Patrick J. **Lestrange**

Researcher · Developer
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Education

University of Washington
Seattle, WA

Ph.D. in Chemistry
Sept. 2012 - June 2017

Thesis: *Modeling core excitations and preserving spin symmetry in molecular systems*

- Helped implement a solver for interior eigenvalues in order to model high energy spectroscopies
- Investigated the abilities of various commonly used models to describe new phenomena (out of sample testing)
- Implemented several nonlinear optimization algorithms (DIIS, Newton-Raphson, L-BFGS) to converge quantum mechanical wave functions in the open-source software package, Chronus Quantum
- Derived and implemented several schemes to better describe the symmetries of non-relativistic wave functions

York College of Pennsylvania
York, PA

B.S. in Chemistry – *Magna Cum Laude*
Sept. 2008 - May 2012

Skills

Scientific Communication	9 accepted peer-reviewed publications, 9 conference presentations
Collaborative Work	Established relationships with other research groups resulting in 5 publications
Mentoring	Mentored 1 high school, 2 undergraduate, and 6 graduate students
Systems Administration	Maintained a 96 node compute cluster with >300 users in >20 academic departments
Technical Editing	Significant editing of others' papers, grants, award applications, etc.
Programming	Python (numpy, scikit-learn, pandas), Perl, C++, Fortran, SQL, LaTeX

Relevant Experience

Gaussian, Inc.
Wallingford, CT

Software Developer
Summer 2012 & Winter 2013

- Developed new algorithms to efficiently solve common quantum mechanical problems and implemented these techniques in a commercial software package, leading to several publications

Publications

10. **P. J. Lestrange**, D. B. Williams-Young, C. A. Jiménez-Hoyos, X. Li, "An Efficient Implementation of Variation After Projection Generalized Hartree-Fock." *Submitted*.
9. J. J. Goings, **P. J. Lestrange**, X. Li, "Real-Time Time-dependent Electronic Structure Theory." *WIREs Comput. Mol. Sci.*, **2017**, e1341. DOI:10.1002/wcms.1341.
8. **P. J. Lestrange**, M. R. Hoffmann, X. Li, "Time-dependent Configuration Interaction using the Graphical Unitary Group Approach: Nonlinear Electric Properties." *Adv. Quantum Chem.*, **2017**, DOI:10.1016/bs.aiq.2017.06.003.
7. D. B. Lingerfelt, **P. J. Lestrange**, J. J. Radler, S. E. Brown-Xu, P. Kim, F. N. Castellano, L. X. Chen, X. Li, "Can Excited State Electronic Coherence be Tuned via Molecular Structural Modification? A First-Principles Quantum Electronic Dynamics Study of Pyrazolate-Bridged Pt(II) Dimers." *J. Phys. Chem. A*, **2017**, *121*, 1932-1939.
6. L. X. Chen, M. L. Shelby, **P. J. Lestrange**, N. E. Jackson, M. W. Mara, K. Haldrup, A. B. Stickrath, D. Zhu, H. Lemke, M. Chollet, B. M. Hoffman, X. Li, "Imaging Ultrafast Excited State Pathways in Transition Metal Complexes by X-ray Transient Absorption and Scattering Using X-ray Free Electron Laser Source." *Faraday Discuss.*, **2016**, *194*, 639-659.
5. M. L. Shelby, **P. J. Lestrange**, N. E. Jackson, M. W. Mara, K. Haldrup, A. B. Stickrath, D. Zhu, H. Lemke, B. M. Hoffman, X. Li, L. X. Chen, "Ultrafast Processes in the Relaxation of a Nickel(II) Porphyrin Described by Femtosecond X-ray Absorption Spectroscopy." *J. Am. Chem. Soc.*, **2016**, *138*, 8752-8764. **Featured in JACS Spotlights.* DOI: 10.1021/jacs.6b07111
4. **P. J. Lestrange**, F. Egidi, X. Li, "The Consequences of Improperly Describing Oscillator Strengths Beyond the Electric Dipole Approximation." *J. Chem. Phys.*, **2015**, *143*, 234103.

