James E. T. Smith

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Education

University of Colorado Boulder **Boulder**
PhD, Chemical Physics *2014–Present*
GPA: 3.94

Davidson College **Davidson, NC**
B.S., Chemistry (Minor in Mathematics) *2010–2014*
Overall GPA: 3.67 *Major GPA:* 3.87

Fellowships

- MolSSI Phase-II Software Fellow (January 2019-July 2020)
- MolSSI Phase-I Software Fellow (July 2018-December 2018)
- GAANN Fellow (2016-2018)

Experience

Graduate

Chemistry Department, University of Colorado Boulder **Boulder**
Research Assistant, Sharma Group *Fall 2016–Present*

- Work on the implementation of Heat-bath configuration interaction (HCI) method in conjunction with PYSCF software and develop embedding methods using HCI to investigate previously intractable systems.
- Maintain the group webpage, the Dice documentation website as well as its GitHub repository.
- Frequently contribute to the PySCF quantum chemistry package.

JILA/ University of Colorado Boulder **Boulder**
Research Assistant, Weber Group *Fall 2014–Fall 2016*

- 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.

University of Colorado Boulder **Boulder**
Head Teaching Assistant *Spring 2016*

- 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.

University of Colorado Boulder **Boulder**
Teaching Assistant *Fall 2014–Spring 2016*

- 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.

Self Employed **Boulder**

Personal Tutor *2015–Present*

- 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.

PhET Interactive Simulations **Boulder**

PhET Developer *Jan.–May 2015*

- 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

Davidson College Chemistry Department **Davidson**

DRI Fellow *May–Aug 2013*

- 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.

Davidson College Math and Science Center **Davidson**

Chemistry and Math Tutor *2012–2014*

- 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.

Davidson College Chemistry Department **Davidson**

Research Assistant *May–Aug 2012*

- 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.

Davidson College Chemistry Department **Davidson**

Lab Assistant for Organic Chemistry II *Jan.–May 2012*

- Taught 14 students introductory organic chemistry lab techniques with Dr. David M. Brown and prepared materials and equipment with Mr. Lee Maiorano.

Computer skills

Programming: C++, Python, Java, JavaScript, HTML

Chemistry Software: PYSCF, Q-Chem, Gaussian, GaussView, TurboMole, GAMESS, LAMMPS, GROMACS, IQmol, Jmol, Avogadro, GabEdit

Other Software Experience: MATLAB, Blender, LabView, Mathematica, Origin

Publications

- 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), 5468-5478. **(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