Fischer-Tropsch Synthesis

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LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Outlook

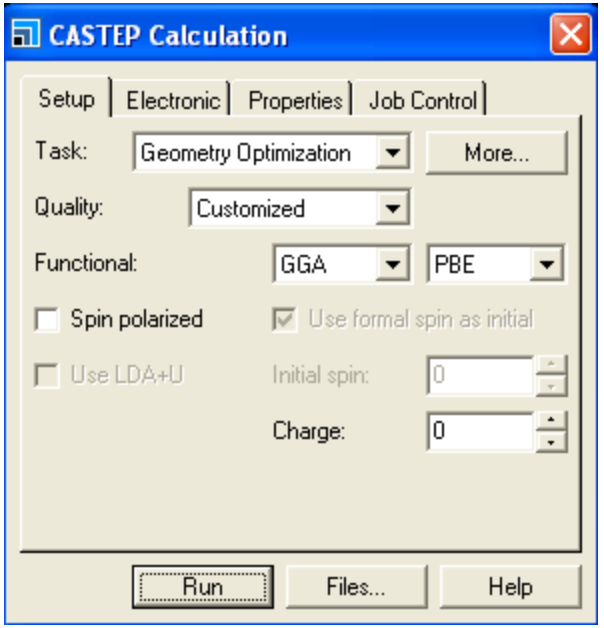
- Introduction
- Methodology
- Results
- Future Plans
- Educational Application

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

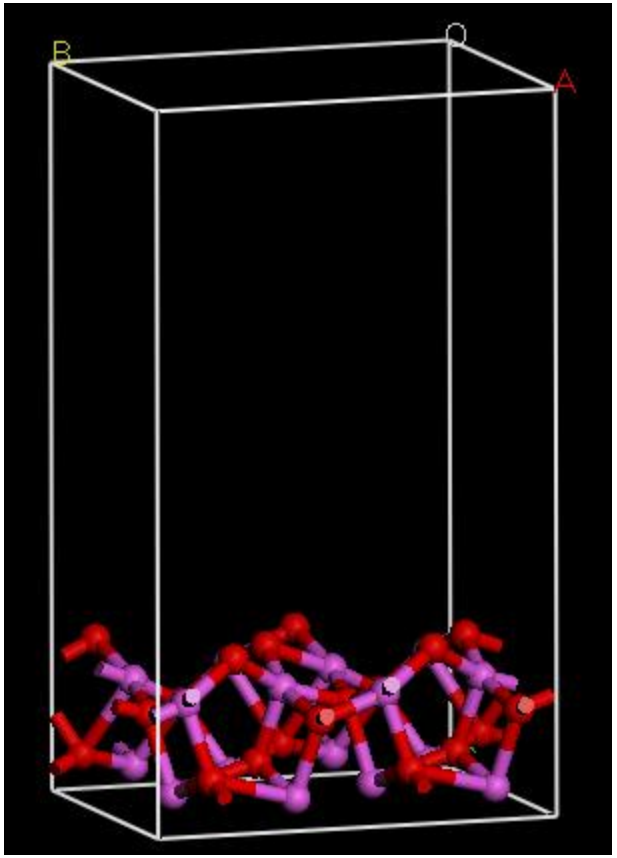
- Material Studio®
  - CASTEP
    - GGA/PBE
    - Geometry Optimizations
      - Medium Quality
      - Gamma k-point



Results

- Al_2O_3
- Imported from Material Studio®
- Lattice Parameters:
  - a= 6.996373 Å
  - b= 10.256929 Å
  - c= 18.302746 Å
- Number of atoms:
  - 35 atoms
- Final Energy:
  - -8793.25 eV

