LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

LOUISIANA TECH UNIVERSITY®

# Lowering the Activation Energy of Fischer Tropsch Reactions through CoRu Core-Shell Catalysts

Mentor: Dr. Daniela Mainardi

REU Student: Tosin Oyeleke

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# Finding the Best Catalyst for Liquid Fuel Production


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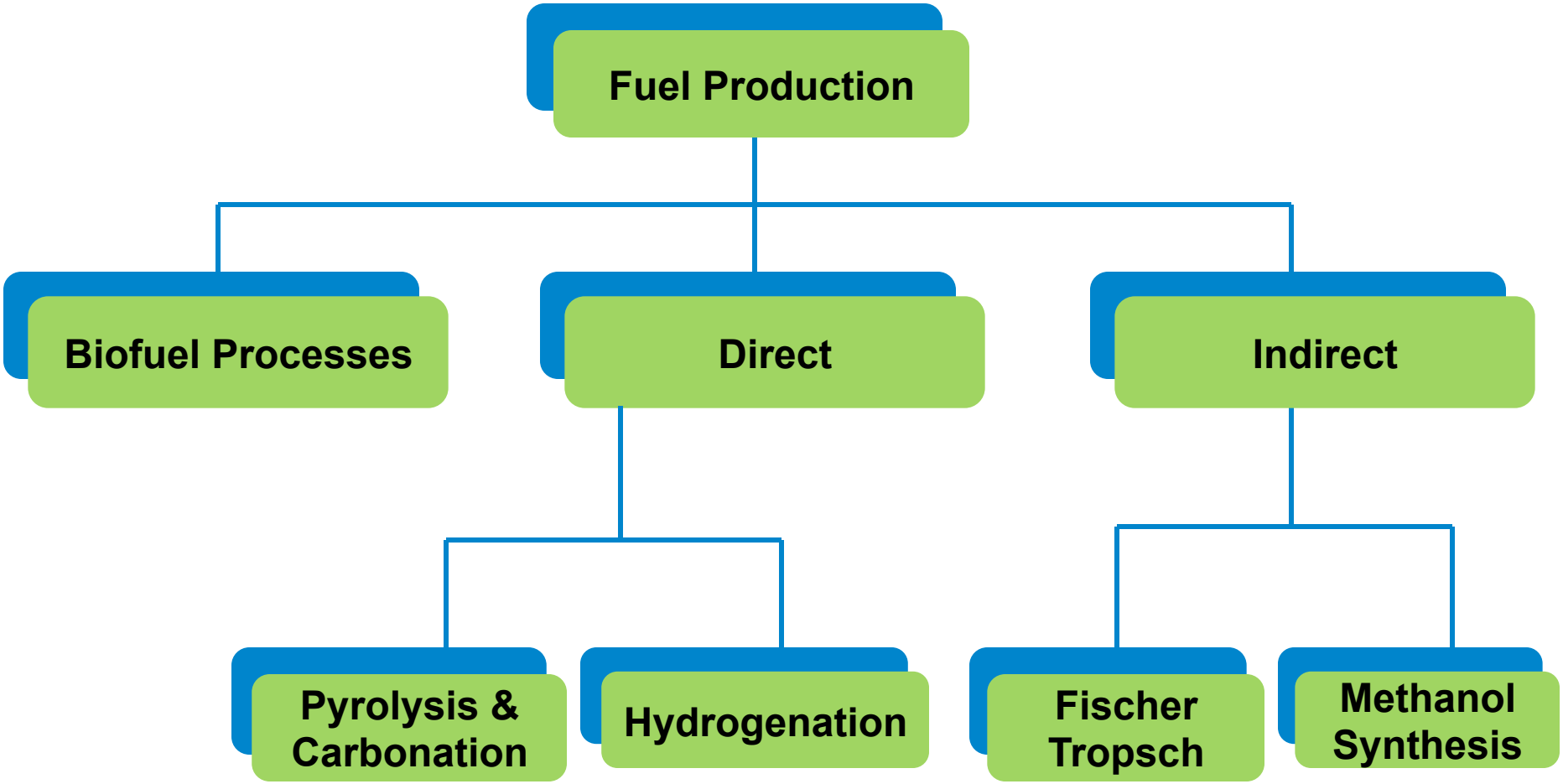
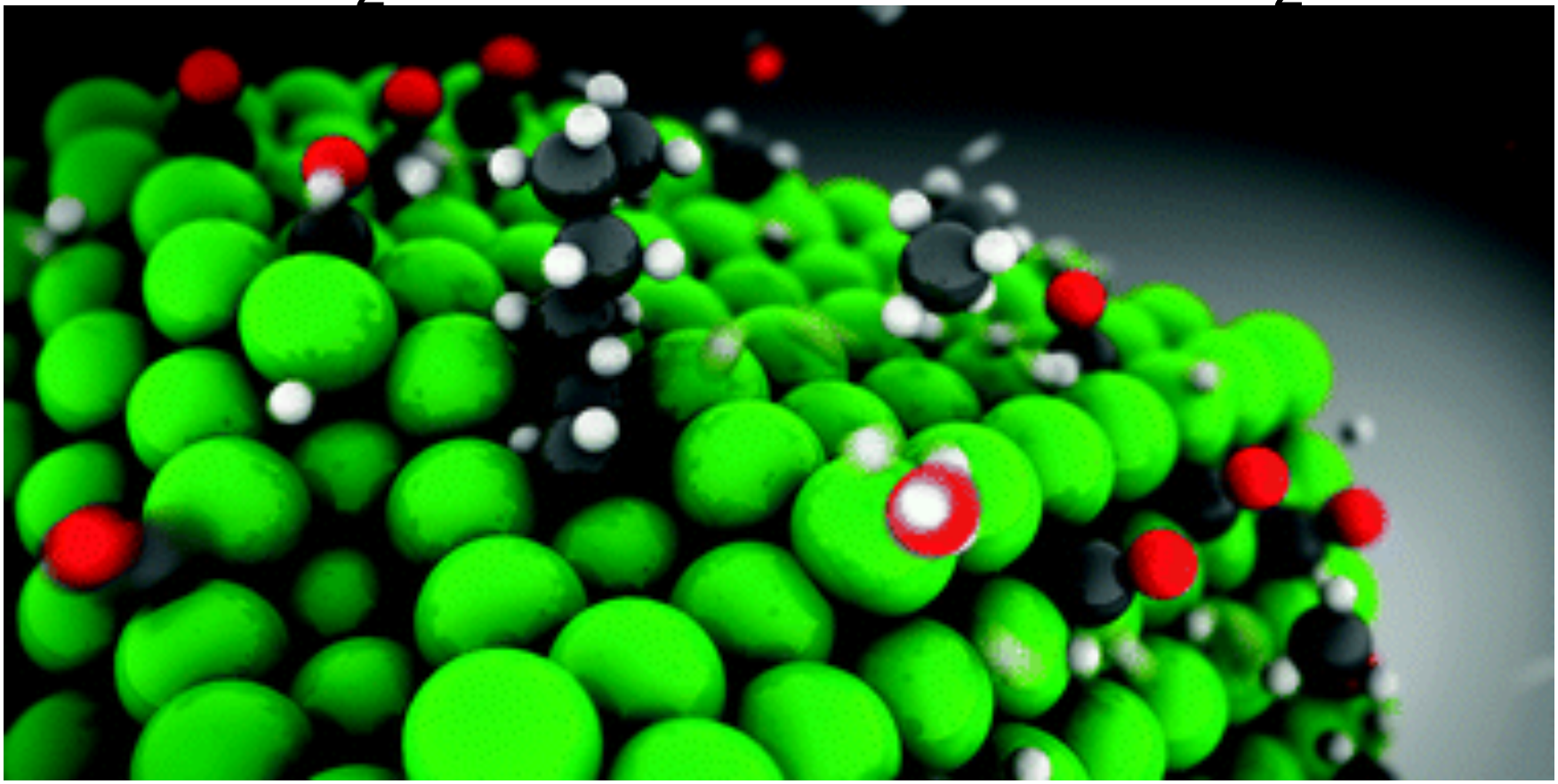
# Methods of Producing Fuel



