

Fischer-Tropsch Synthesis

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The logo for LA-SIGMA features a stylized central element consisting of a black diamond shape with three colored triangles (blue, orange, and green) pointing upwards from its top vertex.

LA-SIGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Outlook

- Introduction
- Methodology
- Results
- Future Plans
- Educational Application

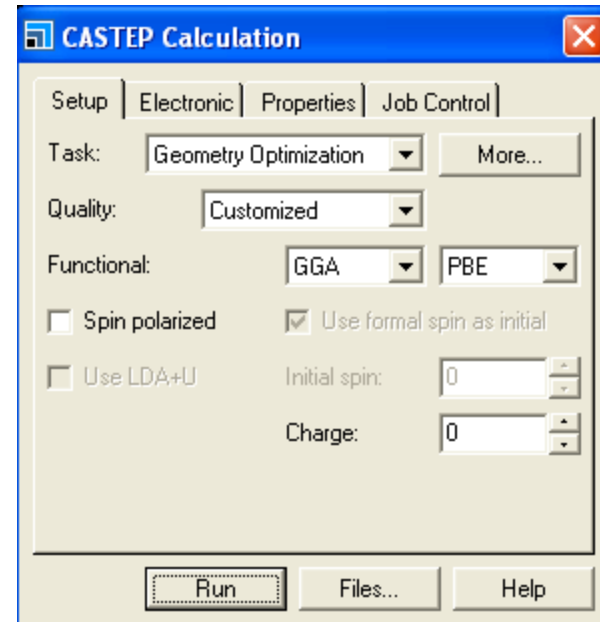
Introduction

- What is Fischer-Tropsch Synthesis?
 - Collection of chemical reactions that converts a mixture of carbon monoxide and hydrogen into liquid hydrocarbons to produce synthetic fuels
 - First produced in the 1920s
 - Used by Germans during WWII



Methodology

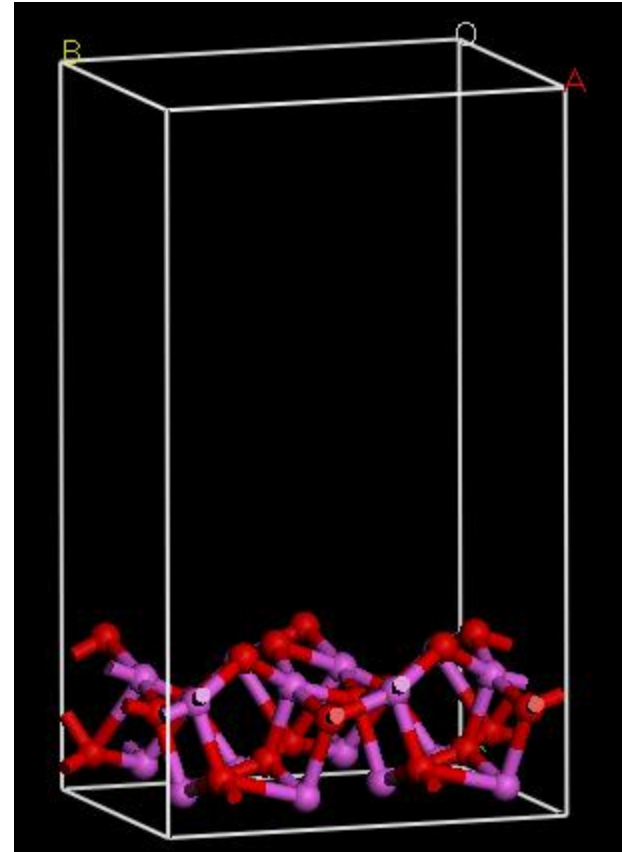
- Material Studio®
 - CASTEP
 - GGA/PBE
 - Geometry Optimizations
 - Medium Quality
 - Gamma k-point



Results

- Al_2O_3
- Imported from Material Studio®
- Lattice Parameters:
 - $a = 6.996373 \text{ \AA}$
 - $b = 10.256929 \text{ \AA}$
 - $c = 18.302746 \text{ \AA}$
- Number of atoms:
 - 35 atoms
- Final Energy:
 - -8793.25 eV

