O. Jonathan Fajen

47 Olmsted Rd, Apt 237 ● Stanford, California 94305 ● (573) 823-0090

ojfajen@stanford.edu

EDUCATION

Stanford University, Stanford, California, 2021-

Ph.D., Theoretical Chemistry

Research advisor: Todd Martinez

University of Missouri, Columbia, Missouri, 2018-2021

Bachelor of Science in Chemistry, Summa Cum Laude with Honors in Chemistry

Minor in Mathematics

GPA: 3.99/4.00

EXPERIENCE

Graduate Student, Martinez Group, June 2021-

Chemistry Department, Stanford University/SLAC

Worked on applying rank-reduction to high-order tensors in electron correlation theories, in particular rank-reduced coupled cluster theory (RR-CC2, RR-CCSD) to calculate electronic excitation energies, properties of large molecular systems.

GPU accelerated CC2, EOM-CC2 code in TeraChem for calculation of ground and excited-state electronic energies.

Undergraduate Research Assistant, Walensky and Brorsen Groups, June 2018-May 2021

Chemistry Department, University of Missouri, Columbia

Synthesized, studied reactivity of, and characterized spectroscopically various novel organoactinide complexes featuring pnictogen- and chalcogen-based ligands.

Investigated electronic and magnetic properties of organoneptunium complexes using computational methods.

Applied coupled cluster and second-order vibrational perturbation theory to predict rovibrational lines of astrochemically-relevant small organic molecules.

Worked on development and benchmarking of *ab initio* multicomponent methods, including orbital-optimized second-order perturbation theory (NEO-OO-MP2), multireference active space approaches (NEO-CASSCF), and coupled cluster theory (NEO-CCSD).

Summer Researcher at the University of Minnesota, Gagliardi Group, June-August 2020

Chemistry Department, University of Minnesota, Minneapolis (Remote)

Applied machine learning to automate active space selection in multireference (CASSCF) calculations.

Graduate Teaching Assistant, September 2021-June 2022

Stanford University

CHEM 31A (General Chemistry I), Fall 2021

CHEM 31B (General Chemistry II), Winter 2022

CHEM 33 (Organic Chemistry I), Spring 2022

Undergraduate Teaching Assistant, August-December 2020

University of Missouri, Columbia

Led recitation and lab sections for General Chemistry II (~50 students)

AWARDS

National Merit Scholar, 2018

Summer Stephen's Fellow (University of Missouri Department of Chemistry), 2018

University of Missouri Honors College Discovery Fellow, 2018-20

University of Minnesota Chemical Theory Center Summer Undergraduate Research Fellowship, 2020

Goldwater Scholar, 2020

Department of Energy Computational Science Graduate Fellowship, 2022

PUBLICATIONS

Rungthanaphatsophon, P., Fajen, O. J., Kelley, S. P., Walensky, J. R. Thorium(IV) and Uranium(IV) Phosphaazaallenes. *Inorganics.* **2019**, *7*, 105.

Fajen, O.J., Brorsen, K.R. Separation of electron-electron and electron-proton correlation in multicomponent orbital-optimized perturbation theory. *J. Chem. Phys.* **2020,** *152,* 194107.

Fajen, O.J., Brorsen, K.R. Multicomponent CASSCF revisited: Large active spaces are needed for qualitatively accurate protonic densities. *J. Chem. Theory Comput.* **2021**, *17*, 965.

Tarlton, M.L., Fajen, O.J., Kelley, S.P., Kerridge, A., Malcomson, T., Morrison, T.L., Shores, M.P., Xhani, X., Walensky, J.R. Systematic investigation of the molecular and electronic structure of thorium and uranium phosphorous and arsenic complexes. *Inorg. Chem*. **2021**, *60*, 10614.

Fajen, O.J., Brorsen, K.R. Multicomponent MP4 and the inclusion of triple excitations in multicomponent many-body methods. *J. Chem. Phys.* **2021**, *155*, 234108.

PRESENTATIONS

Fajen, O.J., Tarlton, M.L., Murray, M.J., Walensky, J.R. Synthesis of new ylides for their reactivity to form actinide-carbene complexes. Presented at the University of Missouri Summer Undergraduate Research Forum, 07/26/18.

Fajen, O.J., Jeong, W.S., Gagliardi, L. Machine learning for automated selection of active spaces in multiconfigurational calculations. Presented virtually at the University of Minnesota Chemical Theory Center Summer Research Symposium, 08/12/2020.

Fajen, O.J., Brorsen, K.R. Separation of electron-electron and electron-proton correlation in multicomponent orbital-optimized perturbation theory. Presented virtually at the Gulf Coast Undergraduate Research Symposium at Rice University, 10/31/20. Awarded "Outstanding Presentation in Theoretical Chemistry."