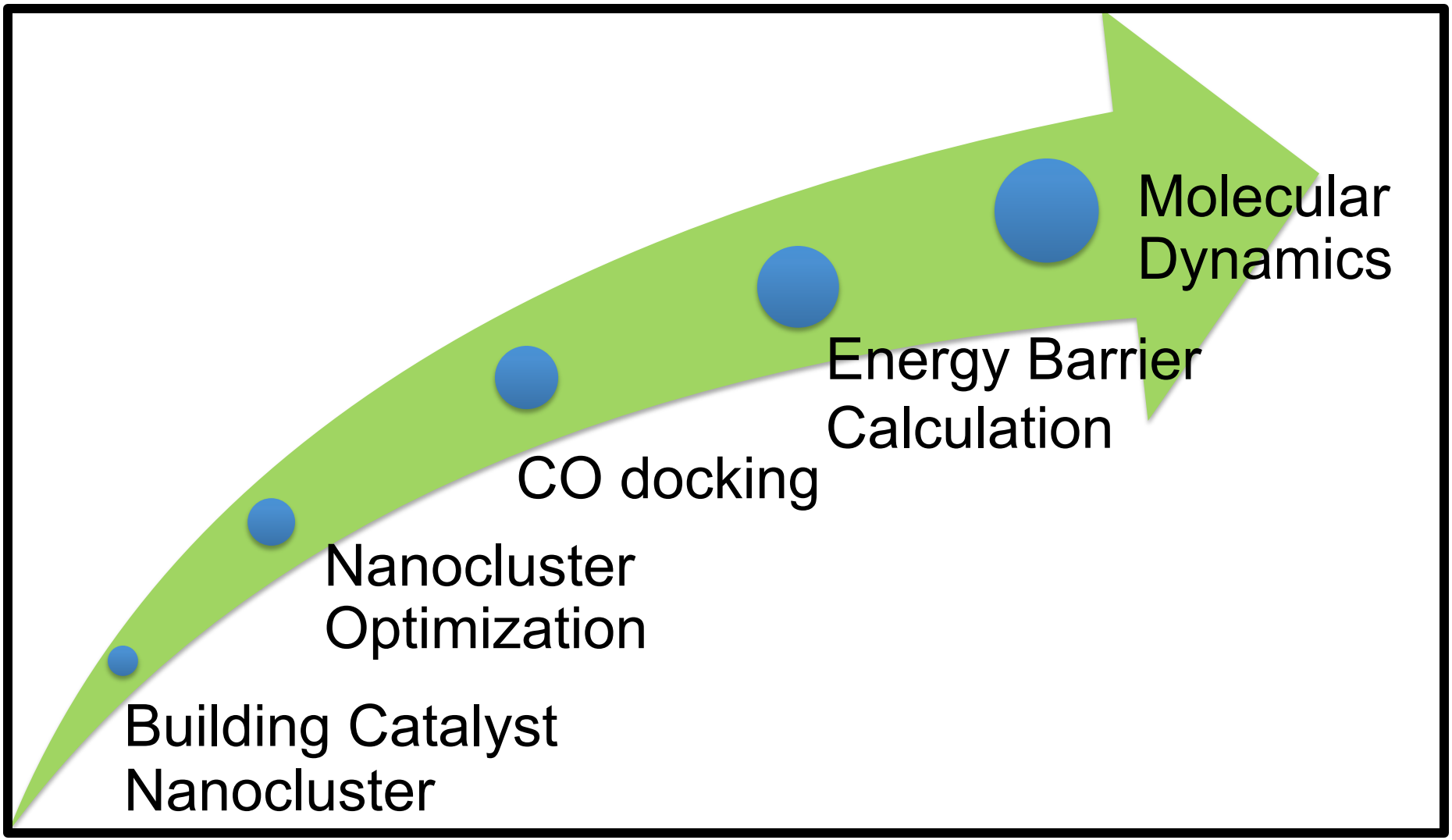
# What is the Fischer Tropsch Process?