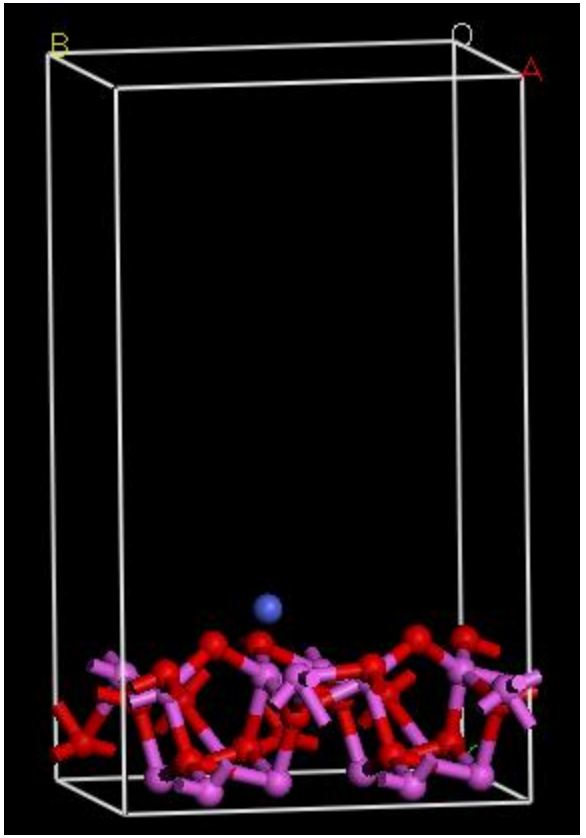
1 1 0 Surface



Addition of Cobalt

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

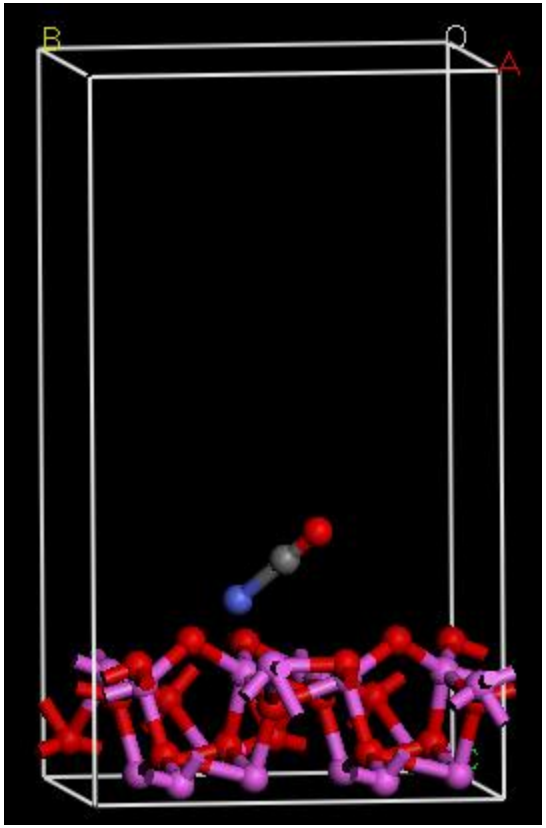
1 1 0 Surface



Addition of Carbon Monoxide

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

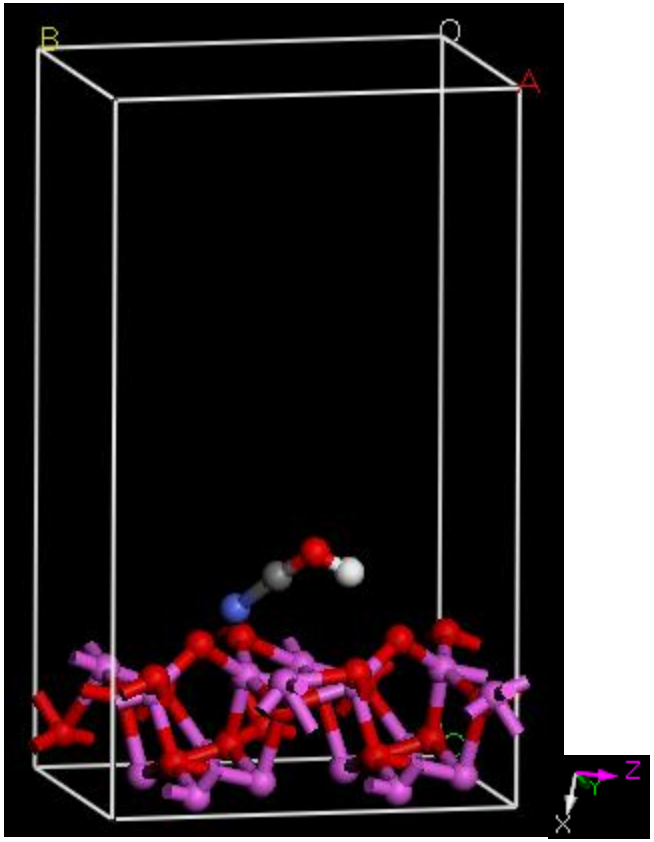
