

Patrick J. Lestrangle

Researcher · Data Scientist

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Education

University of Washington

Ph.D. in Chemistry – Defending May 2017

Seattle, WA

Sept. 2012 - present

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

York College of Pennsylvania

B.S. in Chemistry – *Summa Cum Laude*

York, PA

Sept. 2008 - May 2012

Skills

Scientific Communication	7 peer-reviewed publications, 9 conference presentations
Collaborative Work	Worked with other universities and national labs resulting in 4 publications
Mentoring	Mentored 1 high school, 2 undergraduate, and 6 graduate students
Technical Editing	Significant editing of others' papers, grants, award applications, etc.
Programming	Python (numpy, scipy, pandas), Perl, C++, Fortran, Javascript, SQL, LaTeX

Relevant Experience

Gaussian, Inc.

Software Developer

Wallingford, CT

Summer 2012 & Winter 2013

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

Publications

7. D. B. Lingerfelt, **P. J. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, "Tracking electronic dynamics with X-rays." Oral presentation at York College of Pennsylvania. *York, PA*
- Dec. 2015 **P. J. Lestrangle**, X. Li, "Transition properties in X-ray spectroscopy." Oral presentation at Pacifichem 2015. *Honolulu, HI*
- Aug. 2014 **P. J. Lestrangle**, 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. Lestrangle**, "Shaping the climate change conversation through social media." Oral presentation at 248th ACS National Meeting. *San Francisco, CA*
- Sept. 2013 **P. J. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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. Lestrangle**, 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

Board Member

U. of Washington

2016-2017

High Performance Computing Club

Vice President and Founding Officer

U. of Washington

2016-2017