$$CO + H_2 \xrightarrow{\text{Catalyst}} \text{Fuel} + H_2O$$

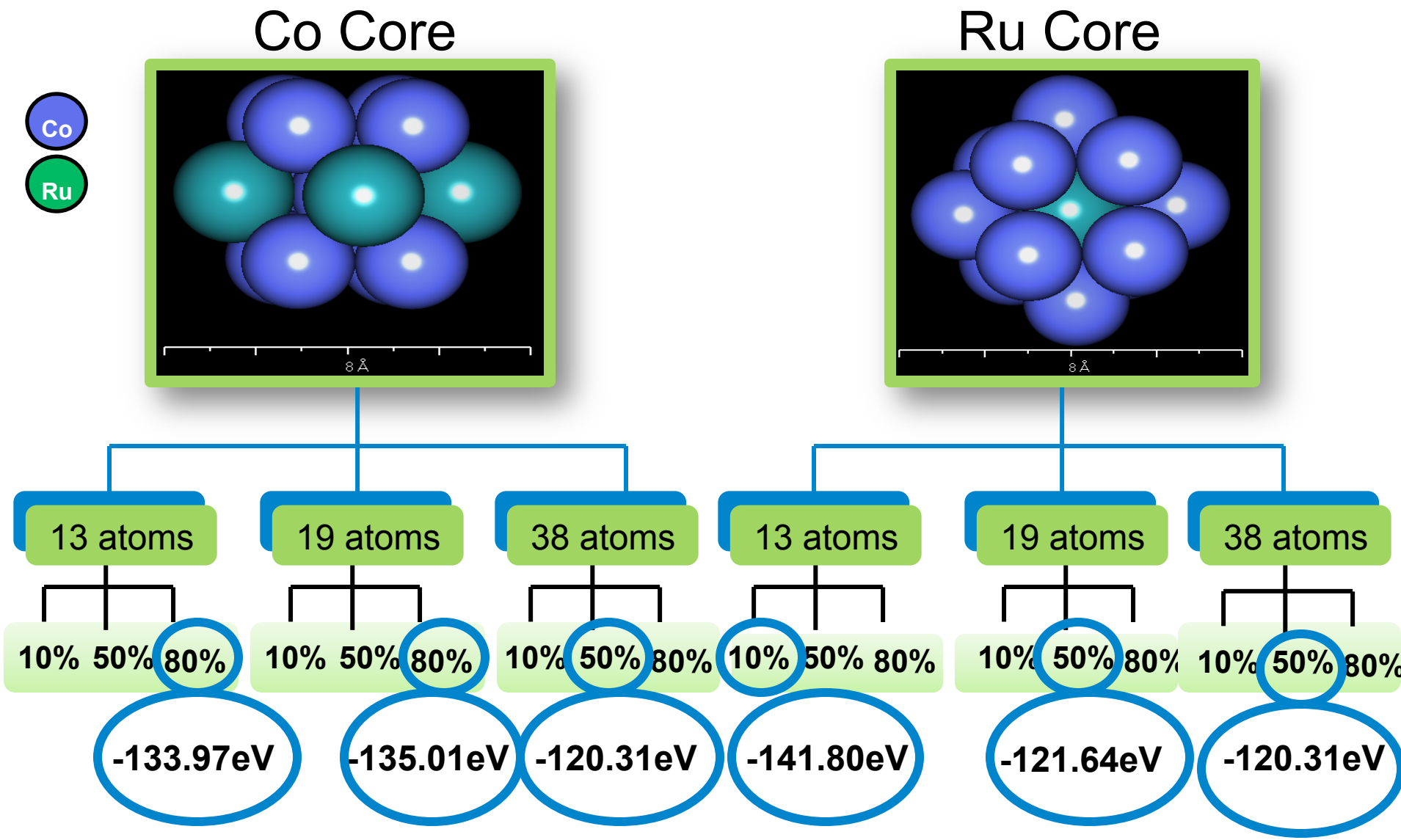


# …Why Computational Modeling?

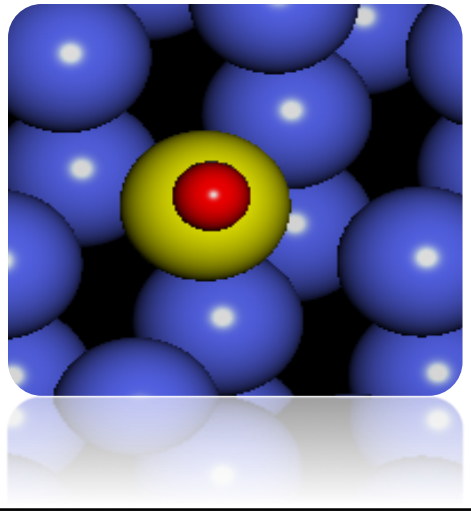
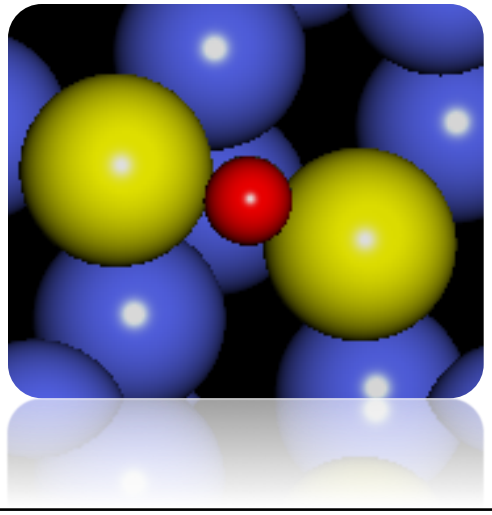
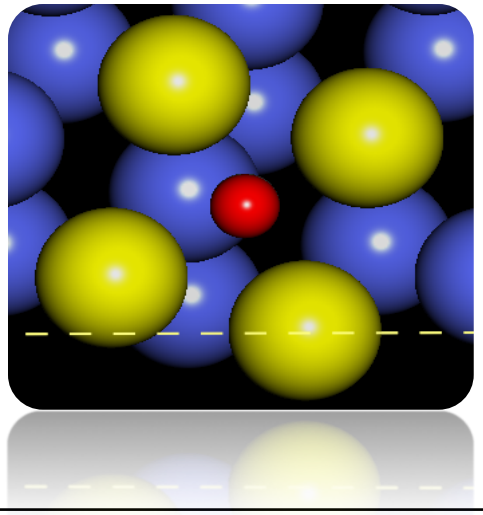
# Methodology Used

