

Abdul Zamani

Ph.D. | Theoretical Chemistry

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Research Interests

Molecular electronic structure; excited states; molecular spectroscopy; electron correlation; spin symmetry; chemical catalysis; high performance computing; software development

Education

University of California, Merced

Ph.D. Chemistry

Merced, California

Aug 2018 – Dec 2023

La Sierra University

B.S. Biochemistry

Riverside, California

Aug 2014 – Jun 2017

Riverside City College

Riverside, California

Jun 2012 – Jun 2014

Research Experience

University of Pittsburgh | Department of Chemistry

Jun 2024 – Present

Postdoctoral Associate | Advisor: Kevin Carter-Fenk

UC Merced | Department of Chemistry and Biochemistry

Jun 2018 – Dec 2023

Graduate Student Researcher | Advisor: Hrant P. Hratchian

La Sierra University | Department of Chemistry and Biochemistry

Jun 2015 – Jun 2017

Undergraduate Student Researcher | Advisor: Marco M. Allard

Publications

A.Y. Zamani and H.P. Hratchian. "Estimating vertical core excitation energies from Møller Plesset theory with spin projection." *Mol. Phys.* e2398142 (2024)

A.Y. Zamani and H.P. Hratchian. " Δ -based composite models for calculating X-ray absorption and emission energies." *J. Chem. Phys.* **159**, 224109 (2023)

H.H. Corzo, A.E. Hillers-Bendtsen, A. Barnes, **A.Y. Zamani**, F. Pawlowski, J. Olsen, P. Jørgensen, K.V. Mikkelsen and D. Bykov. "Coupled Cluster Theory on Modern Heterogeneous Supercomputers." *Front. Chem.* **11**, 1154526 (2023)

A.Y. Zamani and H.P. Hratchian. "Assessing the performance of Δ SCF and the diagonal second-order self-energy approximation for calculating vertical core excitation energies." *J. Chem. Phys.* **157**, 084115 (2022)

Teaching Experience

UC Merced | Department of Chemistry and Chemical Biology

Aug 2018 – Present

Graduate Teaching Assistant

- CHEM 001 – Preparatory Chemistry
- CHEM 002, 010 – General Chemistry I, II
- CHEM 112 – Quantum Chemistry and Spectroscopy

La Sierra University | Department of Chemistry and Biochemistry

Jun 2015 – Jun 2017

Undergraduate Teaching Assistant

- CHEM 281L, 282L, 283L – Organic Chemistry I, II, III Laboratory

Other Employment

University of Redlands | Department of Biology and Chemistry

Sep 2017 – May 2018

Laboratory Assistant

Selected Honors and Awards

Chemistry and Chemical Biology Summer Research Fellowship | UC Merced *2019 - 2020*

Chemistry Graduate Student Travel Award Fellowship | UC Merced *2019*

Competitive Edge Summer Bridge Fellowship | UC Merced *2018*

Leland Wilson Memorial Chemistry & Biochemistry Scholarship | La Sierra University *2017*

Greater Riverside Dollars for Scholars Scholarship *2012*

Presentations

63rd Sanibel Symposium | St. Augustine Beach, FL | Poster *Feb 2024*

West Coast Theoretical Chemistry Meeting | Davis, CA | Poster *May 2023*

Advanced Light Source User Meeting | Virtual | Poster *Aug 2022*

10th Conference on Molecular Quantum Mechanics | Blacksburg, VA | Poster *Jun 2022*

ACS National Meeting | San Diego, CA | COMP: Contributed Talk *Mar 2022*

ACS National Meeting | San Diego, CA | COMP & Sci-Mix Poster *Aug 2019*

Service Activities

Competitive Edge Summer Bridge Program | Graduate Mentor *Jul 2022 – Aug 2022*

Assisting incoming students with their transition into graduate studies at UC Merced

ACS National Meeting | San Diego, CA | COMP Session Presider *Aug 2019*

Symposium – *Exploring Transition Metal Chemistry & Spectroscopy with Quantum Chemistry*

Science Outreach Volunteer *May 2017 – May 2019*

Chemistry demonstrations at CA elementary schools – Weaver USD (May 2017), Alvord USD (May 2019); Science Fair Volunteer – Donn B. Chenoweth Elementary School (Nov 2018)

Workshops

9th BerkeleyGW Tutorial Workshop | DOE C2SEPPEM | CSUEB Oakland Center *Feb 2023*

Qiskit Global Summer School | IBM Research | Virtual *Jul 2020*

MolSSI Software Summer School | UT Austin | Texas Advanced Computing Center *Jul 2019*

Technical Skills

Programming Languages – Fortran 90/03 (proficient), Python (basic), C++ (basic)

Tools and Environments – Linux, Slurm, Sun Grid Engine, Nvidia HPC SDK, OpenMP, Vim, git, conda, bash, HTML, L^AT_EX, Gaussian, Q-Chem, UQUANTCHEM, Orca, DoNOF, Mathematica, GaussView, IQmol, Inkscape

Data Science Techniques – Exploratory Data Analysis, Supervised Machine Learning (regression, classification, cross-validation); Libraries – pandas, scikit-learn, NumPy, SciPy