# Ubaidullah S. Hassan

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## EDUCATION

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

## AWARDS

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

**Outstanding Presentation in Computational/Theoretical Chemistry**, GCURS Rice University 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 K. Sharma September 2024 - Present

- Used differentiable molecular dynamics (JAX-MD) to map sequences to network structures analogous to amino acid sequences to three-dimensional protein structures
- Developed original code to simulate and optimize network structures using gradient descent
- Created a model to simulate protein evolution in the presence of mutational stresses

**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
- Explained, for the first time, the patterns for peaks 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

**Stony Brook Institute of Advanced Computational Sciences** Stony Brook, NY
*Undergraduate Researcher (NSF REU),* Advisor: Benjamin G. Levine May – August 2024

- 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

**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 optical properties of samples of Dirac semimetals fabricated via different methods

**Purdue Energetics Research Center** West Lafayette, IN
*Undergraduate Researcher (DEVCOM funded),* Advisor: Stephen Beaudoin May – August 2022

- Studied particle adhesion in mock polymer-bonded explosives by quantifying Van der Waals forces
- Independently operated an atomic force microscope for 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 atmospheric ammonium fluoride clusters by helping with theoretical aspects and carrying out simulated annealing Monte Carlo methods

**The Cooper Union Department of Chemistry** New York, NY
*Physical Chemistry Tutor* 2024 – Present

- Helped students in introductory quantum chemistry with topics such as particle in a box, harmonic oscillator, rigid rotator, variational methods, and perturbation theory

**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*, 128, 9184-9194 (2024). DOI: 10.1021/acs.jpca.4c04630

**TALKS** (presenters' name underlined)

[5] **Hassan, U. S.**; Mehmood, A.; and Levine, B. G. *Computational Insights into the Photodynamics of 2-Hydroxyazobenzene*. Gulf Coast Undergraduate Research Symposium, Rice University, Houston, TX, 2024.

[4] Topper, R. Q.; 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] **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, LaGuardia Community College, 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

[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, JAX-MD, Bash, Linux, Excel

**Quantum Chemistry Codes:** ORCA, TeraChem, Spartan, OpenMolcas, Psi4

**Lab:** AFM, FTIR, UV-VIS, MS, SEM, XRD

## RELEVANT COURSEWORK

**Chemistry:** Computational Chemistry & Statistical Mechanics (Graduate 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