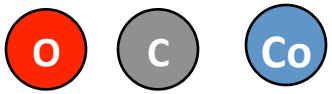


# Building Cluster Library Using Genetic Algorithm Optimizers

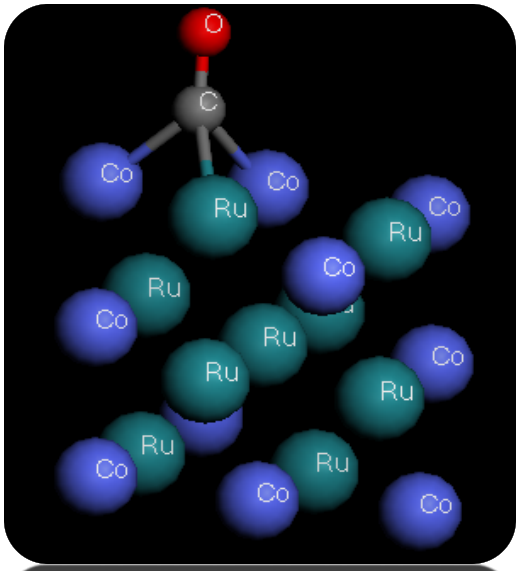
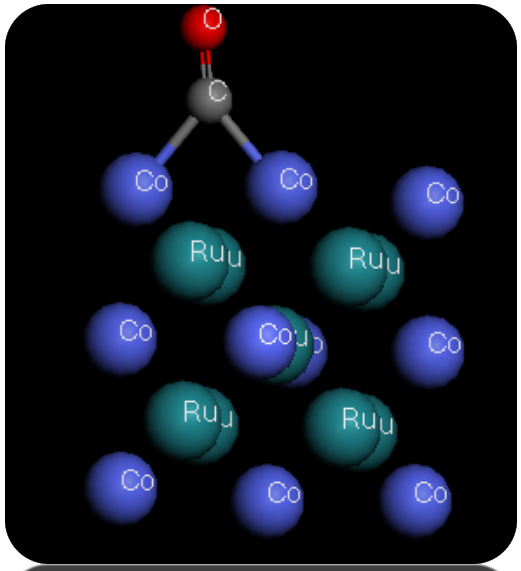
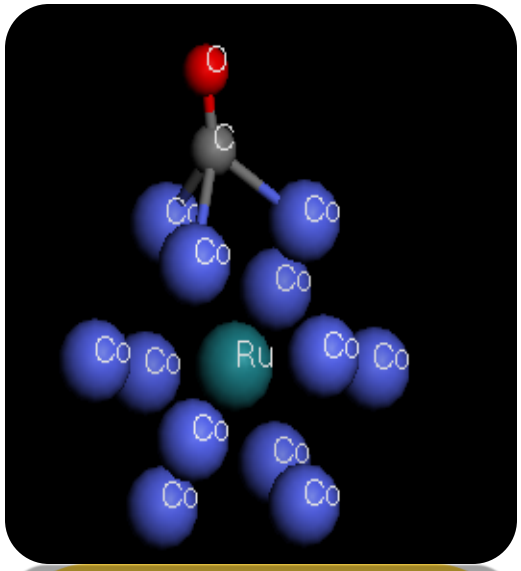


# Docking of CO Molecules on the Shell

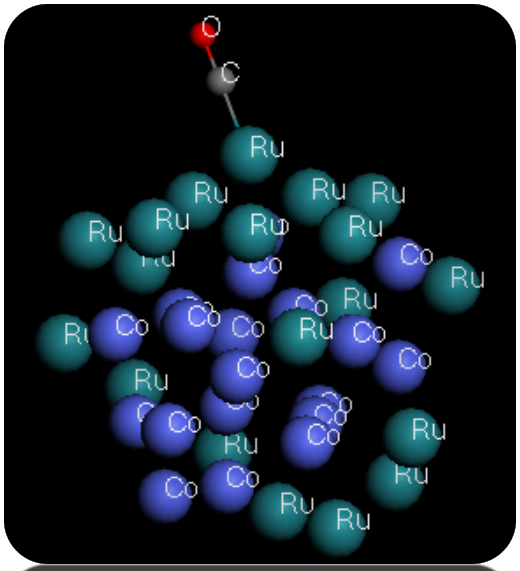
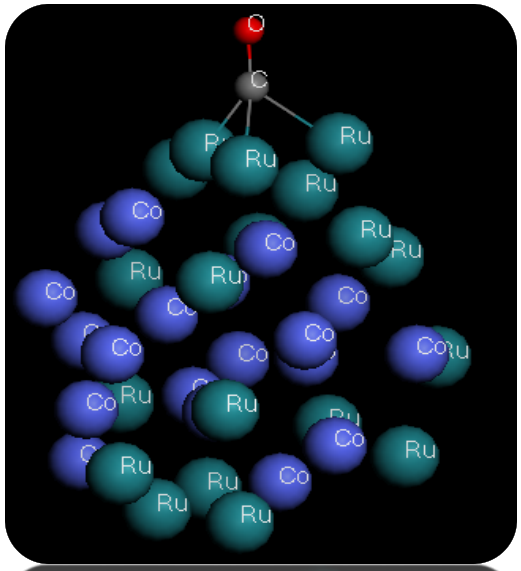
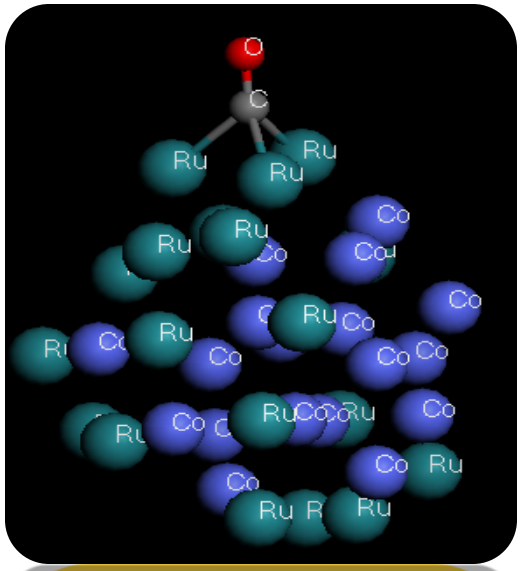
| Top | Bridge | Hollow |
| --- | --- | --- |
|  |  |  |



