Ubaidullah S. Hassan

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EDUCATION

University of Pennsylvania — Philadelphia, PA
Ph.D., Theoretical Chemistry — 2025 - Present

The Cooper Union for the Advancement of Science and Art — New York, NY
B.E., Chemical Engineering, *Summa Cum Laude* — 2021 – 2025
Minors in Mathematics and Chemistry

FELLOWSHIPS AND SCHOLARSHIPS

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

Full Tuition Scholarship, *The Cooper Union* 2024

AWARDS

New York ACS Excellence in Chemistry, *New York Section of American Chemical Society* 2025

Outstanding Presentation in Computational/Theoretical Chemistry, *GCURS Rice University* 2024

Norman Perry ChE '49 Internship Fund, *The Cooper Union* 2024

Daniel E. Kowler ChE ’65 Memorial Prize Fund, *The Cooper Union* 2023

RESEARCH EXPERIENCE

University of Pennsylvania Department of Chemistry — Philadelphia, PA
Graduate Researcher, Advisor: Andrew M. Rappe — 2025 - Present

- Developing a machine learned force field for ferroelectric HfO2 by generating density functional theory (DFT) data and fitting to an artificial neural network
- Computational material science techniques such as pseudopotential planewave DFT to study the relationship between surface chemistry and ferroelectric switching in wurtzite aluminum nitride
- Integrated first-principles simulations with analytical “pencil and paper” theory to study surface charge passivation on AlN slab models relevant for surface engineering for electronic devices

The Cooper Union Department of Chemical Engineering — New York, NY
Undergraduate Researcher, Advisor: Abhishek K. Sharma — 2024 - 2025

- 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

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 in an independently led project studying the photochemistry of 2-hydroxyazobenzene
- 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 - 2024

- Analyzed the decomposition and growth pathways of ammonium nitrate clusters using simulated annealing Monte Carlo and density functional theory in an independently led project
- 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 morphologies

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

University of Pennsylvania Department of Chemistry Philadelphia, PA
Graduate TA 2025 – Present

- Lectured recitations and graded for General Chemistry covering atomic structure, Bohr model, particle-in-a-box, bonding, gas laws, thermochemistry, chemical kinetics, and electrochemistry

The Cooper Union Department of Chemistry New York, NY
Physical Chemistry Tutor 2024 – 2025

- 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 – 2025

- 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)*

[2] Vazquez, J. M.; Ellis, Lucas G.; **Hassan, U. S.**; Sapp, J. R.; Jensen, R. J.; Vaz, S.; Corti, D. S.; and Beaudoin, S. P. The Effect of Particulate Solids and Plasticizer Content of Polymer Formulation on the Measured Forces Via AFM. *The Journal of Adhesion Science and Technolog. (Submitted 2025)*

[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

[5] **Hassan, U. S.**; Behrendt, D.; and Rappe, A. M. *Polar AlN Surfaces and Defect Migration*. The Center for 3D Ferroelectric Microelectronics Manufacturing (3DFeM^2) Thrust 1, Virtual, 2025.

[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.

[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.

[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.

TECHNICAL SKILLS

Computational: Python, Bash, Slurm, High-Performance Computing, JAX-MD, Excel

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

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

RELEVANT COURSEWORK

Graduate level

Quantum Chemistry I, Statistical Mechanics I, Computational Chemistry, Mathematics for Chemistry

Undergraduate

Chemistry: Statistical Mechanics, Physical Chemistry I & II, Organic Chemistry I & II, Organometallic Chemistry, Biochemistry

Mathematics: Linear Algebra, Abstract 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

Engineering: Material Science, Chemical Reaction Engineering, Heat and Mass Transfer, Fluid Dynamics, Separation Principles, Chemical Process Evaluation and Design I & II, Chemical Process Simulation, Chemical Dynamics & Control