1 1 0 Surface



Addition of Hydrogen

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

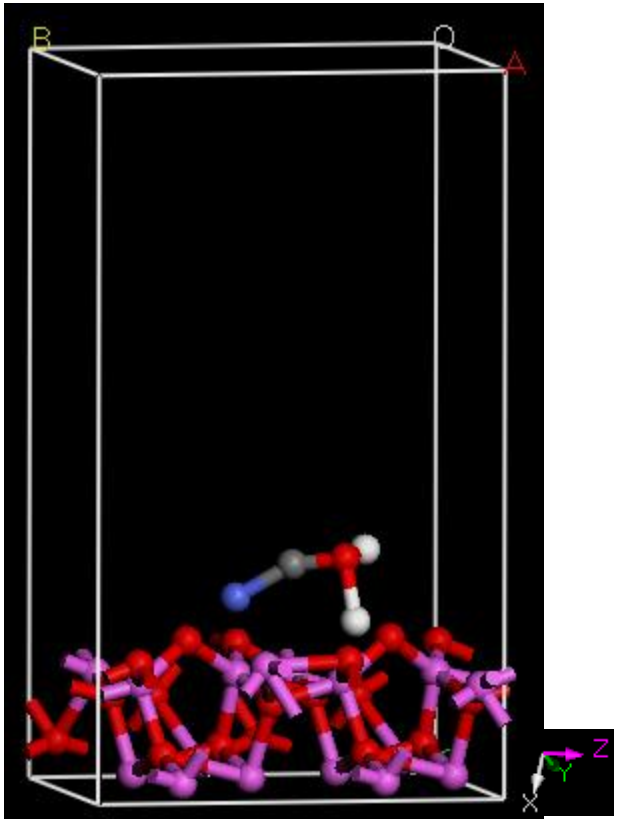
1 1 0 Surface



Addition of Hydrogen

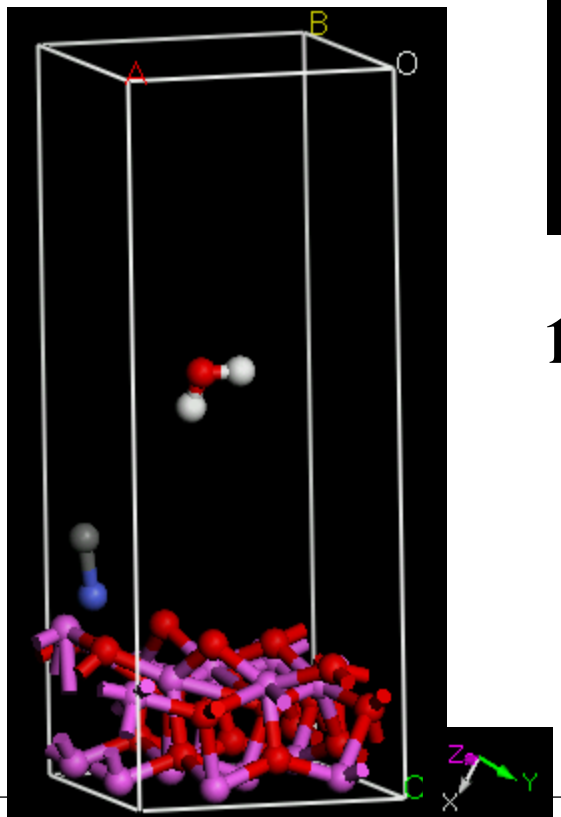
- Second hydrogen atom added
- Final Energy:
  - -10455.42 eV