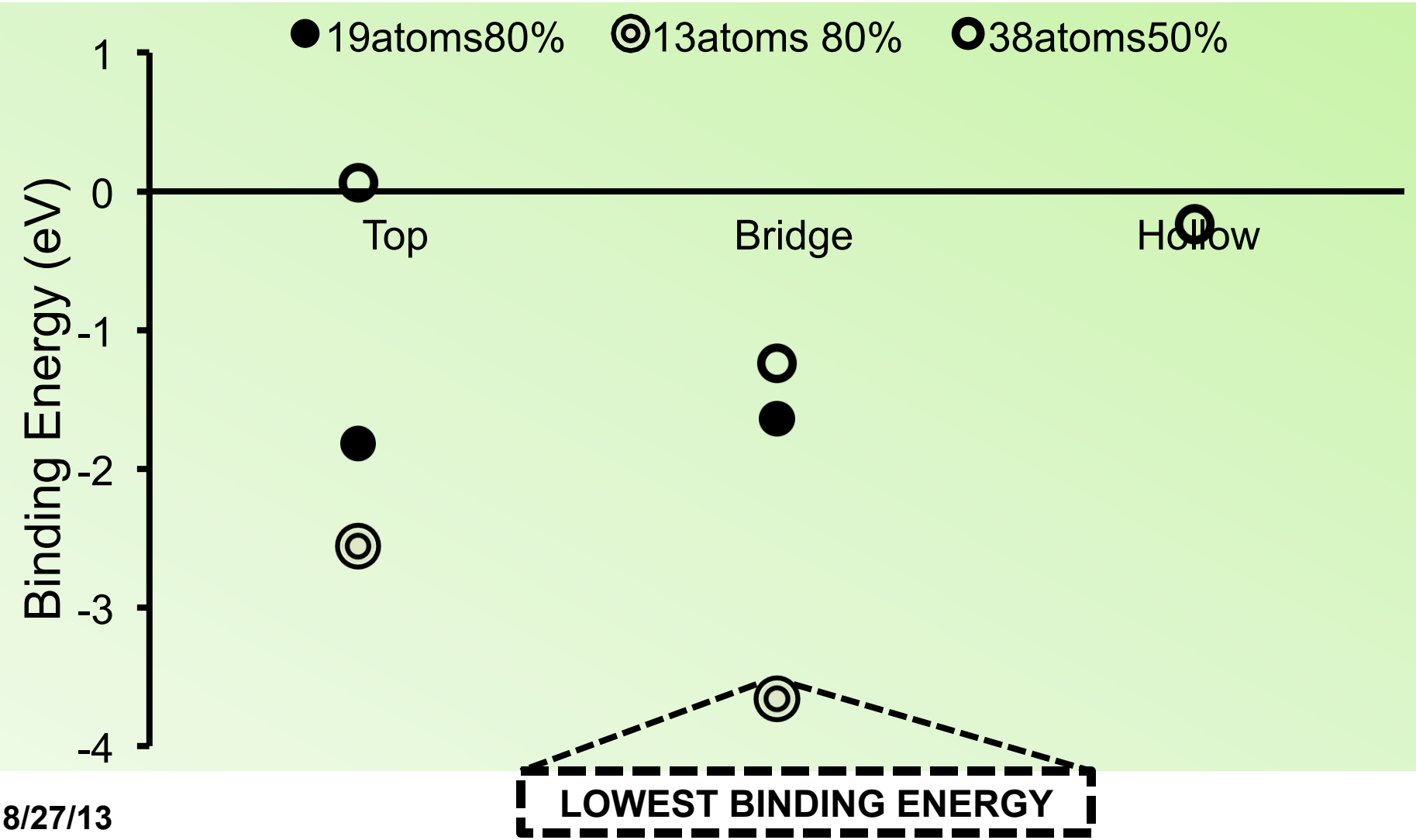
# Docking of CO Molecules on Ru Core Nanoclusters

| 13 Atoms 10% | | |
|---|---|---|
| Top | Bridge | Hollow |
|  |  |  |
| -1.86 eV | -2.92 eV | -2.99 eV |

