Benjamin P. Pritchard

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Employment

Molecular Sciences Software Institute at Virginia Tech — **Blacksburg, VA**
Software Scientist — *2017–current*

- TBD

Georgia Institute of Technology — **Atlanta, GA**
Postdoctoral Associate — *2015–2017*

- Mentor: Dr. Edmond Chow
- Development of the Simint open-source two-electron integral library and the Pulsar computational chemistry framework

Virginia Polytechnic Institute and State University — **Blacksburg, VA**
Postdoctoral Associate — *2014–2015*

- Mentor: Dr. T. Daniel Crawford
- Development of the PANACHE open-source density fitting & approximate integral library

University at Buffalo, State University of New York — **Buffalo, NY**
Teaching Assistant — *2008–2012*

- Assisted in undergraduate general chemistry, as well as upper-level physical chemistry (including laboratory)

Xerox Corporation — **Webster, NY**
Analytical Polymer Chemist — *2005–2008*

- Analyzed toner formulations using modern instrumentation and wet lab techniques

Education

University at Buffalo, State University of New York — **Buffalo, NY**
Ph.D. – Computational Chemistry — *February 2014*

- Mentor: Dr. Jochen Autschbach
- GPA: 3.89/4.00

Rochester Institute of Technology — **Henrietta, NY**
Bachelor of Science – General Chemistry — *June 2008*

- Graduated with Honors (GPA: 3.49/4.00). Placed on Dean's List 6 times
- Undergraduate Research (2007 – 2008)
- Teaching Assistant for Quantitative Analysis (2007 – 2008)

Medina High School — **Medina, NY**
New York State Regents Diploma — *June 2003*

- Majored in Math, Science, Music, and Spanish
- National Honor Society, Scholar/Athlete, and AP Scholar with Distinction awards

Research Interests

My main research interests involve the development of open-source software for use in computational chemistry. This includes applying modern programming practices and techniques to high-level issues such as software architecture, program design, and clean interfaces, while also taking into consideration efficiency and optimization when required.
My research projects include:

- Development of the Simint library (https://www.bennyp.org/simint)
  - Efficient calculation of electron repulsion integrals. Speedup is obtained on specific microarchitectures through the use of both manual and automatic vectorization
  - Emphasis on a simple, straightforward C interface
  - Developed as part of the Intel Parallel Computing Center at Georgia Tech
- Development of the Pulsar framework (https://github.com/pulsar-chem)
  - C++/Python framework for computational chemistry
  - Highly modular (via plugins), which allows for fast prototyping and development, particularly when distributed among different developers and research groups
  - Designed for interoperability between different libraries and between full computational chemistry packages.
- Development of the PANACHE library
  - Allows for easy and efficient incorporation of density fitting and Cholesky decomposition into existing computational chemistry packages
  - High-level C++11 code, with interfaces for C and Fortran
- Calculation of ESR/EPR and NMR properties of transition metal, lanthanide, and actinide complexes using DFT and multi-determinant methods
- Code development for ADF and MolCAS, along with custom applications
  - Implemented initial hyperfine tensor support in MolCAS
  - Added functionality to generate natural orbital plots that included spin-orbit coupling and allowed for mixing of spin-orbit states (MolCAS)
  - Added the ability to plot spin magnetization in ADFView
  - Implementation and benchmarking of magnetic properties in ADF and NWChem
  - Custom C/C++ programs to calculate vibrationally-resolved optical spectra and to calculate PNMR shifts (including ZFS contributions) from the outputs of computational chemistry software

Skills

- Excellent computer programming skills. Experienced C/C++ programmer (including C++11/14), and experience with Python, Fortran (77, 90, 2003), Mathematica, and GUI programming (ncurses, Qt). Workflow optimization with BASH & Python
- Practical experience with high-performance computing, including MPI programming and job/batch scheduling
- Experience developing for the Intel Xeon Phi (KNC and KNL), including setup and maintenance
- Familiar with industry-standard tools such as git, CMake, and modern compilers, debuggers, and profilers
- Experience with many of the commonly-used computational chemistry codes, such as Psi4, ADF, NWChem, MolCAS, Turbomole, and Gaussian, including installation and troubleshooting
- Passionate about teaching and mentoring others
- Lifelong, self-directed learner, particularly with new programming languages and techniques

