

Patrick J. Lestrangle

Researcher · Developer

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Education

University of Washington

Ph.D. in Chemistry

Seattle, WA

Sept. 2012 - June 2017

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

- Developed models to describe high energy spectroscopies and accurately represent experimental findings
- Helped develop open-source software (Chronus Quantum on Github) to solve multivariate optimization problems in order to predict the properties of quantum mechanical systems

York College of Pennsylvania

B.S. in Chemistry – *Magna Cum Laude*

York, PA

Sept. 2008 - May 2012

Skills

Scientific Communication	8 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, scipy, pandas), Perl, C++, Fortran, Javascript, SQL, LaTeX

Relevant Experience

Aarhus University

Visiting Scholar

Aarhus, Denmark

Aug. 2016 - Oct. 2016

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

9. J. J. Goings, **P. J. Lestrangle**, X. Li, "Real-Time Time-dependent Electronic Structure Theory." *Submitted*.
8. **P. J. Lestrangle**, M. R. Hoffmann, X. Li, "Time-dependent Configuration Interaction using the Graphical Unitary Group Approach: Nonlinear Electric Properties." *Adv. Quantum Chem.*, **2017**, Just Accepted.
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

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| 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. | <i>San Francisco, CA</i> |
| Apr. 2016 | P. J. Lestrangle , "Tracking electronic dynamics with X-rays." Oral presentation at York College of Pennsylvania. | <i>York, PA</i> |
| Dec. 2015 | P. J. Lestrangle , X. Li, "Transition properties in X-ray spectroscopy." Oral presentation at Pacificchem 2015. | <i>Honolulu, HI</i> |
| 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. | <i>San Francisco, CA</i> |
| Aug. 2014 | P. J. Lestrangle , "Shaping the climate change conversation through social media." Oral presentation at 248th ACS National Meeting. | <i>San Francisco, CA</i> |
| 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. | <i>Palermo, Italy</i> |
| 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. | <i>San Diego, CA</i> |
| Mar. 2012 | P. J. Lestrangle , K. Peterman, G. Foy, "Student climate change engagement via UN platform." Panel discussion at 243rd ACS National Meeting. | <i>San Diego, CA</i> |
| 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. | <i>Denver, CO</i> |

Honors & Awards

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| 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