Krista Bullard
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Education

University of Pittsburgh (Pittsburgh, PA) Graduation: April 2017
BS in Chemistry
GPA: 3.5

Georgia Institute of technology (Atlanta, GA) Fall 2017 – present
Projected Ph.D in Chemistry

Research Experience

Georgia Institute of Technology, Gutekunst Research Group (co-advised with Mohan Srinivasarao)
Fall 2017-present
Polymer/cellulose nanocrystals composites using host-guest complexes

University of Pittsburgh, Lambrecht Research Group (in collaboration with Dr. Emily Pentzer at Case Western University)
Fall 2016-Spring 2017
Simulation of ketene polymerization

- The group is examining the synthesis of three different polymers, poly(α-silyl β-ketones), poly(ketene acetals), and poly(alkenyl esters) from silyl ketene
- Specifically, I am comparing the relative energies to polymerize the C=C or C=O bonds using the quantum chemistry software packages MOPAC and Q-CHEM
- By altering the internal and external factors computationally, the experimental synthesis can be altered to favor formation of different polymer products

Department of Energy, National Energy Technology Lab – Mickey Leland Energy Fellowship
Summer 2016
Electrochemistry of CO_2 with AuNP

- I used quantum mechanics in combination with computational electrochemistry techniques were to obtain an atomic-level picture of CO_2 electro reduction to CO with Au nanoparticle catalyst
- Using density functional theory (DFT) implemented in QCHEM, I modeled the target Au13 nanoparticle and preformed frequency calculations on each step of the reduction
- By implementing the raw data calculated from QCHEM and using the computational hydrogen electrode method, I calculated the free energies of each step of the CO2 to CO electroreduction, showing that the Au13 catalyst lowered the over potential of the reduction when compared to bulk Au

University of Pittsburgh, Lambrecht Research Group (in collaboration with Dr. Sean Garrett-Roe)
Spring 2014-Spring 2015
CO_2 absorption in Ionic Liquids

- I modeled CO_2 in a series of 1-butyl-3-methylimidazolium-based ionic liquids ([C4C1im][X] and used computational DFT frequency analysis utilizing QCHEM to calculate the v3 frequency of CO_2 in each IL
- The group used this information to develop molecular pictures of CO2 solvation in ILs based on computational modeling in combination with experiment

Teaching Experience

Graduate Teaching Assistant – Quantitative Analysis Fall 2017
Undergraduate Teaching Assistant – Intro Analytical Chemistry Lab Fall 2016 – Spring 2017

Publications

Polymerization of silyl ketenes using alkoxide initiators: a combined computational and experimental study. Xiang, Y.; Burrill, D.; **Bullard, K.**; Albrecht, B.; Tragesser, L.; Drout, R.; McCaffrey, J.; Densmore, T.; Lambrecht, D.; Pentzer, E. *in preparation*

Modeling Carbon Dioxide Vibrational Frequencies in Ionic Liquids: I. *Ab Initio* Calculations. Berquist, E.; Daly, C.; Brinzer, T.; **Bullard, K.**; Campbell, Z.; Corcelli, S.; Garrett-Roe, S.; Lambrecht, D. Journal of Physical Chemistry. *Accepted and pending publication*

References

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Dominic Alfonso, Ph.D
Computational Chemist at NETL
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