Computational Catalysis with Density Functional Theory

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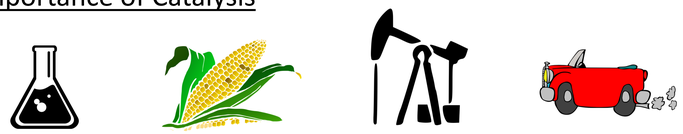
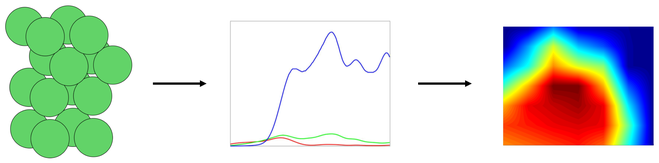
Background & Motivation

Importance of Catalysis



- 90% of all chemical and fuel production[1]
- 30% of U.S. Gross National Income[1,2]
- $4.5 trillion/year in U.S. products[2]
- $1 spent is $1000 earned[2]

Studying Catalysis with Computational Methods



- Ideal catalysts are highly active, selective, and stable
- Predictions from computation drastically reduce the number of possibilities that must be tried experimentally
- Even with computation, the sample space is too large to examine by brute-force methods
- Using descriptors allows us to screen new catalyst candidates efficiently

Problem Statement

Computational methods currently used to study catalysis require specialized software packages and high-performance computing resources, making them less accessible for students and beginning researchers.

Objectives

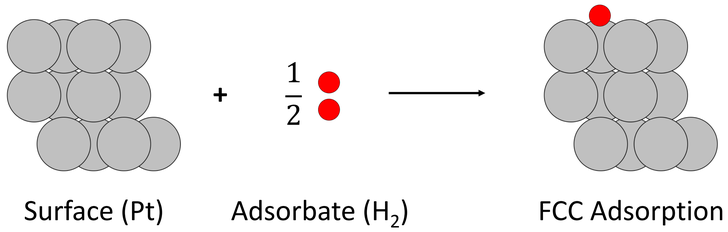
1. Create a tool on nanoHUB that can calculate properties of interest to catalysis.
2. Make the tool versatile for use in both research and education.

Methods & Approach

Generating Structures

Density Functional Theory

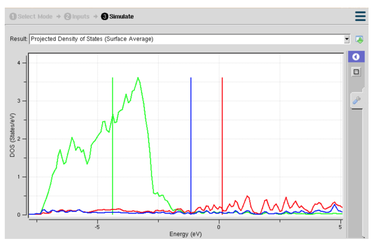
Calculating Adsorption Energy



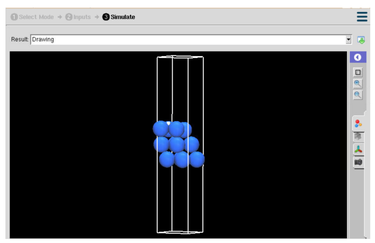
$$\Delta E_H = E_{surf+H} - E_{surf} - \frac{1}{2}E_{H_2}$$

Results & Analysis

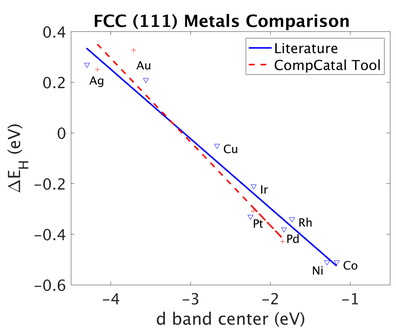
Projected Density of States



Structure Viewer



Calculating Catalytic Properties



- *d* band center is important for predicting catalytic properties
- Results from nanoHUB tool match closely with literature values[3,4]

Results & Analysis (cont.)

Usability in Education and Research

Basic Inputs (Education):
- Surface
- Adsorbate
- Adsorbate position
- Distance from surface
- Energy of surface
- Energy of adsorbate

Advanced Inputs (Research):
- All basic inputs
- Lattice parameter
- Miller indices
- Supercell dimensions
- Number of layers
- Vacuum thickness

Conclusions

- Tool is able to calculate adsorption energy and *d* band center with comparable accuracy to literature values
- Basic and Advanced modes of operation enable use of the tool in both research and educational settings
- Tool removes the barriers to studying catalysis (specialized software and high-performance computing resources no longer required)

Try out the tool for yourself!
https://nanohub.org/tools/compcatal

Future Work

- Perform additional benchmarking to test accuracy with other adsorbates and metals
- Access Rappture tool through Jupyter notebook for improved visualization capabilities

References

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4. Ruban, A.; Hammer, B.; Stoltze, P.; Skriver, H. .; Nørskov, J. . Surface Electronic Structure and Reactivity of Transition and Noble Metals. *J. Mol. Catal. A Chem.* 1997, *115* (3), 421–429.

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