3. B. Peng, **P. J. Lestrange**, J. J. Goings, M. Caricato, X. Li, "Energy-Specific Equation-of-Motion Coupled-Cluster Methods for High-Energy Excited States: Application to K-edge X-ray Absorption Spectroscopy." *J. Chem. Theory Comput.*, **2015**, *11*, 4146-4153.

2. **P. J. Lestrange**, P. D. Nguyen, X. Li, "Calibration of Energy-Specific TDDFT for Modeling K-edge XAS Spectra of Light Elements." *J. Chem. Theory Comput.*, **2015**, *11*, 2994-2999.

1. **P. J. Lestrange**, B. Peng, F. Ding, G. W. Trucks, M. J. Frisch, X. Li, "Density of States Guided Møller–Plesset Perturbation Theory." *J. Chem. Theory Comput.*, **2014**, *10*, 1910-1914.

Presentations

Apr. 2017	**P. J. Lestrange**, D. B. Williams-Young, X. Li, "An Efficient Implementation of Variation After Projection Generalized Hartree-Fock." Poster presentation at 253rd ACS National Meeting. *Awarded the ACS Chemical Computing Group Excellence Award.	*San Francisco, CA*
Apr. 2016	**P. J. Lestrange**, "Tracking electronic dynamics with X-rays." Oral presentation at York College of Pennsylvania.	*York, PA*
Dec. 2015	**P. J. Lestrange**, X. Li, "Transition properties in X-ray spectroscopy." Oral presentation at Pacifichem 2015.	*Honolulu, HI*
Aug. 2014	**P. J. Lestrange**, D. B. Lingerfelt, P. D. Nguyen, X. Li, "Electronic excitations in transition metal complexes." Poster presentation at 248th ACS National Meeting.	*San Francisco, CA*
Aug. 2014	**P. J. Lestrange**, "Shaping the climate change conversation through social media." Oral presentation at 248th ACS National Meeting.	*San Francisco, CA*
Sept. 2013	**P. J. Lestrange**, X. Li, "Density of States Guided Second-Order Møller-Plesset Perturbation Theory." Poster at European Summer School of Quantum Chemistry.	*Palermo, Italy*
Mar. 2012	**P. J. Lestrange**, J. B. Foresman, "New benchmarks for calibrating methods used to simulate VCD spectra." Poster presentation at 243rd ACS National Meeting.	*San Diego, CA*
Mar. 2012	**P. J. Lestrange**, K. Peterman, G. Foy, "Student climate change engagement via UN platform." Panel discussion at 243rd ACS National Meeting.	*San Diego, CA*
Aug. 2011	**P. J. Lestrange**, T. Cumming, G. Foy, "Sustainability and IYC-2011: A York College Chemistry Society production." Oral presentation at 242nd ACS National Meeting.	*Denver, CO*

Honors & Awards

2017	**Excellence Award**, American Chemical Society Chemical Computing Group
2016	**Independent Study Fellowship**, Scan|Design Foundation
2015	**Clean Energy Institute Graduate Fellowship**, University of Washington
2014	**Brian R. Reid Endowed Fellowship**, University of Washington
2014	**Honorable Mention**, National Science Foundation Graduate Research Fellowship
2013	**Honorable Mention**, National Science Foundation Graduate Research Fellowship
2012	**Benton Seymour Rabinovitch Endowed Fellowship**, University of Washington
2012	**Outstanding Chemistry Major**, Southeastern Pennsylvania Section of the ACS
2010-2016	**Robert A. Grassman Scholarship**, Steamfitters Local 475

Affiliations

Hyak Supercomputer Governance Board — *U. of Washington*
Board Member — *2016-2017*

High Performance Computing Club — *U. of Washington*
Vice President and Founding Officer — *2016-2017*