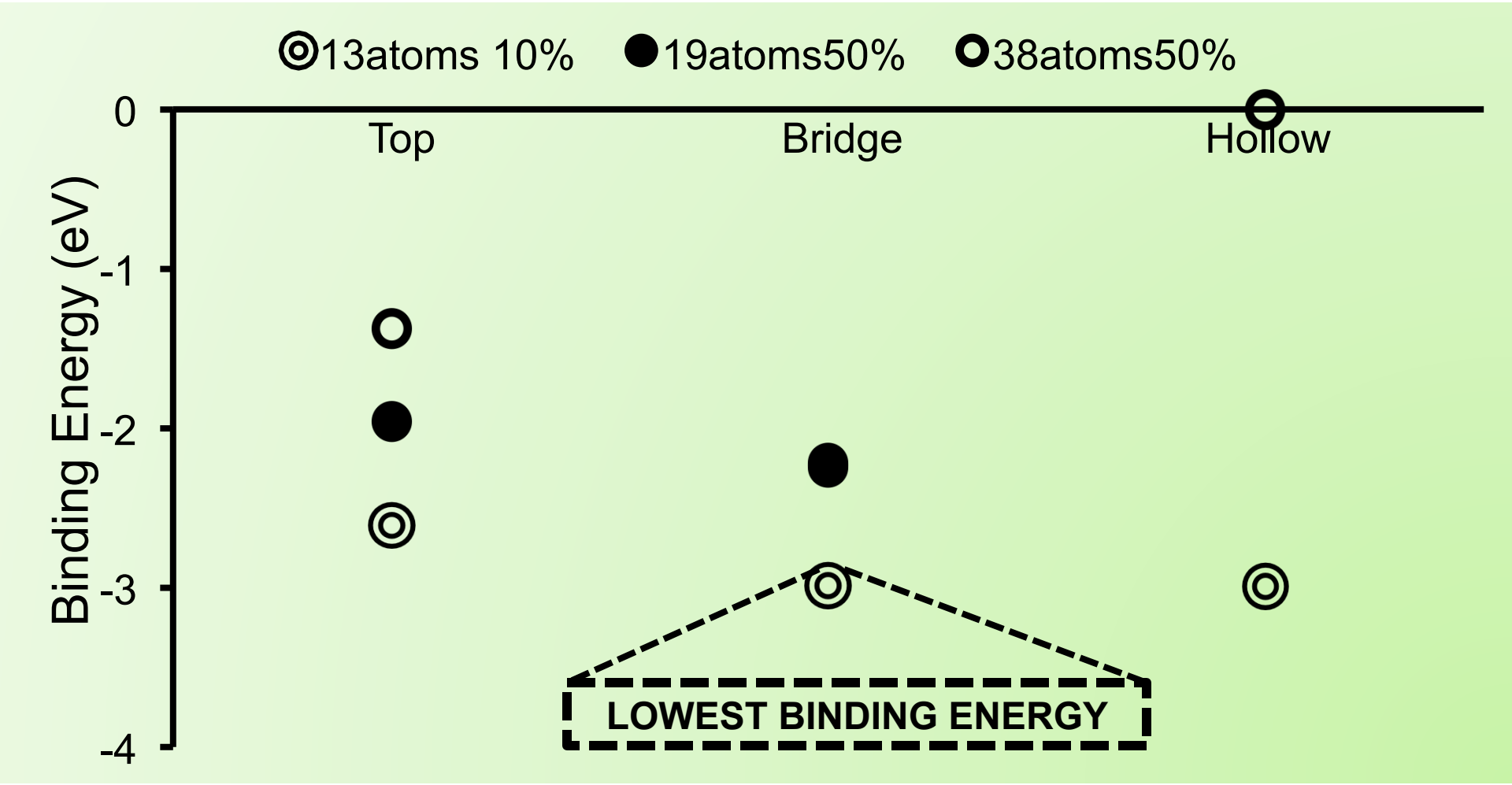
# Docking of CO Molecules on Co Core Nanoclusters

| 13 Atoms 80% | | |
|---|---|---|
| Top | Bridge | Hollow |
|  |  |  |
| -1.86 eV | -1.64 eV | -0.24 eV |

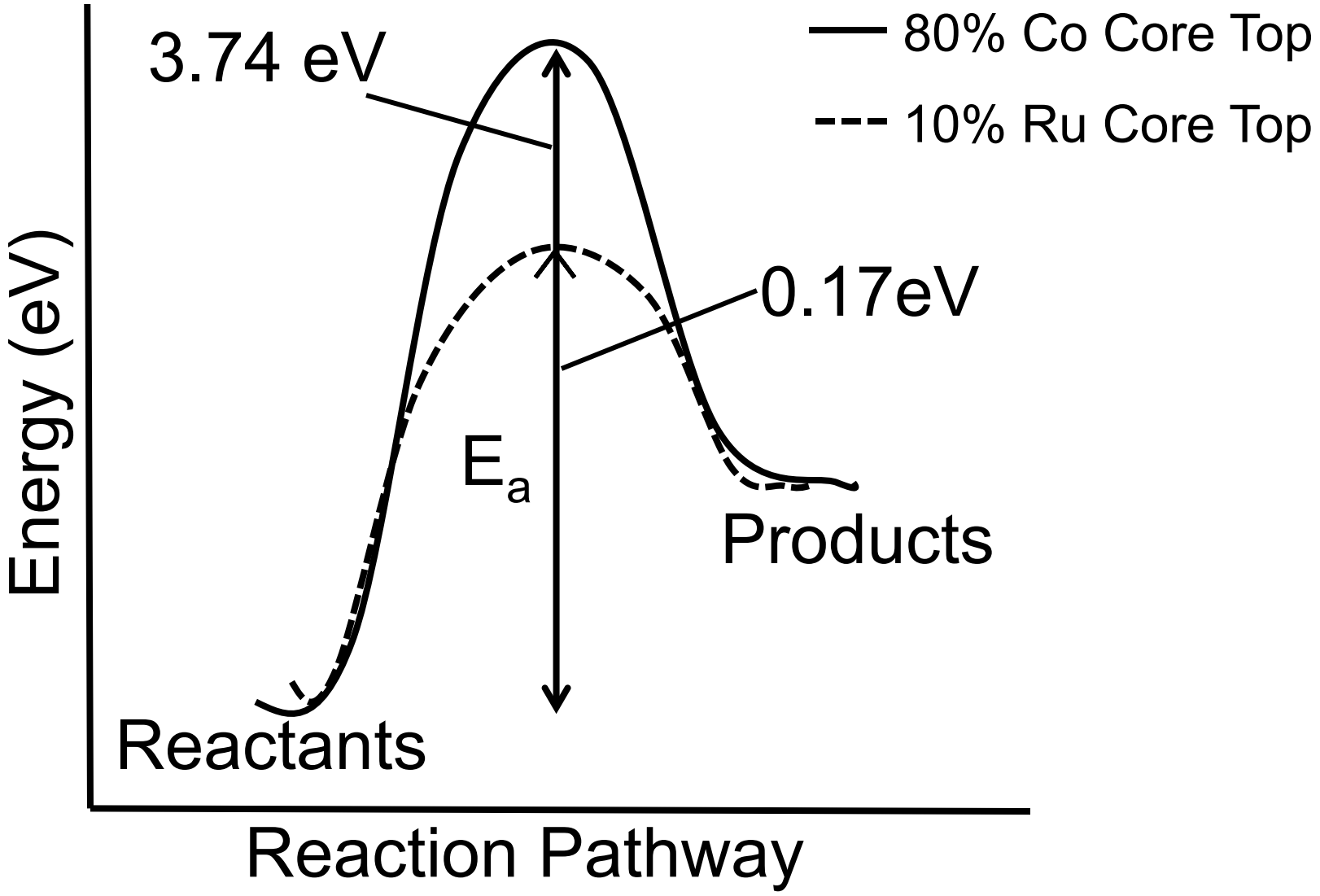
# Binding Energies for Optimized CO Docked Molecules Co Core