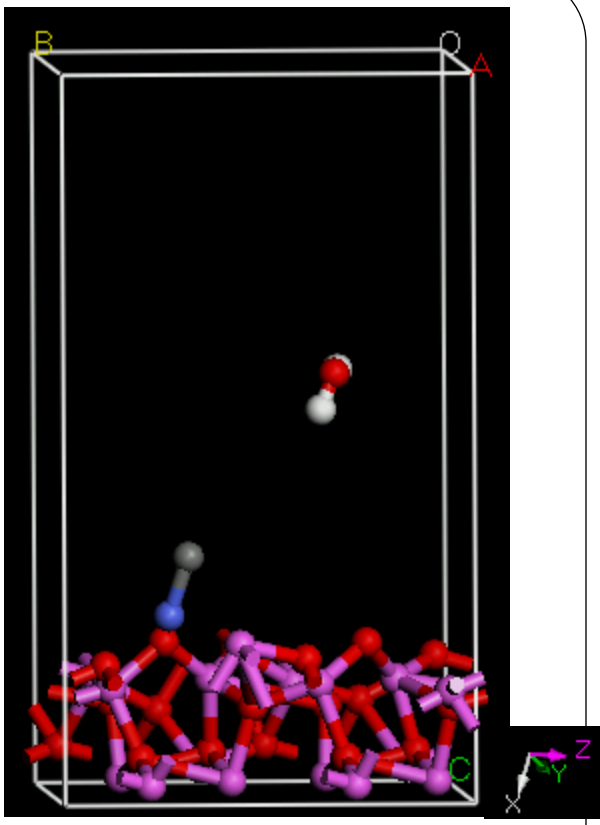
1 1 0 Surface



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 Al_2O_3

= E(surface + Co) – [E(surface) + E(Co)]

= -5.25 eV = -121.01 kcal/mol

Binding Energy of CO to Co

= E(surface + Co + CO) – [E(surface + Co) + E(CO)]

= -4.09 eV = -94.32 kcal/mol

Binding Energy of H to O

= E(surface + Co + CO + H) – [E(surface + Co +CO) + E(H)]

= -2.18 eV = -50.27 kcal/mol

Calculations (Single Cobalt Surface) Continued

Binding Energy of second H to O

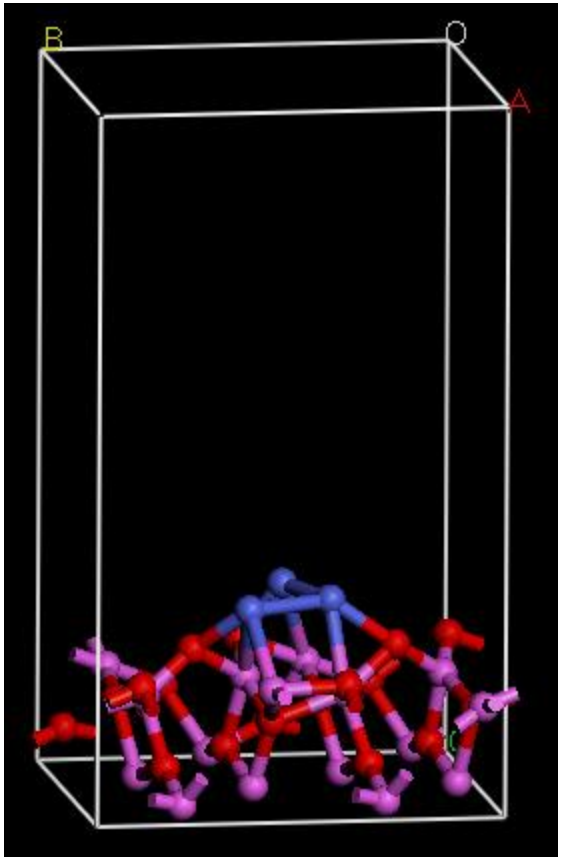
$= E(\text{surface} + Co + CO + H_2) - [E(\text{surface} + Co + CO + H) + E(H)]$

