# James E. T. Smith

2020 Lawrence St. Unit 624
Denver 80205
1 (508) 596 7110
james.e.smith@colorado.edu

## Education

2014–Present **PhD**, *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.

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 MATLAB, Blender, LabView, Mathematica

## 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