Patrick J. **Lestrange**

Researcher · Data Scientist
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Education

University of Washington — *Seattle, WA*
Ph.D. in Physical Chemistry – Defending May 2017 — *Sept. 2012 - present*

York College of Pennsylvania — *York, PA*
B.S. in Chemistry – *Summa Cum Laude* — *Sept. 2008 - May 2012*

Skills

Scientific Communcation 7 peer-reviewed publications, 8 conference presentations
Collaborative Work Worked with other universities and national labs leading to 3 publications
Programming Python (numpy, scipy, pandas), Perl, C++, Fortran77, Javascript, SQL, LaTeX

Relevant Experience

Gaussian, Inc. — *Wallingford, CT*
Software Developer — *Summer 2012 & Winter 2013*

- Worked with other scientists to develop new methods to numerical model quantum mechanical systems
- Implemented these techniques in a commercial software package leading to several publications

Presentations

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 presentation 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*

Publications

8. **P. J. Lestrange**, D. B. Williams-Young, C. A. Jiménex-Hoyos, G. E. Scuseria, X. Li, "Improving the Efficiency of Variation After Projection Hartree-Fock." **2017**, *In preparation for submission to J. Chem. Theory Comput.*

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**, *Just Accepted Manuscript*.

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.

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*