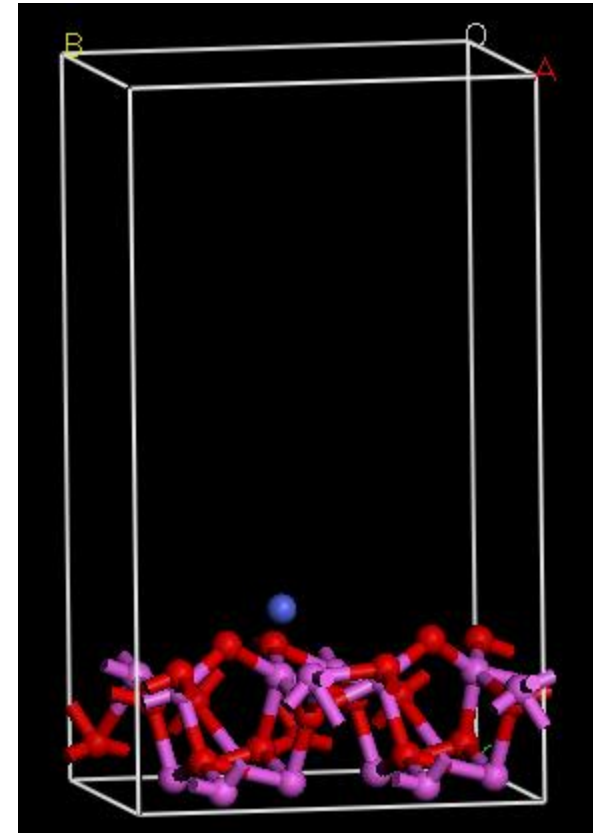
1 1 0 Surface



Addition of Cobalt

- Cobalt atom added near the surface of alumina above an oxygen atom
- Final Energy:
 - -9833.51 eV