$= -2.14\ eV = -49.35\ kcal/mol$

Addition of Cobalt

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

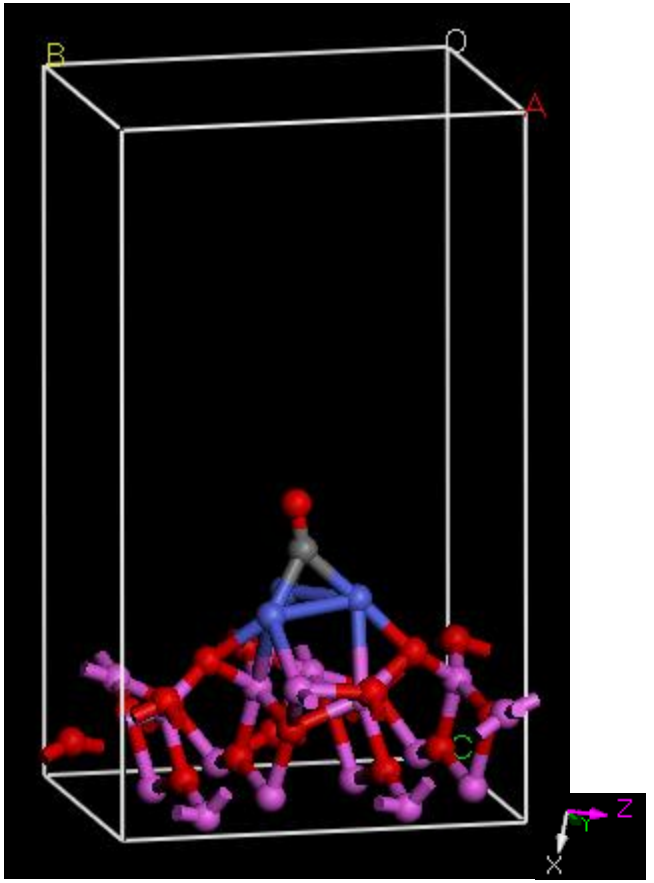
1 1 0 Surface



Addition of Carbon Monoxide

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

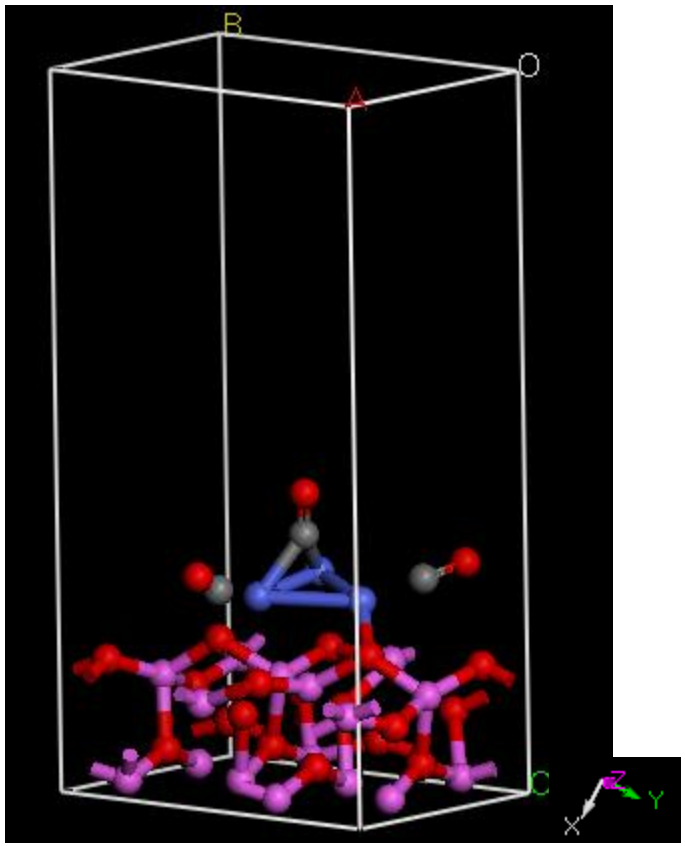
1 1 0 Surface



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 Al_2O_3

$= E(surface + Co) - [E(surface) + E(Co)]$

= -5.25 eV = -121.01 kcal/mol

Binding Energy of second Co to Al_2O_3

$= E(surface + Co_2) - [E(surface + Co) + E(Co)]$

= -5.55 eV = -127.98 kcal/mol

Binding Energy of third Co to Al_2O_3

$= E(surface + Co_3) - [E(surface + Co_2) + E(Co)]$

= -5.25 = -121.01 kcal/mol

Calculations (Three Cobalt Surface) continued

Binding Energy of CO to Co

$= E(\text{surface} + Co_3 + CO) - [E(\text{surface} + Co_3) + E(CO)]$

= -3.99 eV = -92.01 kcal/mol

Binding Energy of second & third CO to Co

$= E(\text{surface} + Co_3 + 3CO) - [E(\text{surface} + Co_3 + CO) + E(2CO)]$

= -6.85 eV = -157.96 kcal/mol

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

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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

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THANK YOU!!!

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Dr. Ayo Hassan

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