Ubaidullah S. Hassan

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EDUCATION

The Cooper Union for the Advancement of Science and Art, New York, NY 2021 – Present
B.E., Chemical Engineering, Minors in Mathematics and Chemistry, GPA: 3.94/4.0

AWARDS

Barry Goldwater Scholar, 2024

Half Tuition Scholarship, 2021-2025

Daniel E. Kowler ChE ’65 Memorial Prize Fund Recipient

RESEARCH EXPERIENCE

The Cooper Union Department of Chemistry, New York, NY August 2022 - Present
Undergraduate Researcher, Advisor: Robert Q. Topper

- Studied decomposition and growth pathways of ammonium nitrate clusters using our groups code for simulated annealing Monte Carlo molecular mechanics geometry optimizations, quantum chemistry methods, and comparison to experimental literature

Stony Brook Institute of Advanced Computational Sciences, Stony Brook, NY May 2024 - Present
Undergraduate Researcher (NSF REU), Advisors: Benjamin G. Levine and Arshad Mehmood

- Static quantum mechanical calculations and non-adiabatic *ab initio* molecular dynamics of 2-hydroxyazobenzene for applications in photochemistry

Penn State University Department of Material Science, State College, PA May – August 2023
Undergraduate Researcher (NSF REU), Advisor: Stephanie Law

- Used Fourier transform infrared spectroscopy and analyzed spectra to examine Dirac semimetals’ potential in infrared photodetection

Purdue Energetics Research Center, West Lafayette, IN May – August 2022
Undergraduate Researcher (U.S. Army Research Labs funded program), Advisor: Stephen Beaudoin

- Studied particle adhesion of mock polymer-bonded explosives by quantifying Van der Waals forces
- Independently operated an atomic force microscope for more than 50 hours to calculate Hamaker constants

PUBLICATIONS

[2] **Hassan, U. S.**; Mehmood A.; and Levine B. G. Static Quantum Mechanical Calculations and Non-Adiabatic Dynamics of 2-Hydroxyazobenzene. *(In preparation).*

[1] **Hassan, U. S.**; Amat, M. A.; and Topper, R. Q. Decomposition and Growth Pathways of Ammonium Nitrate Clusters and Nanoparticles. *(In preparation).*

TALKS

[3] **Hassan, U. S.**; Trice, R.; and Law, S. *The Potential of Dirac Semimetals for Infrared Photodetection*. Penn State Materials Research Institute 2D Materials REU Talks, State College, PA, 2023.

[2] **Hassan, U. S.** and Topper, R. Q. *Computational Analysis of Mass Spectra and Growth Patterns of Ammonium Nitrate Nanoparticles.* New York Chapter of ACS Undergraduate Symposium, Queens, NY, 2023.

[1] **Hassan, U. S.**; Vazquez J. M.; and Beaudoin S. *Adhesion of Mock Polymer-Bonded Explosives.* Purdue Energetics Research Symposium, West Lafayette, IN, 2022.

POSTER PRESENTATIONS

[5] **Hassan, U. S.**; Amat, M. A.; and Topper, R. Q. *Decomposition and Growth Pathways of Aerosolized Ammonium Nitrate Particles.* American Conference on Theoretical Chemistry, North Carolina, 2024.

[4] **Hassan, U. S.** and Topper, R. Q. *Patterns in Growth of Ammonium Nitrate Clusters.* Virtual Winter School on Computational Chemistry, 2024.

[3] **Hassan, U. S.**; Amat, M. A.; and Topper, R. Q. *Growth and Decomposition Pathways for Ammonium Nitrate Clusters.* AIChE Annual Conference, Orlando, FL 2023.

[2] **Hassan, U. S.**; Trice, R.; and Law, S. *Dirac Semimetals Potential in Infrared Photodetection.* Penn State REU Symposium, State College, PA, 2023.

[1] **Hassan, U. S.**; Vazquez J. M.; and Beaudoin S. *Quantifying Van der Waals Adhesion of Energetic Particles.* Purdue Energetics Research Symposium, West Lafayette, IN, 2022.

SKILLS

Interests: Quantum Chemistry, *Ab initio* Molecular Dynamics, Non-adiabatic and excited state dynamics, Simulated annealing and Monte Carlo methods, Density functional theory
General: Excel, Linux, High-Performance Computing, LaTeX, Word
Programming Languages: Python and Bash
Computational Chemistry Codes: ORCA, TeraChem, Spartan, OpenMolcas, Psi4
Lab: AFM, FTIR, UV-VIS Spectroscopy, MS, SEM, XRD

RELEVANT COURSEWORK

Chemistry: Computational Chemistry & Statistical Mechanics (Grad level), Organic Chemistry, Physical Chemistry, Organometallic Chemistry, Biochemistry
Mathematics: Linear Algebra, Real Analysis, Differential Equations, Discrete Math, Probability, Vector Calculus
Physics: Quantum Mechanics, Electricity and Magnetism, Optics and Modern Physics, Mechanics