Lixue Cheng, Ph.D.

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Google Scholar sherrylixuecheng
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Work & Research Experiences

August 2025 – Present
Assistant Professor in Chemistry, The Hong Kong University of Science and Technology.
AI for Physical Science lab: A lab focuses on physics-driven multi-scale modeling strategies via highly accurate simulators, emulators, predictors and evaluators/agents to achieve a collaborative effort of AI, computational chemistry and experimentalists.

June 2023 – May 2025
Researcher, Microsoft Research AI4Science Lab (Berlin).
AI for quantum chemistry: DeepQMC and MLFF; LLMs for Science: ability of GPT-4 in chemistry.

July 2022 – April 2023
Research Scientist, Tencent Quantum Lab, Tencent.
Machine learning assisted quantum computing algorithm design for quantum chemistry.

August 2017 – March 2022
PhD Student, Miller Group, California Institute of Technology.
MOB-ML: Molecular Orbital-Based Machine Learning; INSPIRE: Computational Parameterization of Nucleic Acid Secondary Structure Models.

January 2013 – July 2017
Undergraduate Researcher, Record Group, University of Wisconsin-Madison.
Interpreting and predicting Hofmeister salt ion, polyol, PEG and sugar effects on biopolymer processes using solubility assay and solute-partitioning model.

August 2015 – May 2016
Undergraduate Researcher, Math studies supervised by Qin Li, University of Wisconsin-Madison.
Randomized Singular Value Decomposition algorithm for low rank matrices & its numerical applications.

Teaching Experiences

2026 Spring
Instructor CHEM 3030 Introductory to AI for Science, The Hong Kong University of Science and Technology.

2019 Fall
TA for Ch. 125b. Elements of Quantum Chemistry, California Institute of Technology.

2017 Spring
TA for Chem 562 Physical Chemistry II, University of Wisconsin-Madison.

2016 Spring
Grader/TA for Math 341 Linear Algebra (Honor) and Math 561 Differential Geometry, University of Wisconsin-Madison.

2015 Fall & 2016 Fall
Grader/TA for Chem/Biochem 565/665 Biophysical Chemistry, University of Wisconsin-Madison.

Education

August 2017 – June 2022
Ph.D. in Chemistry, California Institute of Technology, Pasadena, CA.
Thesis: *Accurate and transferable molecular-orbital-based machine learning for molecular modeling* [Link]

Education (continued)

September 2012 – May 2016

Bachelor of Sciences in Honors, University of Wisconsin-Madison, Madison, WI, GPA: 3.933/4.0.
Majors: Chemistry (Honor), Mathematics (Honor), Biochemistry, Molecular Biology. Minor (Certificate): Computer Sciences.

Publications

Google Scholar Citations: 1032; h-index: 13; i10-index: 17

24 C. Wang, L. Huang, X. Wei, T. Qin, **L. Cheng**, and J. Zhang, Scalable machine learning force fields for macromolecular systems through long-range aware message passing, 2025.

23 Z. Song, J. Lu, Y. Du, B. Yu, T. Pruyn, Y. Huang, K. Guo, X. Luo, Y. Qu, Y. Qu, Y. Wang, H. Wang, J. Guo, J. Gan, P. Shojaee, D. Luo, A. Bran, G. Li, Q. Zhao, S.-X. L. Luo, Y. Zhang, X. Zou, W. Zhao, Y. Zhang, W. Zhang, S. Zheng, S. Zhang, S. Khan, M. Rajabi-Kochi, S. Paradi-Maropakis, T. Baltoiu, F. Xie, T. Chen, K. Huang, W. Luo, M. Fang, X. Yang, **L. Cheng**, J. He, S. Hassoun, X. Zhang, W. Wang, C. Reddy, C. Zhang, Z. Zheng, M. Wang, L. Cong, C. Gomes, C.-Y. Hsieh, A. Nandy, P. Schwaller, H. Kulik, H. Jia, H. Sun, S. Moosavi, and C. Duan, Evaluating large language models in scientific discovery, 2025. arXiv: 2512.15567.

22 Y. Chen, **L. Cheng**, Y. Jing, and P. Zhong, "Benchmarking a foundation potential against quantum chemistry methods for predicting molecular redox potentials," *arXiv preprint arXiv:2510.24063*, 2025.

21 G. M. Jacobson, A. W. Webb, **L. Cheng**, and A. B. McCoy, "Diffusion monte carlo study of the structure and spectroscopy of h3o–," *The Journal of Physical Chemistry A*, vol. 129, no. 47, pp. 10 928–10 939, 2025. DOI: 10.1021/acs.jpca.5c06590.

20 G. N. C. Simm, J. Hélie, H. Schulz, Y. Chen, G. Simeon, A. Kuzina, E. Martinez-Baez, P. Gasparotto, G. Tocci, C. Chen, Y. Li, **L. Cheng**, Z. Wang, B. H. Nguyen, J. A. Smith, and L. Sun, Simpoly: Simulation of polymers with machine learning force fields derived from first principles, 2025. arXiv: 2510.13696 [physics.chem-ph].

19 A. Foster, Z. Schätzle, P. B. Szabó, **L. Cheng**, J. Köhler, G. Cassella, N. Gao, J. Li, F. Noé, and J. Hermann, "An ab initio foundation model of wavefunctions that accurately describes chemical bond breaking," *arXiv preprint arXiv:2506.19960*, 2025.

18 J. Sun, **L. Cheng**, and S.-X. Zhang, "Stabilizer ground states for simulating quantum many-body physics: Theory, algorithms, and applications," *Quantum*, vol. 9, p. 1782, 2025.

17 G. M. Jacobson, **L. Cheng**, V. C. Bhethanabotla, J. Sun, and A. B. McCoy, "Machine learning approaches for developing potential surfaces: Applications to oh–(h2o) n (n= 1–3) complexes," *J. Phys. Chem. A*, vol. 129, no. 12, pp. 2958–2972, 2025.

16 **L. Cheng**, P. B. Szabó, Z. Schätzle, D. P. Kooi, J. Köhler, K. J. Giesbertz, F. Noé, J. Hermann, P. Gori-Giorgi, and A. Foster, "Highly accurate real-space electron densities with neural networks," *J. Chem. Phys.*, vol. 162, no. 3, 2025.

15 **L. Cheng**, Y.-Q. Chen, S.-X. Zhang, and S. Zhang, "Quantum approximate optimization via learning-based adaptive optimization," *Comm. