Pyuskulyan, Arthur

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Education

- **University of California, Merced** — **Merced, CA**
  Ph.D., Chemistry — 2021 - current
- **University of California, Irvine** — **Irvine, CA**
  B.S. Physics — 2016 - 2019
- **Los Angeles City College** — **Los Angeles, CA**
  Transfer — 2012 - 2016

Research Experience

- **Department of Chemistry and Biochemistry, UC Merced** — **Merced, CA**
  Graduate Student Researcher, Professor Christine Isborn's group — 7/2021 - 12/2027
  - Performing ground and excited state classical and quantum molecular dynamics simulations for molecules in the gas and condensed phases, modeling electronic structure, dynamics, linear, and nonlinear spectroscopy.
  - Writing and optimizing scalable code to streamline data analysis and enhance computational workflows.
  - Collaborating on research projects, contributing to publications, and advancing methodologies for understanding molecular dynamics, electronic structure, and spectroscopy, while comparing models to experiments.
  -Codeveloping projects, writing, and contributing to publications.
- **Department of Chemistry, and Physics and Astronomy, UC Irvine** — **Irvine, CA**
  Undergraduate Researcher, Professor Kieron Burke's group — 1/2019 - 2/2020
  • Performed calculations on diamagnetic molecules using density functional theory to compute electric field gradients, nuclear magnetic resonance chemical shifts, and magnetic anisotropies.
  • Utilized various functionals and pseudopotentials, and analyzed the data with scripting and statistical methods.
  • Delivered insights into the relationship between computational methods and physical properties, contributing to the development of accurate predictive models.
- **Department of Physics and Astronomy, UC Irvine** — **Irvine, CA**
  Undergraduate Researcher, Professor Jing Xia's group — 5/2017 - 9/2018
  -Synthesized crystals, spots welded and soldered, prepared experiments in a dilution fridge, and analyzed the data (mainly for determining topological effects of topological insulators).

Technical Skills

- Programming Languages: Python, Mathematica, Fortran
- Technical Programs: TeraChem, Gaussian, AMBER, LaTeX, Bash

Presentations

- "Comparison of trajectory-based correlation function and Franck-Condon methods in optical spectroscopy: insights into spectral broadening and molecular interactions," oral presentation at the American Chemical Society Spring Meeting, San Diego, California, March 2025
- "Static and Dynamic Condensed Phase Linear and Nonlinear Optical Spectroscopy Through Second-Order Cumulant-Based Correlation Function and Franck-Condon Methods," poster at the West Coast Theoretical Chemistry Conference, UC Merced, California May 2024
- "Condensed Phase Optical Absorption and Emission Spectra: Comparison of Trajectory-based Correlation Function and Franck-Condon Methods," oral presentation at the American Chemical Society Spring Meeting, New Orleans, Louisiana, March 2024
- Condensed Phase Optical Spectroscopy Modeled by Dynamic Cumulant Correlation Function and Static Ensemble Franck-Condon Methods," poster at the Time Dependent Density Functional Theory School and Workshop, Rutgers University, New Jersey, June-July 2023
- "Predicting Nuclear Magnetic Resonance Parameters in Ceramics Using Density Functional Theory," poster at the SoCal Undergraduate Chemistry Research Symposium, UC Irvine, California 2019
- "Predicting Nuclear Magnetic Resonance Parameters in Ceramics Using Density Functional Theory," poster at the University of Southern California's SoCal Theo Chemistry Conference, University of Southern California, May 2019
- "Band Gap Evolution in Ytterbium Hexaboride Under Uniaxial Strain," poster at the UC Irvine's Undergraduate Research Symposium 2018

Honors and Awards

- Chemistry and Biochemistry department travel award — March 2024
- Chemistry and Biochemistry department summer fellowship — Summer 2023
- Chemistry and Biochemistry department travel award — July 2023
- UC Irvine Undergraduate Research Opportunities Program research grant — 2018
- National Science Foundation S-STEM Program Scholarship — 9/2017 - 6/2019
- Phi Theta Kappa College Honors Society President — 9/2014 - 6/2016
- Nathaniel Kirshner Scholarship — 3/2015
- Ralph Bunche Scholars Program — 3/2014 - 6/2015

Teaching and Service

- **UC Merced Undergraduate Research Opportunities Program** — **Merced, CA**
  Mentor for the Summer Undergraduate Research Institute — Summer 2024
  -Mentored undergraduate student starting summer 2024 (I still mentor him today, as he is still in our research group) in research to perform molecular dynamics simulations, electronic structure calculations, model spectroscopy, and perform analysis.
- **American Chemical Society** — **Merced, CA**
  Mentor for the Summer Experiences for the Economically Disadvantaged — Summer 2024

-Mentored local high school student from Merced High School (who is currently a UC Merced freshman) in research to perform molecular dynamics simulations, electronic structure calculations, model spectroscopy, and perform analysis.

- **American Chemical Society** **New Orleans, Louisiana**
  Spring March meeting session presider March 2024
  -Presider for a Quantum Mechanics session
- **University of California, Merced** **Merced, CA**
  Teaching assistant
  Chem 1 Preparatory chemistry Fall 2022, Spring 2023
  Chem 2H Honors General chemistry 1 lab and discussion Fall 2024
  Chem 10 General chemistry 2 lab and discussion Fall 2021, Spring 2022
  Chem 10H Honors General chemistry 2 lab and discussion Spring 2025
  Chem 112 Quantum chemistry and spectroscopy Fall 2023
  Chem 130 Organic spectroscopy and computation Spring 2023
- **University of California, Merced** **Merced, CA**
  Secretary of the graduate chemistry club Ground State Spring 2022 - Spring 2024
  -Helped organize social and professional events
- **Mission Academy Charter High School** **Pacoima, CA**
  Teaching assistant and tutor 6/2020 - 11/2020
  -Helped teach algebra and geometry, tutored students, and graded assignments
- **Resonance Mentoring Program, Department of Physics, UC Irvine** **Irvine, CA**
  Mentor 1/2018 - 12/2019
  -Mentored freshmen to junior students, tutored them with their courses, and helped students overcome hardships associated with being a first-generation student or other socioeconomic factors
  -Helped students join research groups, familiarizing them with research and resources such as applying for scholarships and grants
- **Grade Potential Tutoring** **Los Angeles, CA**
  Tutor 12/2019 - 4/2021
  -Tutored high school and college students with their physics, chemistry, and math courses

Publications

Christopher A. Myers, Shao-Yu Lu, Sapana Shedge, **Arthur Pyuskulyan**, Katherine Donahoe, Ajay Khanna, Liang Shi, and Christine M. Isborn. Axial H-bonding Solvent Controls Inhomogeneous Spectral Broadening, While Peripheral H-bonding Solvent Controls Vibronic Broadening: Cresyl Violet in Methanol. *The Journal of Physical Chemistry B*, 128(23):5685–5699, 2024