Exploring Characteristics of Adsorption Sites for Atomically Dispersed Mₓ/TiO₂ (M = Ag, Au, Co, Cu, Ir, Ni, Pd, Pt, Rh) Catalysts

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Introduction

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 TiO₂ 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 TiO₂
- Discovering correlations between binding energy and other site dependent electronic and chemical properties
- Static Density Functional Theory to visualize atomic structure and determine binding sites with two types of O and Ti atoms
- Platform’s OVITO and ASE utilized to open these visualizations and determine any duplicates
- 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

Methods/Skills Learned

- Static Density Functional Theory to visualize atomic structure and determine binding sites with two types of O and Ti atoms
- Platform’s OVITO and ASE utilized to open these visualizations and determine any duplicates
- Collected closest neighboring Oxygen and Titanium distances from single atom catalyst using python and functions of ASE
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Figure 2: Stoichiometric TiO₂, with atoms T1_, T1c, Obr, and Oba shown across a column respectively.

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

Figure 4: The six non vacancy sites visualized on a single cell of TiO₂, PC: Selin Bac Bilgi [1]

Figure 5: Equations used to calculate the coordination numbers for Oxygen and Titanium

Figure 6: As site for Pt/TiO₂, 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 Ludden

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Next Steps and Results

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

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.

Study data with cluster analysis methods

Planning to use machine learning methods to study data as well

References