

JOHN HYMEL

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EDUCATION

Georgia Institute of Technology

- Atlanta, Georgia
- Ph.D. Graduate Student
- Physical Chemistry
- Expected May 2025

University of Tennessee, Knoxville (2019)

- Knoxville, Tennessee
- B.S. in Chemistry, ACS Certified
- Minor: Mathematics
- GPA: 3.77/4.00, Magna Cum Laude

EXPERIENCE

Graduate Teaching Assistant,

August 2020 - Present

Georgia Institute of Technology, School of Chemistry and Biochemistry

Led two classes of 24 students through Chemical Principles I in a virtual setting.

Higher Education Research Experience (HERE) Intern,

February 2020 - May 2020

Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, Nanomaterials Theory Institute

Advisor: Dr. Bobby Sumpter

Studied applications of vibrational electron energy loss (VEEL) spectroscopy in electron beam - matter interactions.

Performed *ab initio* molecular dynamics simulations on small molecules to understand how changes in beam geometry and strength excite vibrational modes in materials. Compared these results with conventional normal mode analysis.

Undergraduate Research Assistant,

May 2018 - December 2019

University of Tennessee, Department of Chemistry

Advisor: Dr. Konstantinos Vogiatzis

Studied CO₂ gas interactions with calixarenes for development of gas separations. Performed molecular dynamics simulations and electronic structure theory calculations to determine binding sites and energies. Wrote python and bash scripts to facilitate these processes. Succeeded in publishing a paper in the *Journal of Physical Chemistry A* as first author.

Chemistry Undergraduate Teaching Assistant,

August 2019 - December 2019

University of Tennessee, Department of Chemistry

Lead a classroom of 24 students through discussion and problem exercises. Guided students in the laboratory section of the course. Proctored exams and graded homework's.

Math Undergraduate Teaching Assistant,

May 2017 - August 2018

University of Tennessee, Department of Mathematics

Assisted the professor in the classroom; helped students with group work problems during in-class activities; graded tests, homework, and in-class assignments.

TECHNICAL SKILLS

Programming: Python3, NumPy, Pandas, SciPy, Git, Unix/Linux, Slurm Workload Manager, Torque-PBS

Chemistry Software: NWChem, TurboMole, Psi4, Gaussian09, LAMMPS, ChemCraft, Avogadro, MolSimplify,

PUBLICATIONS

- (1) Townsend, J.; Micucci, C. P.; Hymel, J. H.; Maroulas, V.; Vogiatzis, K. D. Representation of Molecular Structures with Persistent Homology for Machine Learning Applications in Chemistry. *Nat. Commun.*, **2020**, 11 (1), 3230. <https://doi.org/10.1038/s41467-020-17035-5>.
 - (2) Hymel, J. H.; Townsend, J.; Vogiatzis, K. D. CO₂ Capture on Functionalized Calixarenes. A Computational Study. *J. Phys. Chem. A* **2019**, 123 (43), 10116-10122. <https://doi.org/10.1021/acs.jpca.9b08670>.
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PRESENTATIONS

Center of Nanophase Materials Sciences Directed Nanoscale Transformations (CNMS DNT) Town Hall (talk)

Virtual meeting with ORNL CNMS staff and collaborators, June 2020

First principles simulation of vibrational response to point-source electric fields

South Eastern Regional Meeting of the American Chemical Society (SERMACS) (talk)

Savannah, Georgia, October 2019

CO₂ Capture on Functionalized Calixarenes. A Computational Study

Eastman-NETSACS Student Research Symposium (poster)

Kingsport, Tennessee, October 2019

CO₂ Capture on Functionalized Calixarenes. A Computational Study

South Eastern Theoretical Chemistry Association (SETCA) Meeting (poster)

Knoxville, Tennessee, May 2019

A Computational Study of CO₂ Interactions with Calixarenes

Exhibition of Undergraduate Research and Creative Achievement (EURECA) (poster)

Knoxville, Tennessee, April 2019

A Computational Study of CO₂ Interactions with Calixarene Molecules

Award of Excellence in Natural Sciences

Office of Research and Engagement Bronze Award

AWARDS

- TACC Computational Research Techniques Fellowship Award (2020)
- Distinction in Undergraduate Research Award (2019)
- ETS-ACS Undergraduate Senior Award (2019)
- C.A. Buehler Chemistry Scholarship (2019)
- Award of Excellence, *EURECA* (2019)
- Office of Research and Engagement Bronze Award, *EURECA* (2019)
- Phi Beta Kappa Honors Society (2018)
- A.D. Melaven-Rhenium Scholarship (2018, 2019)
- CRC Press General Chemistry Award (2016)

ORGANIZATIONS

Student Members of the American Chemical Society (SMACS), *University of Tennessee*

Member (2015-2020), President (2018-2019)

Responsibilities included planning events and meetings for the club; arranging for guest speakers, faculty, and graduate students to present at club meetings; arranging and planning a high school mentoring day for local high school students to tour the UTK chemistry department facilities; fundraising through the sale of molecular modeling kits to organic chemistry students at University of Tennessee.

VOLUNTEERING

Chemistry Outreach, *University of Tennessee*

August 2016 – May 2020

Assisted Dr. Al Hazari in performing roughly fifteen chemistry “magic shows” for audiences ranging from 50 - 100 parents and young children showcasing simple but visually stimulating chemical reactions. Heavily involved in planning and preparation of reagents and apparatuses as well as on-stage demonstrations.

Science Olympiad, *University of Tennessee*

May 2018, May 2019

Worked with other volunteers to ensure the safety of 48 teams of high school and middle school students while they participated in a chemistry-based competition. Judged results of the competition upon completion.

South Appalachian Science and Engineering Fair (SASEF), *University of Tennessee*

April 2019

Served as a judge for a science fair consisting of 132 teams. Duties included interviewing teams about their projects and working with other judges to determine rankings for projects. Gave two special awards as a representative of the East Tennessee Section of the American Chemical Society.
