Utilizing Density Functional Theory to Compute the Efficacy of a Practical Material for Industrial Direct Air Capture via a Copper Metal Organic Framework

Eugene Agravante, Mechanical Engineering
Mentor: Houlong Zhuang, Assistant Professor
Arizona State University - Fulton School of Engineering

Background

• Global warming poses a threat to humanity.
• One way to reverse the effects of global warming is to capture Carbon Dioxide from the air.
• That process is called Direct Air Capture and some materials are better suited for it than others.
• Literature in the field has proved that materials made from Metal Organic Frameworks can excel in this process, but still can be optimized [1].
• A visual of this in action can be found to the right [2].

Research Question

• Can the structure of a metal organic framework with a copper core be optimized for the process of direct air capture to help proliferate climate change fighting technologies?

Research Methods and Findings Thus Far

• First, the following copper metal organic framework was modelled via VESTA.
• The blue circles represent the copper atoms, and the red and bronze circles represent the organic ligands attached to the copper.
• Then the structure was simulated to undergo the DAC process via DFT.
• The magenta highlighted regions indicate areas of high charge distribution (presence of electrons). This implies that the area is more chemically reactive compared to the other areas when undergoing the DAC process.

Acknowledgements and References

• I would like to thank the ASU FURI program for accepting my proposal and allowing me to work on this, I greatly appreciate it.
• I would also like to thank Dr. Houlong Zhuang for being an excellent mentor and answering any questions and providing necessary expertise during this endeavor.

Works Cited