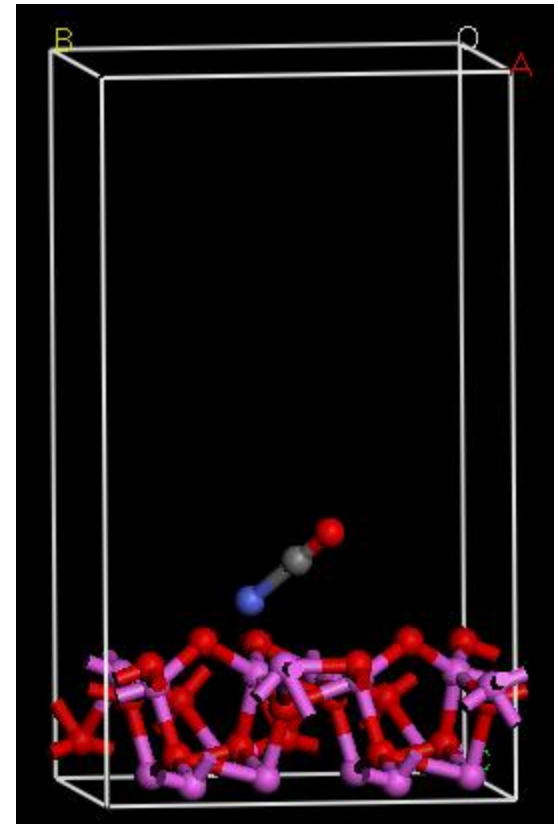
1 1 0 Surface



Addition of Carbon Monoxide

- Carbon monoxide added near cobalt atom
- Final Energy:
 - -10426.68 eV

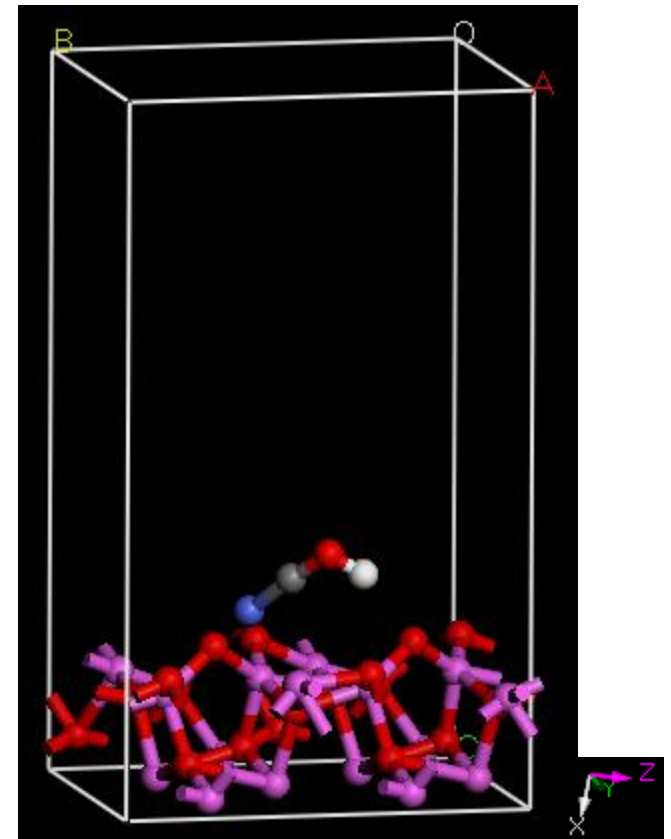
1 1 0 Surface



Addition of Hydrogen

- Hydrogen atom added to oxygen
- Final Energy:
 - -10441.07 eV

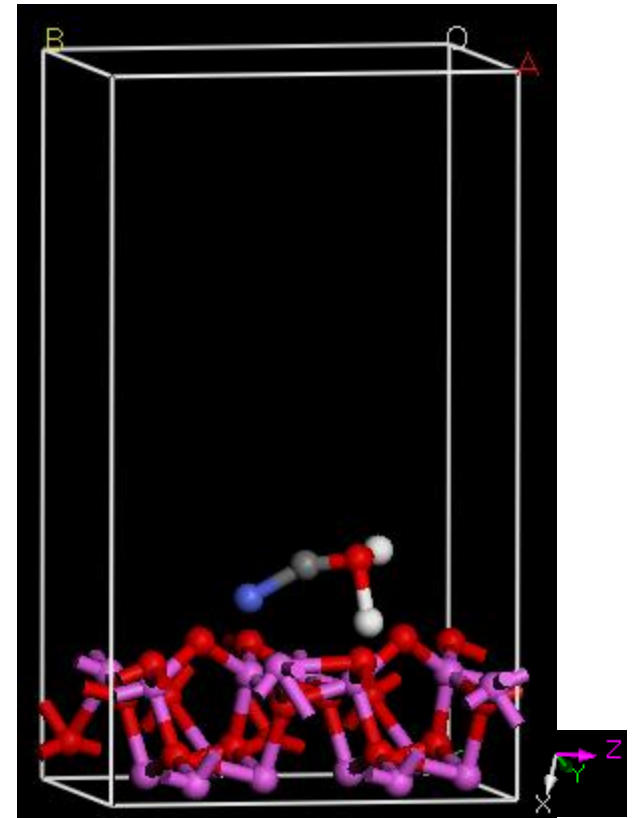
1 1 0 Surface



Addition of Hydrogen

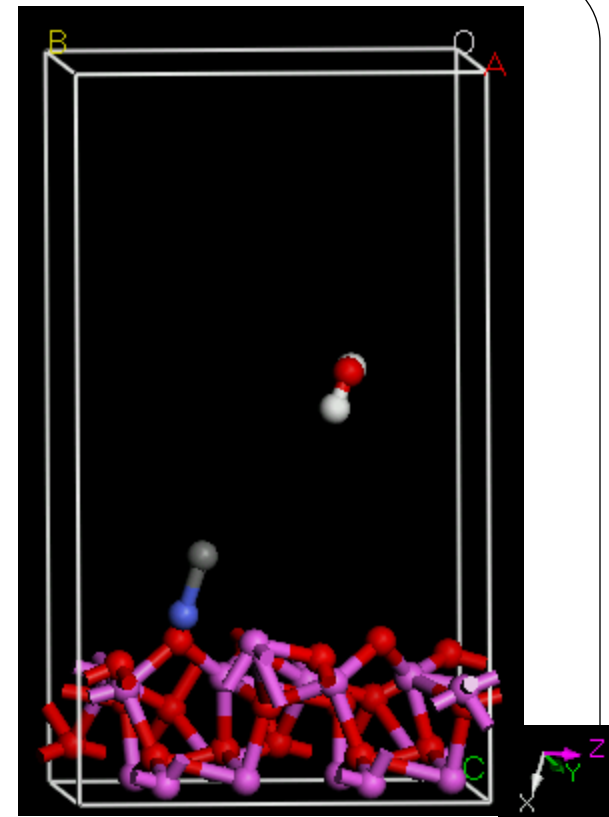
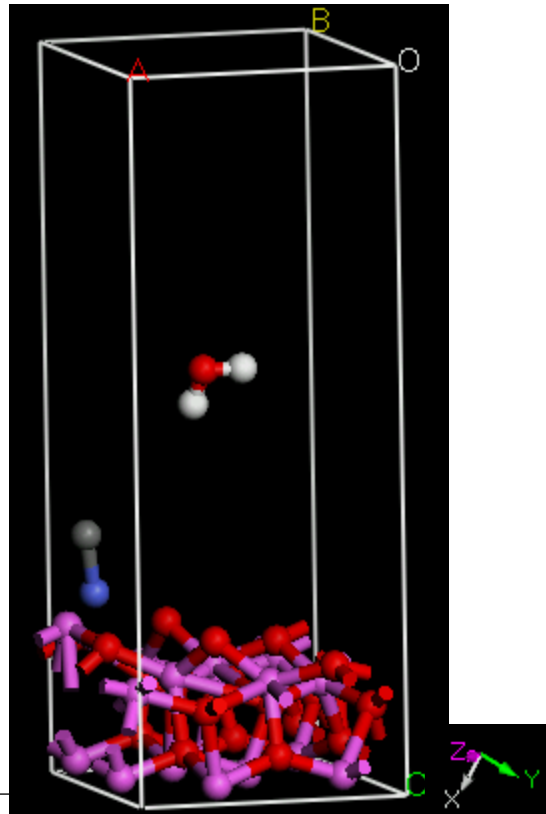
- Second hydrogen atom added
- Final Energy:
 - -10455.42 eV

1 1 0 Surface



Removal of Water

- Water molecule separated from carbon.
- Final energy:
 - -10456.17 eV



1 1 0 Surface

Calculations (Single Cobalt Surface)

Binding Energy of Co to Al₂O₃

$$\begin{aligned} &= E(\text{surface} + \text{Co}) - [E(\text{surface}) + E(\text{Co})] \\ &= -5.25 \text{ eV} = -121.01 \text{ kcal/mol} \end{aligned}$$

Binding Energy of CO to Co

$$\begin{aligned} &= E(\text{surface} + \text{Co} + \text{CO}) - [E(\text{surface} + \text{Co}) + E(\text{CO})] \\ &= -4.09 \text{ eV} = -94.32 \text{ kcal/mol} \end{aligned}$$

Binding Energy of H to O

$$\begin{aligned} &= E(\text{surface} + \text{Co} + \text{CO} + \text{H}) - [E(\text{surface} + \text{Co} + \text{CO}) + E(\text{H})] \\ &= -2.18 \text{ eV} = -50.27 \text{ kcal/mol} \end{aligned}$$