Selected Publications

- Benjamin P. Pritchard and Edmond Chow. Horizontal vectorization of electron repulsion integrals. *Journal of Computational Chemistry*, 37(28):2537–2546, 2016
- Francesco Aquilante, Jochen Autschbach, Rebecca K. Carlson, Liviu F. Chibotaru, Mickaël G. Delcey, Luca De Vico, Ignacio Fdez. Galván, Nicolas Ferré, Luis Manuel Frutos, Laura Gagliardi, Marco Garavelli, Angelo Giussani, Chad E. Hoyer, Giovanni Li Manni, Hans Lischka, Dongxia Ma, Per Åke Malmqvist, Thomas Müller, Artur Nenov, Massimo Olivucci, Thomas Bondo Pedersen, Daoling Peng, Felix Plasser, Ben Pritchard, Markus Reiher, Ivan Rivalta, Igor Schapiro, Javier Segarra-Martí, Michael Stenrup, Donald G. Truhlar, Liviu Ungur, Alessio Valentini, Steven Vancoillie, Valera Veryazov, Victor P. Vysotskiy, Oliver Weingart, Felipe Zapata, and Roland Lindh. Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, 37(5):506–541, 2016
- Kamal Sharkas, Ben Pritchard, and Jochen Autschbach. Effects from spin–orbit coupling on electron–nucleus hyperfine coupling calculated at the restricted active space level for kramers doublets. *Journal of Chemical Theory and Computation*, 11(2):538–549, 2015
- Benjamin P. Pritchard, Scott Simpson, Eva Zurek, and Jochen Autschbach. Computation of chemical shifts for paramagnetic molecules: A laboratory experiment for the undergraduate curriculum. *Journal of Chemical Education*, 91(7):1058–1063, 2014
- Ben Pritchard and Jochen Autschbach. Theoretical investigation of paramagnetic NMR shifts in transition metal acetylacetonato complexes: Analysis of signs, magnitudes, and the role of the covalency of ligand–metal bonding. *Inorganic Chemistry*, 51(15):8340–8351, 2012
- Fredy Aquino, Ben Pritchard, and Jochen Autschbach. Scalar relativistic computations and localized orbital analyses of nuclear hyperfine coupling and paramagnetic NMR chemical shifts. *Journal of Chemical Theory and Computation*, 8(2):598–609, 2012
- Jochen Autschbach, Serguei Patchkovskii, and Ben Pritchard. Calculation of hyperfine tensors and paramagnetic NMR shifts using the relativistic zeroth-order regular approximation and density functional theory. *Journal of Chemical Theory and Computation*, 7(7):2175–2188, 2011
- Jochen Autschbach and Benjamin Pritchard. Calculation of molecular g-tensors using the zeroth-order regular approximation and density functional theory: expectation value versus linear response approaches. *Theoretical Chemistry Accounts*, 129(3):453–466, 2011
- Benjamin Pritchard and Jochen Autschbach. Calculation of the vibrationally resolved, circularly polarized luminescence of d-camphorquinone and (s,s)-trans-β-hydrindanone. *ChemPhysChem*, 11(11):2409–2415, 2010

Conferences & Presentations

2010 Chemistry Graduate Student Symposium (Oral Presenter)

2010 Recruitment Weekend (Poster)

2011 Chemistry Graduate Student Symposium (Oral Presenter)

2011 Recruitment Weekend (Poster)

2012 RIT Graduate Research and Creativity Symposium (Oral Presenter)

2012 Conference for Teaching Assistants: Strategies for Effective Teaching (Attended)

2014 Psi4 Developer's Conference (Oral Presenter)

2015 Psi4 Developer's Conference (Oral Presenter)

2016 Psi4 Developer's Conference (Oral Presenter)

2017 SIAM Conference on Computational Science and Engineering (Planned, Oral Presenter)