Lixin Lu

Pronouns: She/Her/Hers

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EDUCATION & TRAINING

Postdoc in theoretical Chemistry, 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*
Dissertation: Approaching Accurate Description of Molecular Spectroscopies with Multi-reference Electronic Structure Methods

MS in Chemistry, University of Washington, Seattle WA
GPA: 3.80 / 4.00, Advisor: Xiaosong Li *Dec. 2019*

BS in Chemistry, Fudan University, Shanghai, China
Major GPA: 3.71 / 4.00, 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*

Exchange Student, University of Hong Kong, Hong Kong
Advisor: Guanhua Chen *Sept. 2016 – Dec. 2016*

HONORS & AWARDS

2022-2023 Graduate Student Merit Award
University of Washington, Department of Chemistry *May 2023*

Chemical Computing Group Excellence Award for Graduate Students
American Chemical Society national meeting *Fall 2022*

CEI Travel Grant 2022 for American Chemical Society National Meeting
Clean Energy Institute, University of Washington *Fall 2022 & Spring 2022*

Nominee, 2023 Schmidt Science Fellowship, University of Washington *2022*

EFRC-Hubs-CMS-CCS PI Meeting Team Science Competition, Student and Postdoc Team Science Contest *2021*

CEI Graduate Student Fellowship 2020-2021, Clean Energy Institute, University of Washington *2020*

Rabinovitch, Benton Seymour Endowed Fellowship, University of Washington *2018*

Xiyuan Scholar for Scientific Research in Chemistry, Fudan University *2017*

Fung Scholar 2016-2017, Victor and William Fung Foundation *2016*

SKILLS & OTHERS

Computer Programming: Excellent in C/C++, Python and Fortran languages, MPI, openMP and TiledArray. Proficient in HTML and JavaScript.
Computational Chemistry: Excellent in Gaussian, Chronus Quantum, openMolCAS, Vienna ab initio simulation package (VASP), Fritz Haber Institute ab initio molecular simulations package (FHI-aims) & Jmol

OUTREACH & SERVICE

As Department of Energy Basic Energy Sciences Early Career Network representative for IDREAM EFRC (Interfacial Dynamics in Radioactive Environments and Materials Energy Frontier Research Center):

- Organized ECN monthly meeting,
- Presented at PNNL Community Science&Technology Seminar,
- Co-leading DOE BES ECN Careers Webinar.

As Clean Energy Institute Fellow:

- Participated in science fairs in primary school,
- Assembled solar battery kits for middle school students,
- Was one of the panelists in virtual "lunch and learn" for high school students.

Full list of publications and presentations

[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 H_4 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.
2^{nd} 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 5^{th} Undergraduate Technology & Academy Forum, Fudan University, Shanghai China. *Nov 12, 2017*