energy and grouped by binding sites PC: Justine L.

How This Relates to Your STEM Coursework

The skills I have acquired while being able to work with the Sharada Lab are lessons that I will be able to carry with me through all my future STEM endeavors. Learning extensively about catalysis while working in the Sharada lab has prepared me deeply for future Chemistry and Biology courses. My ability to participate in group lab meetings has allowed me to become more comfortable asking questions. In addition, I participated in a Python basics course and a Python data analysis course, both of which increased my knowledge of Computer Science and will help me in my academic pursuits.

Next Steps and Results

- No immediate relationships discovered
- Continue to look for more correlations
- Study data with cluster analysis methods



Scan here to view my python scripts!

Figure 8: Graph generated in python plotting Bader charge against binding energy and grouped by catalyst, PC: Justine Ludden

- Planning to use machine learning methods to study data as well

Acknowledgements

I would like to sincerely thank Professor Sharada and the Sharada lab for allowing me to participate and learn about their work, I am so grateful! I would also like to thank my mentor Selin Bac Bilgi for her patience and for being such an amazing teacher. Lastly, thank you to my center mentor Aislinn Knight, Monica Lopez, and Dr. Mills for being so supportive and offering guidance over the last seven weeks.

1. Humphrey, N., et al. (2020). J. Phys. Chem. C, *124*(44), 24187-24195