Calculations (Single Cobalt Surface) Continued

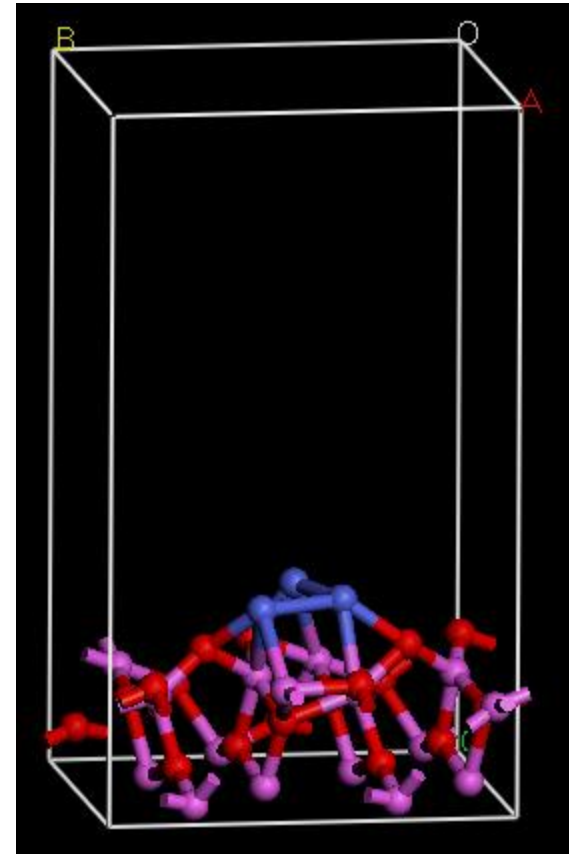
Binding Energy of second H to O

$$\begin{aligned} &= E(\text{surface} + \text{Co} + \text{CO} + \text{H}_2) - [E(\text{surface} + \text{Co} + \text{CO} + \text{H}) + E(\text{H})] \\ &= -2.14 \text{ eV} = -49.35 \text{ kcal/mol} \end{aligned}$$

Addition of Cobalt

- Three cobalt atoms added near the surface of alumina above an oxygen atom
- Final Energy:
 - -11914.33 eV

