

Lixin Lu

Pronouns: She/Her/Hers

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EDUCATION & EXPERIENCES

Postdoctoral Scholar, Stanford University, Stanford CA

Advisor: Todd J. Martínez

Aug. 2023 – present

PhD in Physical Chemistry, University of Washington, Seattle WA

Advisor: Xiaosong Li

Sept. 2018 – Jun. 2023

BS in Chemistry, Fudan University, Shanghai, China

Advisors: Igor Ying Zhang & Xin Xu

Sept. 2014 – Jun. 2018

Visiting Researcher, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Advisors: Igor Ying Zhang & Matthias Scheffler

Jun. 2017 – Sept. 2017

HONORS & AWARDS

2022-2023 Graduate Student Merit Award, UW

2023

Chemical Computing Group Excellence Award for Graduate Students

ACS Division of Computers in Chemistry

Fall 2022

Clean Energy Institute Travel Grant for ACS National Meetings, UW

Fall 2022 & Spring 2022

2023 Schmidt Science Fellows, Nominee

2022

EFRC-Hubs-CMS-CCS PI Meeting Student and Postdoc Team Science Competition, DOE BES 2021

Clean Energy Institute Graduate Student Fellowship 2020-2021, UW

2020

Rabinovitch, Benton Seymour Endowed Fellowship, UW

2018

Xiyuan Scholar for Scientific Research in Chemistry, Fudan University

2017

Fung Scholar 2016-2017, Victor and William Fung Foundation

2016

OUTREACH & SERVICE

UW Clean Energy Institute Fellow:

- Participated in science fairs in a primary school in Kent, Washington.
- Prepared solar battery kits for middle school students during COVID.
- Prepared materials for a CEI educational lesson to introduce spectroscopic techniques.
- Was one of the panelists in virtual “lunch and learn” for high school students.

Department of Energy (DOE) Basic Energy Sciences (BES) Early Career Network (ECN) Representative for IDREAM EFRC from 2022 to 2023:

- Leader of the 2023 DOE BES ECN Career Paths Webinar with 337 attendees from various institutions.
 - Invited to present at PNNL Community Science & Technology Seminar series.
 - Organized ECN monthly meetings and outreach activities.
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SKILLS & OTHERS

Computer Programming: C/C++, Python, Fortran languages. Proficient in MPI, openMP, HTML and JavaScript.

Computational Chemistry: Excellent in Gaussian, Chronus Quantum, TeraChem. Proficient in PySCF, BAGEL, Q-Chem, openMolCAS, Vienna ab initio simulation package (VASP), Fritz Haber Institute ab initio molecular simulations package (FHI-aims) & Jmol

Full list of publications and presentations

- [8] S. Li*, L. Lu*, S. Bhattacharyya*, C. I. Pearce, K. Li, E. T. Nienhuis, G. Doumy, R. D. Schaller, S. Moeller, M. -F. Lin, G. Dakovski, D. J. Hoffman, D. Garratt, K. A. Larsen, J. D. Koralek, C. Y. Hampton, D. Cesar, J. Duris, Z. Zhang, N. Sudar, J. P. Cryan, A. Marinelli, X. Li, L. Inhester, R. Santra, L. Young. Attosecond-pump Attosecond-probe X-ray Spectroscopy of Liquid Water. *Science* **2024**, *383*, 1118-1122
- [7] C. E. Hoyer*, L. Lu*, H. Hu*, K. D. Shumilov, S. Sun, S. Knecht, and X. Li. Correlated Dirac-Coulomb-Breit Multiconfigurational Self-Consistent-Field Methods. *J. Chem. Phys.* **2023**, *158*, 044101
- [6] C. E. Hoyer, H. Hu, L. Lu, S. Knecht, and X. Li. Relativistic Kramers-Unrestricted Exact-Two-Component Density Matrix Renormalization Group. *J. Phys. Chem. A* **2022**, *126*, 30, 5011–5020
- [5] L. Lu, H. Hu, A. J. Jenkins, and X. Li. Relativistic Exact-two-component Multi-reference Second-order Perturbation Theory. *J. Chem. Theory Comput.* **2022**, *18*, 5, 2983–2992
- [4] A. J. Jenkins, H. Hu, L. Lu, M. J. Frisch, and X. Li. Two-Component Multireference Restricted Active Space Configuration Interaction for the Computation of L-edge X-ray Absorption Spectra. *J. Chem. Theory Comput.* **2022**, *18*, 1, 141–150
- [3] R. A. Beck, L. Lu, P. V. Sushko, X. Xu, and X. Li. Defect-Induced Magnetic Skyrmion in a Two-Dimensional Chromium Triiodide Monolayer. *JACS Au* **2021**, *1*, 9, 1362–1367
- [2] L. Lu*, A. Wildman*, A. J. Jenkins, L. Young, A. E. Clark, and X. Li. The “Hole” Story in Ionized Water from the Perspective of Ehrenfest Dynamics. *J. Phys. Chem. Lett.* **2020**, *11*, 22, 9946–9951
- [1] R. A. Beck, L. Lu, A. Petrone, A. C. Ong, P. J. Pauzauskie, and X. Li. Spectroscopic Signatures of the B and H₄ Polyatomic Nitrogen Aggregates in Nanodiamond. *J. Phys. Chem. C* **2020**, *124*, 33, 18275–18283

Note: * – Co-first author

PRESENTATIONS

- [8] Relativistic many-body perturbation theory and its applications in heavy-element spectroscopy. *2nd International Workshop on Theory Frontiers in Actinide Science: Chemistry & Materials*, poster, Santa Fe, NM. Feb 27, 2023
- [7] Unraveling the Complex Chemistry of Hanford Site Nuclear Tank Waste. *PNNL Community Science&Technology Seminar Series*. Nov 15, 2022
- [6] Relativistic many-body perturbation theory and its applications in heavy-element spectroscopy. *Quantum Chemistry: Current & Future Frontiers*, 2022 ACS Fall Chicago. Aug 22, 2022
- [5] Relativistic many-body perturbation theory and its applications in heavy-element spectroscopy. *PHYS Sci-Mix poster*, 2022 ACS Fall Chicago. Aug 22, 2022
- [4] Exact-two-component multi-reference second-order perturbation theory to study fine structure splitting of heavy elements. *Quantum Mechanics*, 2022 ACS Spring San Diego. Mar 24, 2022
- [3] From the “hole” story in Ionized water to the ultrafast dynamics upon radiolysis in complex solution. *Geochemistry in Extreme Environments*, 2022 ACS Spring San Diego. Mar 23, 2022
- [2] Radiolysis Across Multiple Timescales in Extreme Environments. *Student and Postdoc Team Science Contest Talks in 2021 EFRC-Hub-CMS-CCS Virtual Principal Investigators’ Meeting*. Oct 19, 2021
- [1] Core and Valence Effect of MP2 Correlation Energy for Solids. *The 5th Undergraduate Technology & Academy Forum*, Fudan University, Shanghai China. Nov 12, 2017