James E. T. Smith, Ph.D.

Research Interests

Numerical linear algebra, high performance computing, quantum chemistry, quantum computing, machine learning.

Fellowships

2019–2020 MolSSI Phase-II Software Fellow.

2018–2018 MolSSI Phase-I Software Fellow.

2016–2018 GAANN Fellow.

Research Experience

Postdoctoral

2020–Present **Flatiron Research Fellow**, *Center for Computational Quantum Physics*, New York, NY.

- Developed novel stochastic methods to reduce to computational cost of coupled cluster quantum chemistry methods.
- Extended the heath-bath configuration interaction (HCI) algorithm for use in periodic solid-state systems to study the electronic excitations of molecular crystals.
- Organized workshops to help members of the Flatiron community better utilize high performance computing resources as part of the Sciware working group.

Graduate

2016–2020 **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.
- Implemented a hybrid MPI-OpenMP parallelized version of the HCI algorithm in Dice
- Frequently contributed to the PySCF quantum chemistry package, implementing new features and handling bug reports.
- Organized and led a workshop on software best practices for graduate students and post doctoral researchers with staff from the Molecular Sciences Software Institute (MolSSI).
- Maintained the group webpage and the Dice documentation website.

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.

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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.

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.

Teaching Experience

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.

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.

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.

Programming and Computing Skills

Languages Python, C++, Git, Julia, HTML5, JavaScript

Other MPI, OpenMP, VTune, Perf, Github Actions, PyTest, Catch2, DocTest, CodeCov

Open Source Projects

C++ FRI-CC - Using tools from randomized numerical linear algebra to accelerate coupled cluster calculations.
NetKet - Machine learning techniques tackling the many-body problem.
Dice - Fast and approximate configuration interaction solver .

Python PySCF - Quantum chemistry package.
CANTHERM - Thermochemical analysis of quantum chemistry calculations .

Certificates

2021 Software Carpentry Instructor.

2021 NVIDIA DLI Certificate - Accelerating CUDA C++ Applications with Multiple GPUs.

2021 NVIDIA DLI Certificate - Fundamentals of Accelerated Computing with CUDA C/C++.

Preprints

2022 Samuel M. Greene, Robert J. Webber, **James E. T. Smith**, Jonathan Weare, Timothy C. Berkelbach. "Full Configuration Interaction Excited-State Energies in Large Active Spaces from Randomized Subspace Iteration". (2022). https://arxiv.org/abs/2201.12164

James E. T. Smith, Joonho Lee, Sandeep Sharma. "Nuclear Gradients of Near-Exact Complete Active Space Self-Consistent Field Wave Functions". (2022). https://arxiv.org/abs/2201.06514 .

Publications

2020 Wyatt Zagorec-Marks, **James E. T. Smith**, Madison M. Foreman, Sandeep Sharma, J. Mathias Weber. "Intrinsic Electronic Spectra of Cryogenically Prepared Protoporphyrin IX Ions in Vacuo – Deprotonation-Induced Stark Shifts". Physical Chemistry Chemical Physics (2020) 22, 20295-20302.

Qiming Sun, Xing Zhang, Samragni Banerjee, Peng Bao, Marc Barbry, Nick S. Blunt, Nikolay A. Bogdanov, George H. Booth, Jia Chen, Zhi-Hao Cui, Janus Juul Eriksen, Yang Gao, Sheng Guo, Jan Hermann, Matthew R. Hermes, Kevin Koh, Peter Koval, Susi Lehtola, Zhendong Li, Junzi Liu, Narbe Mardirossian, James D. McClain, Mario Motta, Bastien Mussard, Hung Q. Pham, Artem Pulkin, Wirawan Purwanto, Paul J. Robinson, Enrico Ronca, Elvira Sayfutyarova, Maximilian Scheurer, Henry F. Schurkus, **James E. T. Smith**, Chong Sun, Shi-Ning Sun, Shiv Upadhyay, Lucas K. Wagner, Xiao Wang, Alec White, James Daniel Whitfield, Mark J. Williamson, Sebastian Wouters, Jun Yang, Jason M. Yu, Tianyu Zhu, Timothy C. Berkelbach, Sandeep Sharma, Alexander Sokolov, Garnet Kin-Lic Chan. "Recent developments in the PySCF program package". *J. Chem. Phys.* 153 (2020) 024109.

Joel W. Clancey, Andrew S. Cavanagh, **James E. T. Smith**, Sandeep Sharma, and Steven M. George. "Volatile Etch Species Produced During Thermal Al_2O_3 Atomic Layer Etching", *J. Phys. Chem. C*, 124, (2020) 287-299. .

2019 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 .

2018 Leah G. Dodson, Wyatt Zagorec-Marks, Shuang Xu, **James E. T. Smith**, J. Mathias Weber, "Intrinsic photophysics of nitrophenolate ions studied by cryogenic ion spectroscopy", *Phys. Chem. Chem. Phys.* 20 (2018) 28535 - 28543 .

2017 **James E. T. Smith,** Bastien Mussard, Adam A. Holmes, Sandeep Sharma, "Cheap and near exact CASSCF with large active spaces", *J. Chem. Theor. and Comp.* 13 (11), (2017) 5468-5478. (ACS Editor's Choice) .

2016 Shuang Xu, **James E. T. Smith**, Samer Gozem, Anna I. Krylov, J. Mathias 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

2016 Graduate Teaching Excellence Award.

2015 Graduate Student General Chemistry Teaching Award.

2014 Senior Award for Excellence in Chemistry
MCLA Academic All American.

2013 David Halbert Howard Jr. Award.

2012 The Porter Vincent Chemistry Award for Unusual Mastery of Chemistry.

2011 Freshman Award for Excellence in Chemistry.