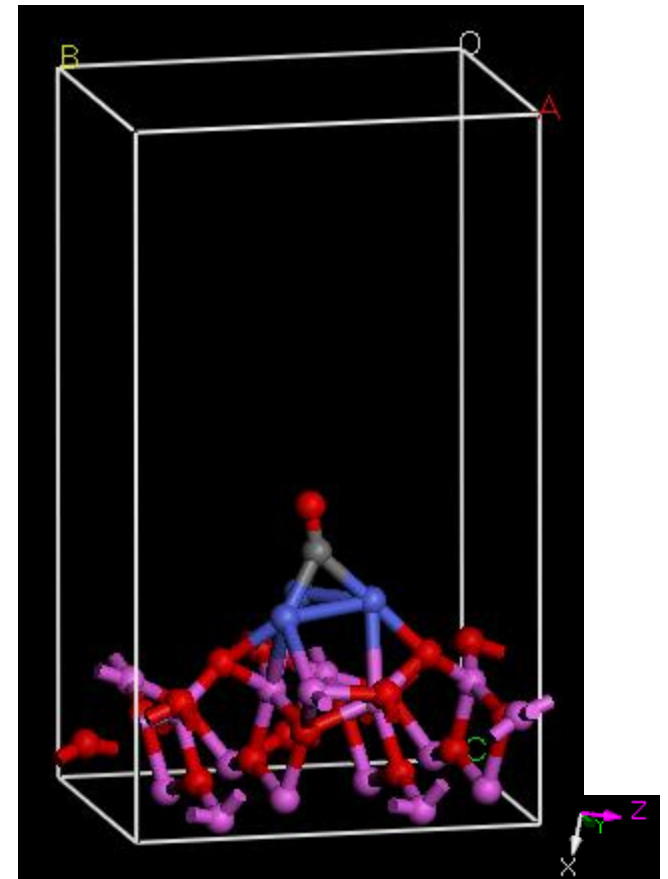
1 1 0 Surface



Addition of Carbon Monoxide

- Carbon monoxide added near cobalt atom
- Final Energy:
 - -12507.40 eV

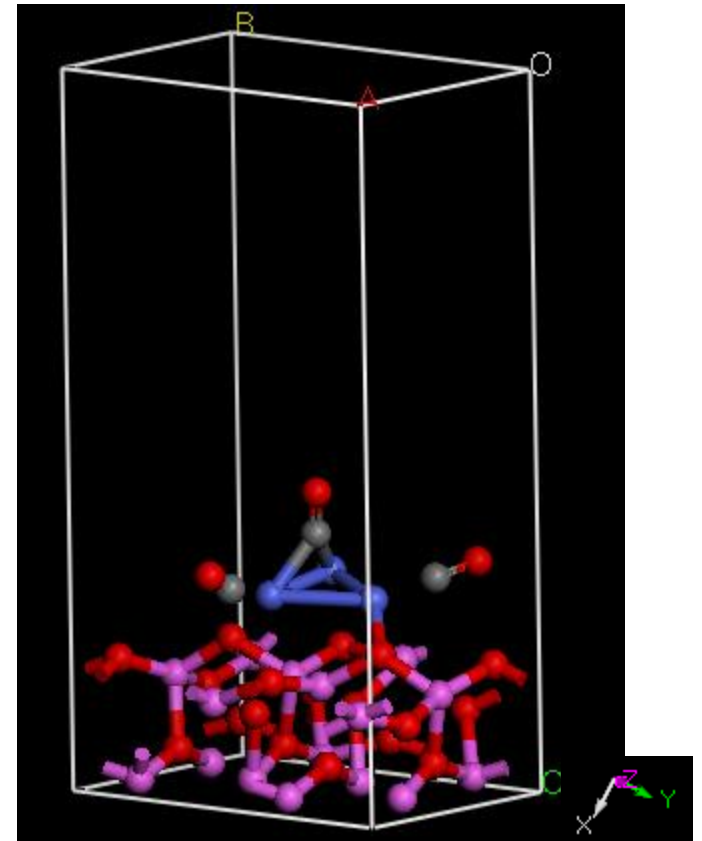
1 1 0 Surface



Addition of Second & Third Carbon Monoxide

- Carbon monoxide added near cobalt atom
- Final Energy:
 - -13692.41

1 1 0 Surface



Calculations (Three Cobalt Surface)

Binding Energy of Co to Al₂O₃

$$\begin{aligned} &= E(\text{surface} + \text{Co}) - [E(\text{surface}) + E(\text{Co})] \\ &= -5.25 \text{ eV} = -121.01 \text{ kcal/mol} \end{aligned}$$

Binding Energy of second Co to Al₂O₃

$$\begin{aligned} &= E(\text{surface} + \text{Co}_2) - [E(\text{surface} + \text{Co}) + E(\text{Co})] \\ &= -5.55 \text{ eV} = -127.98 \text{ kcal/mol} \end{aligned}$$

Binding Energy of third Co to Al₂O₃

$$\begin{aligned} &= E(\text{surface} + \text{Co}_3) - [E(\text{surface} + \text{Co}_2) + E(\text{Co})] \\ &= -5.25 = -121.01 \text{ kcal/mol} \end{aligned}$$

Calculations (Three Cobalt Surface) continued

Binding Energy of CO to Co

$$\begin{aligned} &= E(\text{surface} + \text{Co}_3 + \text{CO}) - [E(\text{surface} + \text{Co}_3) + E(\text{CO})] \\ &= -3.99 \text{ eV} = -92.01 \text{ kcal/mol} \end{aligned}$$

Binding Energy of second & third CO to Co

$$\begin{aligned} &= E(\text{surface} + \text{Co}_3 + 3\text{CO}) - [E(\text{surface} + \text{Co}_3 + \text{CO}) + \\ &E(2\text{CO})] \\ &= -6.85 \text{ eV} = -157.96 \text{ kcal/mol} \end{aligned}$$

Conclusions

- 1 1 0 surface is manageable for FT synthesis
- Binding energies are within an acceptable range

Future Plans

- Continue computational studies on Fischer-Tropsch
- Determine most effective catalysts for reactions

Educational Application

- Microbial Fuel Cell Kit
 - Investigate cellular respiration
 - Explore an alternative fuel source
 - See microbes in a new light



Prices:

- Kit: \$260.00
- Refill: \$27.95

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Educational Application continued...

- Bio-Energy Kit
 - Demonstrates how energy can be created from ethanol without combustion—and works, nonstop, for hours



Prices:

Kit: \$99.99



Educational Application continued...

- Preparation and Properties of Biodiesel Fuel - Student Laboratory Kit
 - The biodiesel fuel methyl stearate is prepared by mixing cooking oil with methyl alcohol and sodium hydroxide.
 - Students use common separation techniques to isolate the biodiesel fuel and then determine the fuel's heat of combustion using calorimeter.



Prices:

Kit: \$30.10



THANK YOU!!!



Dr. Ramu

Dr. Wick

Fernando Soto

Dr. Ayo Hassan

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