Understanding Coking in Propane Conversion

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BACKGROUND

- In hydrocarbon conversion reactions such as cracking or reforming, there is often carbon residue left on the surface of a catalyst. This process is known as coking.
- The problem with coking is that these carbon deposits can lower the activity of the catalyst by blocking active sites.
- The catalysts utilized in our calculations is pure platinum as it strong in breaking hydrocarbon bonds.
- Our project is centered around DFT which is a theory centered around molecular interactions.
- Through software tools utilizing the principles of DFT, these molecular interactions can be studied.

GOAL

Understanding how **coke** forms and grows to design better **catalysts** that last longer and work better in the near future.

OBJECTIVE

- Computational Framework Setup: Utilize Linux to conduct the appropriate DFT calculations.
- Validation and Optimization: Validate computational results against experimental data and optimize simulation parameters for improved accuracy.

METHODS

Utilizing Computer Simulations we will study the formation of carbon on the surface of a catalyst through the usage of DFT.

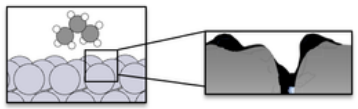
Bulk Calculations:

Calculates the energy produced by an element in its standard form, or as a whole not divided into sections.

Surface Slab Calculations:

Using an accurate lattice constant provided by the bulk calculation, the binding energy can be calculated by splitting the element into sections

Coking On A Molecular Level



[1] Figure 1. Carbon Atoms Blocking The Active Site on the Catalyst.

PROJECT RESULTS

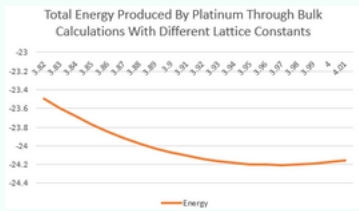


Figure 2. Lattice Constant Convergence

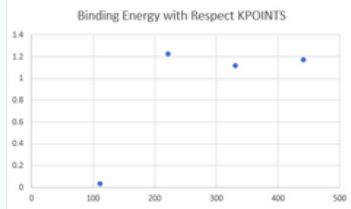


Figure 3. KPOINTS Parameter Convergence

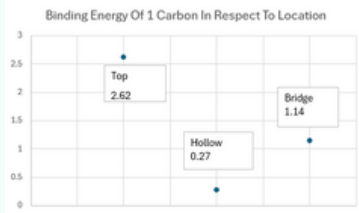


Figure 4. 2 Carbon Atoms Test

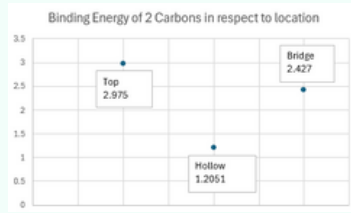


Figure 5. 3 Carbon Atoms Test

According to the surface slab calculations, the most optimal site would be the hollow since it provided the lowest binding energy

Conclusion

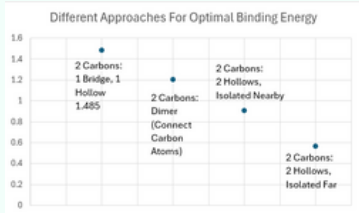


Figure 6. Different Approaches

- The presence of the hollows on the catalyst lowered the binding energy.
- The dimer would be the least favorable choice since it had the highest binding energy
- The 2 isolated carbon further apart from each other would be the most favorable choice for binding energy.

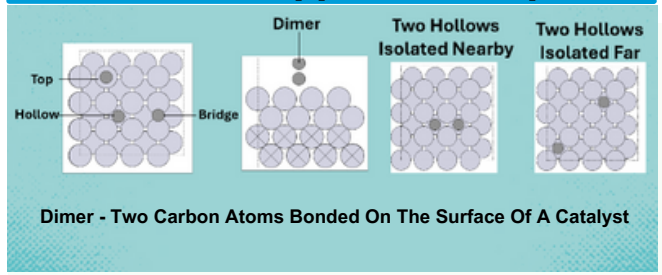
Key Terms:

Lattice Constant - A parameter used in DFT calculations which defines the (size of the) crystal structure of a simple cubic metal.

Binding Energy - The amount of energy needed to break particle(s) apart.

ENERGY FOR OUR GROWING WORLD

Most Common Approaches Explained



Dimer - Two Carbon Atoms Bonded On The Surface Of A Catalyst

IMPACTS & FUTURE

Impacts:
- Increased productivity for catalysts
- Less strain on nuclear reactors
- Less energy consumption

Future:
- Adopt sustainable practices to reduce environmental impact
- Shift toward cleaner propane conversion
- Potentially using platinum alloys

PERSONAL PROGRAM EXPERIENCE

- Gained insight on graduate school
- Developed relationships among peers and mentors
- Met with speakers in both industry and graduate school to gain a general idea on what to pursue post undergrad
- Networked with likeminded individuals
- Given a true perspective on the routine of a graduate student
- Participated in seminars that helped prepare me for the future

ACKNOWLEDGEMENTS

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- Yu-Hsiang Cheng and Ravion Hyatt for helping out during the labs, and being a pillar of support throughout the project.
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References

- [1] Cheng, Y.-H., & Greeley, P. J. (2023). PhD Qualifying Examination-Report First Principles Analysis of Coke Formation on Pt-based Catalysts for Propane Dehydrogenation.

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