JOHN HYMEL

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EDUCATION

University of Tennessee, Knoxville (Class of 2019)
B.S. in Chemistry, ACS Certified
Minor: Mathematics
GPA: 3.77/4.00, Magna Cum Laude

EXPERIENCE

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 CO_2 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 (bash scripting), Slurm Workload Manager, Torque-PBS
Chemistry Software: NWChem, TurboMole, Psi4, Gaussian09, LAMMPS, ChemCraft, Avogadro, MolSimplify, LigParGen

ORGANIZATIONS

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

Student Physics Society (SPS), *University of Tennessee*
Active Member (2015–2019)
Participated in science outreach and leading interactive science experiments at local elementary school; assisted with Boy Scout merit badge seminars for Electricity, Electronics, and Energy merit badges.

AWARDS

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

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.

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. CO_2 Capture on Functionalized Calixarenes. A Computational Study. *J. Phys. Chem. A* **2019**, *123* (43), 10116–10122. https://doi.org/10.1021/acs.jpca.9b08670.

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
CO_2 Capture on Functionalized Calixarenes. A Computational Study

Eastman-NETSACS Student Research Symposium (poster)
Kingsport, Tennessee, October 2019
CO_2 Capture on Functionalized Calixarenes. A Computational Study

South Eastern Theoretical Chemistry Association (SETCA) Meeting (poster)
Knoxville, Tennessee, May 2019
A Computational Study of CO_2 Interactions with Calixarenes

Exhibition of Undergraduate Research and Creative Achievement (EUReCA) (poster)
Knoxville, Tennessee, April 2019
A Computational Study of CO_2 Interactions with Calixarene Molecules
Award of Excellence in Natural Sciences
Office of Research and Engagement Bronze Award

Undergraduate Research Symposium, University of Tennessee (talk)
Knoxville, Tennessee, April 2019
Elucidating the Nature of the Interaction between CO_2 and Functionalized Calixarene Species