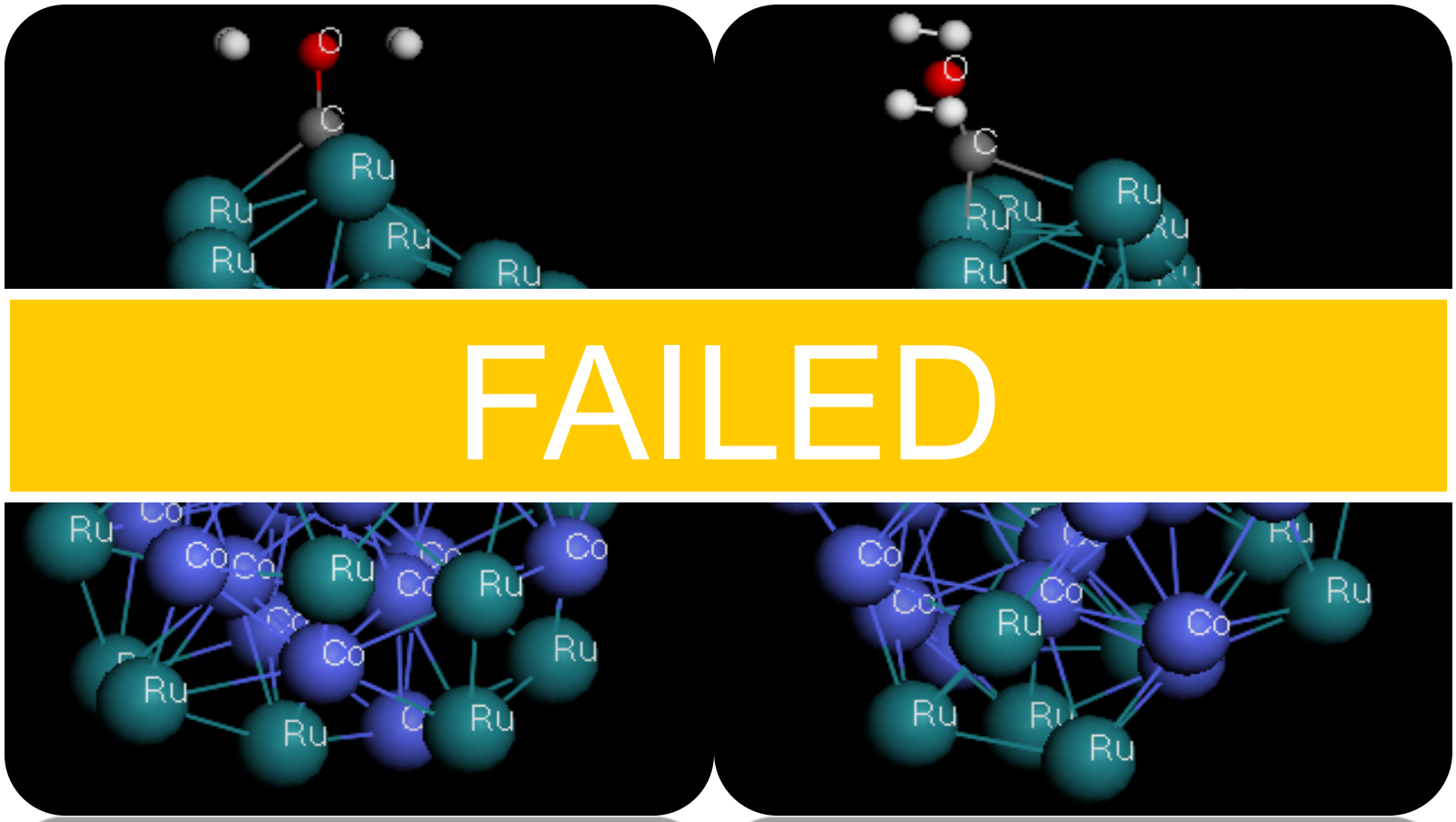
# Binding Energies for Optimized CO Docked Molecules Ru Core



