Carbon Dioxide Capture with Graphene Systems: Computational Studies

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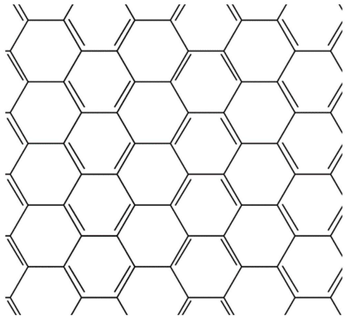
Background

Possibilities for CO2 Capture with Graphene Systems

- Porous graphene and bilayer systems [1]
- Graphene oxide [2]

Graphene

- Virtually two dimensional
- High surface area per mass
- Unique electronic properties
- Functionalized graphene has applications in multiple fields including nanotechnology and biochemistry



Computational Chemistry

- Electronic Structure Calculations
  - Describe the ground state geometry and energy of a system

Objectives

- **Characterize anion-CO_2 reaction for:**
  - **Larger, radially symmetric graphene segments**
  - **Systems with edge functionalities**
- Expand upon computational & functionalization methods: Trousdale's 2018 summer work (below), Teague's 2010 study [3]

Methods

Web Based Interface

WebMO

Computational Engine

Q-CHEM — A QUANTUM LEAP INTO THE FUTURE OF CHEMISTRY

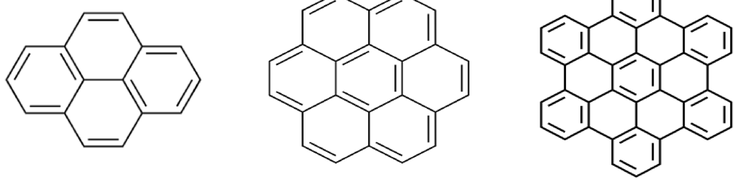
Graphene Scaffold: Polycyclic Aromatic Hydrocarbons

Pyrene (4 hexagonal rings)
Coronene (7)
Hexabenzocoronene (13)

Density Functional Theory

- Method: Becke 3-parameter Lee-Yang-Parr
- Basis Set: 6-31G(d)

Anion bound to central carbon



Calculations

Molecular Energy- calculates the energy of an atomic assembly
Geometry optimization- calculation performed to find the most stable energy of a given system
Vibrational frequency- calculations performed to ensure that geometry optimization yielded a minimum e was obtained

- CO_2-anion complexes created by placing linear CO_2 1.2 Å from the anion

Data Evaluated

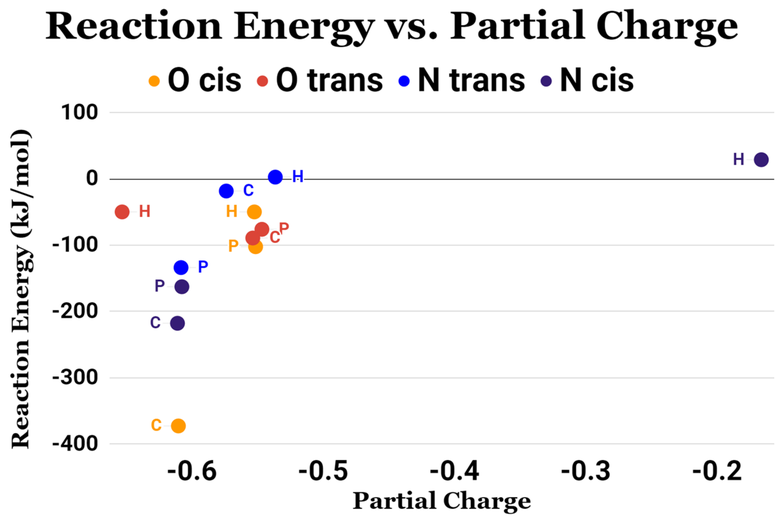
- Reaction energies

Reaction: $CO2 + Anion \rightarrow Complex$

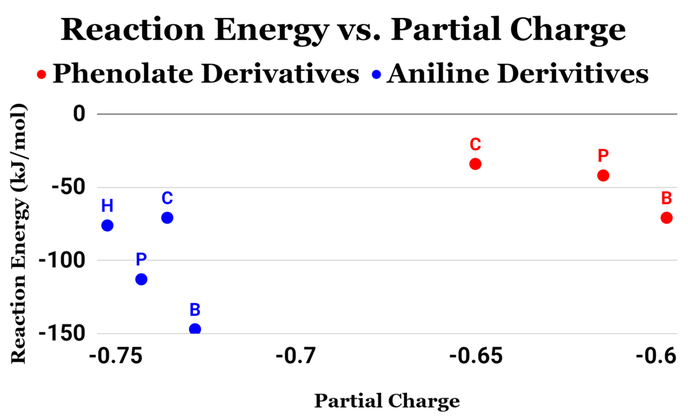
- Geometry of the complex
  CO2 bond angle and C-Anion Bond length

Results

Surface Functionalized Graphene



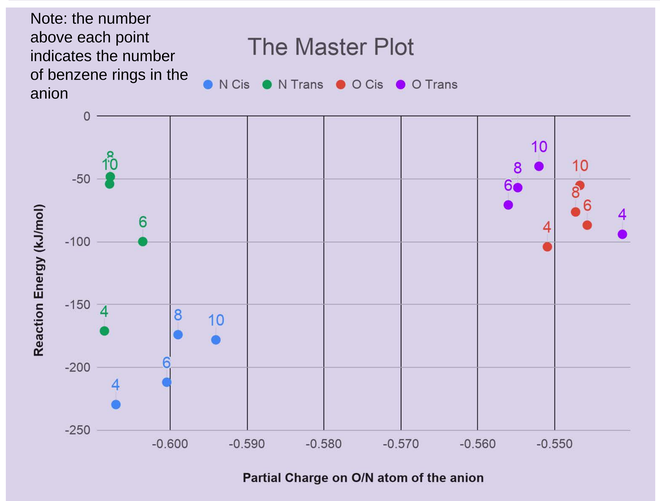
Edge Functionalized Graphene

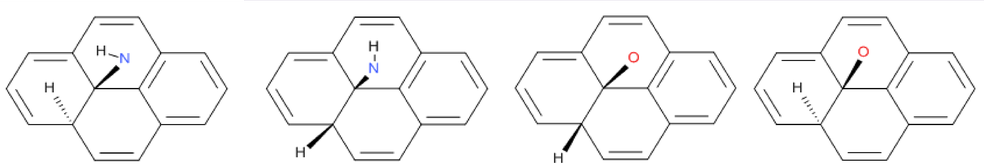


Future Research

- Explore the binding affinities of all moieties found in graphene oxide which include:
  - Epoxides
  - Hydroxyls
  - Carboxyls
  - Ketones
- Explore literature on graphene compatible polymers/moieties

Initial Studies





Structures

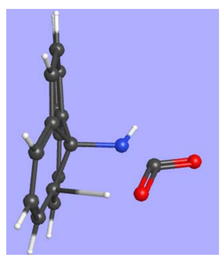
- 4, 6, 8 & 10 ring structures with functionalizations as above
- 2 benzene rings added successively to the original structure in a diagonal fashion

Result

- A trend was observed that related the size of the graphene sheet to the reaction energy

Future Improvements

- Create a system where the carbon scaffold better resembles graphene



References

1 Jiang, Cooper, and Dai, Nano Lett. **2009,** *9*, 4019
2 Li et al. J. Memb. Sci. **2015**, *479*, 1
3 Teague, Dai, and Jiang, J. Phys. Chem. A **2010,** *114*, 11761

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