

James E. T. Smith

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Education

- 2014–2020 **PhD (Expected)**, *University of Colorado Boulder, Boulder, Chemical Physics.*
GPA: 3.94
- 2010–2014 **B.S.**, *Davidson College, Davidson, NC, Chemistry (Minor in Mathematics).*
Overall GPA: 3.67 Major GPA: 3.87

Fellowships

- 2019–2020 **MolSSI Phase-II Software Fellow.**
- 2018–2018 **MolSSI Phase-I Software Fellow.**
- 2016–2018 **GAANN Fellow.**

Experience

Graduate

- 2016–Present **Research Assistant, Sharma Group, Chemistry Dept., University of Colorado Boulder, Boulder, CO.**
- Worked on the implementation of Heat-bath configuration interaction (HCI) method in conjunction with [PySCF](#) software and developed embedding methods using HCI to investigate previously intractable systems.
 - Maintained the group webpage and the [Dice](#) documentation website.
 - Frequently contribute to the [PySCF](#) quantum chemistry package.
- Summer 2019 **Research Intern, Center for Computational Quantum Physics, Flatiron Institute, New York, New York.**
- Studied the applicability of correlated molecular methods to strongly interacting materials under the supervision of Prof. Tim Berkelbach and Dr. Xaio Wang.
 - Implemented a quantum chemistry interface between the [NetKet](#) package and [PySCF](#) under the supervision of Dr. Giuseppe Carleo.
- 2014–2016 **Research Assistant, Weber Group, JILA/University of Colorado Boulder, Boulder, CO.**
- Studied the effect of solvation on water oxidation catalysts and fundamental physical phenomena involved in trapping and cooling ions.
 - Organized "super-group" meetings between the Weber, Bierbaum, Ellison, and Lineberger Groups.
- Spring 2016 **Head Teaching Assistant, University of Colorado Boulder, Boulder, CO.**
- Organized the weekly TA meetings and mentored younger TAs.
 - Helped the lab instructor and coordinator prepare labs and course material.
 - Taught one section of laboratory and recitation for General Chemistry 2.
- 2014–2016 **Teaching Assistant, University of Colorado Boulder, Boulder, CO.**
- Taught two sections of laboratory and recitation for General Chemistry 1 or 2 (CHEM 1114 and 1134) each semester.
 - Met each week with course instructor and other TAs to discuss the curriculum and modify it to improve its effectiveness for future semesters.

- 2015–Present **Personal Tutor**, *Self Employed*, Boulder, CO.
- Work with high school and college students in personal and small group tutoring sessions to improve understanding of fundamental chemical concepts, develop good studying and test-taking strategies, and foster an interest in science and math.
- Spring 2015 **PhET Developer**, *PhET Interactive Simulations*, Boulder, CO.
- Updated simulations created by the PhET department and made them more accessible to students by porting them from Java to HTML5.
 - Collaborated with full time developers to improve the functionality of simulations by modifying the original simulation code.
- Undergraduate**
- Summer 2013 **DRI Fellow**, *Chemistry Dept., Davidson College*, Davidson, NC.
- Built a Resonance Raman Spectrometer and used it in conjunction with Gaussian09 to develop a model for various dyes used in dye-sensitized solar cells so more efficient dyes could be predicted for future solar cells.
 - Worked with one other researcher to improve the current technique of assembling dye-sensitized solar cells and created an instrument to measure the efficiency of these cells.
- 2012–2014 **Chemistry and Math Tutor**, *Math and Science Center, Davidson College*, Davidson.
- Position only offered to students recommended by multiple faculty members.
 - Tutored individual and small groups of students in all levels of calculus, organic and inorganic chemistry on a regular weekly schedule.
- Summer 2012 **Research Assistant**, *Chemistry Dept., Davidson College*, Davidson, NC.
- Worked collaboratively in a two-person team to design an experiment that characterized the pathways and products of the oxidation of isoprene to try to find new methods of aerosol reduction in the atmosphere.
- Spring 2012 **Lab Assistant for Organic Chemistry II**, *Chemistry Dept., Davidson College*, Davidson, NC.
- Taught 14 students introductory organic chemistry lab techniques with Dr. David M. Brown and prepared materials and equipment with Mr. Lee Maiorano.

Computer skills

- Languages C++, Python, Java, JavaScript, HTML
- Collaborative Projects [NetKet](#), [PySCF](#), [Dice](#)
- Other MPI, OpenMP, VTune, MATLAB, Mathematica, Blender, LabView

Publications

- Giuseppe Carleo, Kenny Choo, Damian Hofmann, James E. T. Smith, Tom Westerhout, Fabien Alet, Emily J. Davis, Stavros Efthymiou, Ivan Glasser, Sheng-Hsuan Lin, Marta Mauri, Guglielmo Mazzola, Christian B. Mendl, Evert van Nieuwenburg, Ossian O'Reilly, Hugo Theveniaut, Giacomo Torlai, and Alexander Wietek, "NetKet: A Machine Learning Toolkit for Many-Body Quantum Systems", *SoftwareX* 10, (2019) 100311.
- L. G. Dodson, W. Zagorec-Marks, S. Xu, J. E. T. Smith, J. M. Weber, "Intrinsic photophysics of nitrophenolate ions studied by cryogenic ion spectroscopy", *Phys. Chem. Chem. Phys.* 20 (2018) 28535 - 28543.
- J. E. T. Smith, B. Mussard, A. A. Holmes, S. Sharma, "Cheap and near exact CASSCF with large active spaces", *J. Chem. Theor. and Comp.* 13 (11), (2017) 5468-5478. **(ACS Editor's Choice)**

- S. Xu, J. E. T. Smith, S. Gozem, A. I. Krylov, J. M. Weber, "Electronic Spectra of Tris(2,2'-bipyridine)-M(II) Complex Ions in Vacuo (M = Fe and Os)", *Inorg. Chem.* 56, (2017) 7029–7037.
- Shuang Xu, James E. T. Smith, J. Mathias Weber, " UV Spectra of Tris(2,2'-bipyridine) M(II) Complex Ions in Vacuo (M = Mn, Fe, Co, Ni, Cu, Zn)," *The Journal of Inorganic Chemistry*, 55, (2016): 11937-11943.
- Shuang Xu, James E. T. Smith, J. Mathias Weber, "Hydration of a Binding Site With Restricted Solvent Access: Solvatochromic Shift of the Electronic Spectrum of a Ruthenium Polypyridine Complex, One Molecule at a Time," *Journal of Physical Chemistry A*, 120 (2016): 7650-7658.
- Shuang Xu, James E. T. Smith, and J. Mathias Weber, "The electronic spectrum of cryogenic ruthenium–tris-bipyridine dications in vacuo," *The Journal of Chemical Physics*, 145 (2016): 024304.
- Shuang Xu, James E. T. Smith, and J. Mathias Weber, "Ligand Influence on the Electronic Spectra of Dicationic Ruthenium Bipyridine-Terpyridine Complexes," *The Journal of Physical Chemistry A*, 120, (2016): 2350-2356.

Awards and Honors

- Graduate Teaching Excellence Award
- Graduate Student General Chemistry Teaching Award
- Senior Award for Excellence in Chemistry
- David Halbert Howard Jr. Award
- The Porter Vincent Chemistry Award for Unusual Mastery of Chemistry
- Freshman Award for Excellence in Chemistry
- MCLA Academic All American