

# James E. T. Smith

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## 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.

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### Computer skills

Languages	C++, Python, Java, JavaScript, HTML
Collaborative Projects	NetKet, PySCF, Dice
Other	MPI, OpenMP, VTune, MATLAB, Mathematica, Blender, LabView

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### 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. **(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