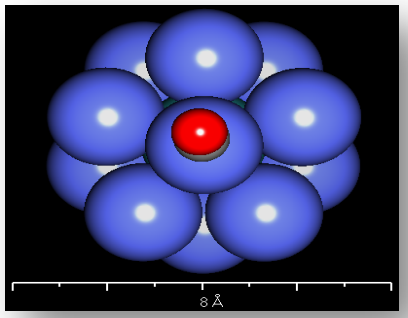
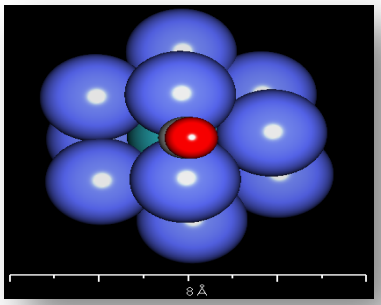
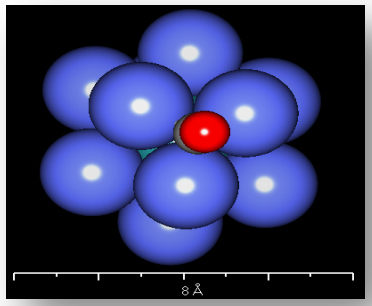
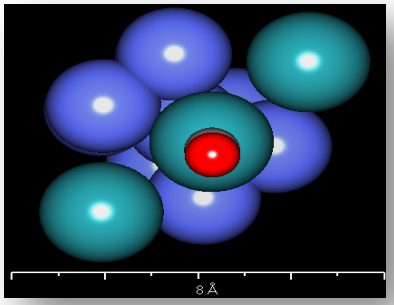
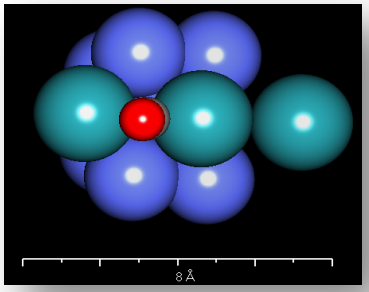
# Transition State: Energy Barriers for 13 Atoms

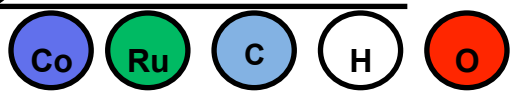


# Molecular Dynamics of 38 Atoms 50% Bridge Co Core at 25°C

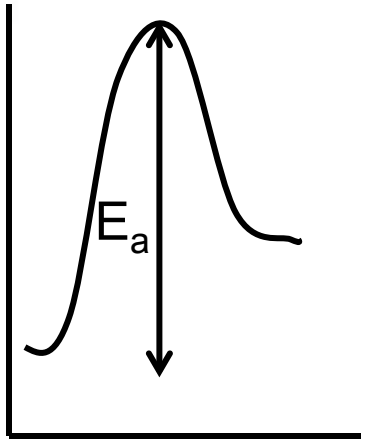


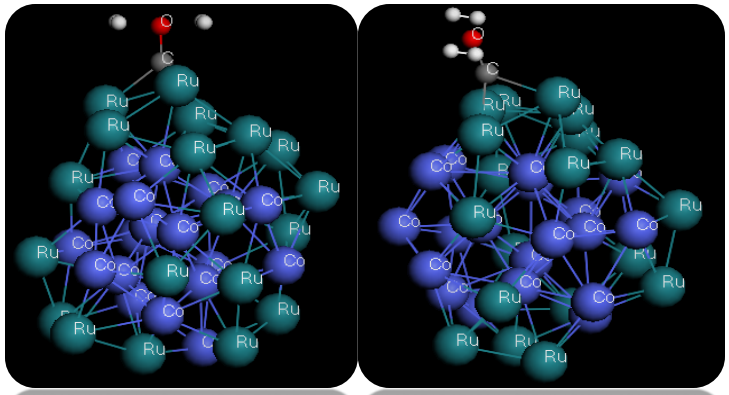
# Conclusion: Favorable Adsorption Site

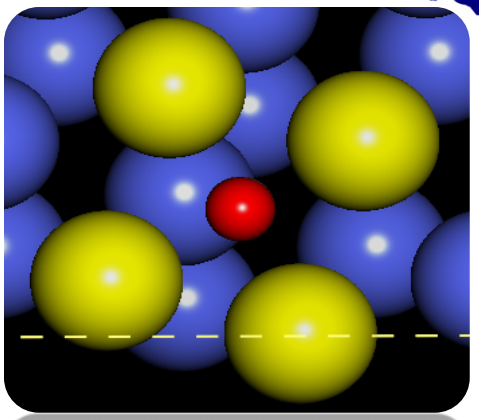
| | Top | Bridge | **Hollow** |
|---|---|---|---|
| Ru Core: |  -2.61 eV |  -2.98 eV |  **-2.99 eV** |
| Co Core: |  -2.56 eV |  **-3.66 eV** | |



# Future Work





- Complete transition states
- Run Molecular Dynamics at 200°C
- Try other CO docking positions

# My Experience so Far

# My Exp

# Acknowledgement

Dr. Daniela Mainardi

Fernando Soto and Suraj Gwajali

Ms. Alicia Boudreaux



- Options: solar energy, wind,fts
- Introduce the two core-shell structures.
- Why fts? and benefits
- The bottleneck of using fts
- Our approach to fix bottleneck
- Our methodology and results
- Graph of binding energies (showing the most postive one) Equation of binding energy
- Graph of transition enrgies.

# Literature Comparison of Bond Lengths

Find

- Hydrogen bond length
  http://itchem.com/calculated_and_experimental_dat
- CO bond length
- Water Bond length
- Co-C Bond Length

http://static.msi.umn.edu/rreports/2007/55.pdf

- Co-Co Bond Length
- Co-Ru Bond Length