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, Calculus I, II, & III

Physics: Quantum Mechanics, Electricity and Magnetism, Optics and Modern Physics, Mechanics