James E. T. Smith, Ph.D.

Research Interests

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

Education

2020 PhD Chemical Physics, *University of Colorado Boulder*, GPA: 3.94

2014 B.S. Chemistry, Minor in Mathematics, *Davidson College*, GPA: 3.67

Experience

July 2022–Present **Member of the Technical Staff**, *Lucata Coporation*, New York, NY

- Worked with a team of five to implement the GraphBLAS library in C/C++ and optimized it for Lucata's custom hardware targets.
- Restructured the build system for the GraphBLAS project and set up continuous integration, testing, and code coverage.
- Collaborated with other teams regularly to address bugs and implement new features in the GraphBLAS library.

Postdoctoral

2020–2022 **Flatiron Research Fellow**, *Center for Computational Quantum Physics*, New York, NY

- Implemented OpenMP parallelized stochastic compression methods for quantum chemistry in the open source C++ package FRI-CC.
- Contributed features, bug fixes, and documentation as one of the primary maintainers for the open source Python/C package PySCF.
- Worked closely with the core team of PySCF developers improve the CMake build system and PyPI distribution after the release of PySCF v2.0.0.
- 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

- Implemented a hybrid MPI-OpenMP parallelized version of the HCI algorithm in the Sharma Group's C++ software Dice
- Built decision tree and graph neural network models to predict etching reaction outcomes and trained these models with experimentally observed data.
- Wrote a new module for the PySCF package to interface with Dice enabling the investigation previously intractable systems.
- 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).

Summer 2019 **Research Intern, Center for Computational Quantum Physics**, *Flatiron Institute*, New York, New York

- Implemented a quantum chemistry interface between the C++/Python package NetKet and PySCF under the supervision of Dr. Giuseppe Carleo.

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

- Developed a suite of Matlab software tools to standardize and automate data analysis for the Weber group.
- Studied ultra-cold molecules with using quantum chemical calculations and optical spectroscopy.

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.

Teaching Experience

2021-Present **Software Carpentries Instructor**, New York, NY

- Taught regularly about software best practices in scientific computing to learners with a broad programming background.
- Taught lessons on shell, Git, Python, and data visualization in Python.

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.

Programming and Computing Skills

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

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

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

Fellowships

2019–2020 MolSSI Phase-II Software Fellow

2018–2018 MolSSI Phase-I Software Fellow

2016–2018 GAANN Fellow

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++

Publications

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 Subspace Iteration with Repeated Random Sparsification". (2022). Journal of Chemical Theory and Computation (2022) DOI: https://doi.org/10.1021/acs.jctc.2c00435

James E. T. Smith, Joonho Lee, Sandeep Sharma. "Nuclear Gradients of Near-Exact Complete Active Space Self-Consistent Field Wave Functions". Journal of Chemical Physics (2022) 157 094104.

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)

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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

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