Ubaidullah S. Hassan

ubaidullah.hassan@cooper.edu | 516-404-6541

EDUCATION

The Cooper Union for the Advancement of Science and Art New York, NY
B.E., Chemical Engineering, Minors in Mathematics and Chemistry, GPA: 3.94 2021 – 2025

AWARDS

Goldwater Scholar, The Barry Goldwater Scholarship and Excellence in Education Foundation 2024

Daniel E. Kowler ChE '65 Memorial Prize Fund Recipient, The Cooper Union 2023

RESEARCH EXPERIENCE

The Cooper Union Department of Chemical Engineering New York, NY
Undergraduate Researcher, Advisor: Abhishek Sharma August 2024 - Present
- Studied the stimulus-response dynamics of networks to gain deeper insights into protein allostery
- Used the JAX-MD library to perform molecular dynamics simulations

Stony Brook Institute of Advanced Computational Sciences Stony Brook, NY
Undergraduate Researcher (NSF REU), Advisor: Benjamin G. Levine May 2024 - Present
- Conducted static electronic structure calculations and non-adiabatic *ab initio* molecular dynamics simulations of 2-hydroxyazobenzene, contributing to advancements in photochemistry applications
- Mapped out the potential energy surfaces by discovering multiple non-radiative relaxation pathways involving photoisomerization and excited-state intramolecular proton transfer

The Cooper Union Department of Chemistry New York, NY
Undergraduate Researcher, Advisor: Robert Q. Topper 2022 - Present
- Analyzed the decomposition and growth pathways of ammonium nitrate clusters using our group's simulated annealing Monte Carlo geometry optimization code
- Identified for the first time, the structures corresponding to the peaks of all detectable species in both the positive and negative ion mass spectra of ammonium nitrate from experimental literature
- Presented the first study on larger ammonium nitrate particles and predicted new particle morphologies with trigonal pyramidal character

Penn State University Department of Material Science State College, PA
Undergraduate Researcher (NSF REU), Advisor: Stephanie Law May – August 2023
- Used Fourier transform infrared (FTIR) spectroscopy and analyzed spectra to assess the potential of Dirac semimetals for infrared photodetection applications
- Compared samples of Dirac semimetals and concluded those fabricated via evaporation had better optical properties than those fabricated via sputtering

Purdue Energetics Research Center West Lafayette, IN
Undergraduate Researcher (DEVCOM funded), Advisor: Stephen Beaudoin May – August 2022
- Conducted research on particle adhesion in mock polymer-bonded explosives by quantifying Van der Waals forces
- Independently operated an atomic force microscope for over 50 hours to determine Hamaker constants

TEACHING AND MENTORSHIP EXPERIENCE

The Cooper Union Department of Chemistry   New York, NY
Research Mentor, Advisor: Robert Q. Topper   2024 – Present
- Mentored an undergraduate researcher, Renee Ma, on a project focused on ammonium fluoride clusters
- Provided instruction on the application of simulated annealing Monte Carlo methods, along with a comprehensive explanation of the underlying theoretical concepts

The Cooper Union Department of Mathematics   New York, NY
Math Tutor   2022 – Present
- Provided tutoring support to undergraduate students in calculus, linear algebra, differential equations, probability, and discrete mathematics
- Delivered clear and effective instruction on mathematical concepts to groups of students in a weekly "Help Room" setting

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. *Journal of Physical Chemistry A*, 2024. *(Submitted)*

TALKS (presenters' name <u>underlined</u>)

[4] <u>Topper, R. Q.</u>; Topper, S.; Lee, S.; **Hassan, U. S.**; Kim, A.; Frost, J.; Wang, W. *TransRot: An open-source project for simulated annealing Monte Carlo calculations of molecular clusters, microhydrated species, and surface adsorbates.* Fall 2024 National Meeting of the American Chemical Society (ACS), Denver, CO, 2024.

[3] <u>**Hassan, U. S.**</u>; 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] <u>**Hassan, U. S.**</u> and Topper, R. Q. *Computational Analysis of Mass Spectra and Growth Patterns of Ammonium Nitrate Nanoparticles.* New York Chapter of ACS Undergraduate Symposium, LaGuardia Community College, NY, 2023.

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

POSTER PRESENTATIONS

[6] **Hassan, U. S.**; Mehmood, A.; and Levine, B. G. *Photochemistry of 2-Hydroxyazobenzene: A Computational Study.* Stony Brook Summer Research Symposium, Stony Brook, NY, 2024.

[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, Chapel Hill, NC, 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

Computational: Python, Bash, Linux, Excel, Word, LaTeX
Quantum 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 I & II, Physical Chemistry I & II, Organometallic Chemistry, Biochemistry
Mathematics: Linear Algebra, Real Analysis I & II, Ordinary and Partial Differential Equations, Discrete Math, Probability, Vector Calculus
Physics: Quantum Mechanics, Electricity and Magnetism, Optics and Modern Physics, Mechanics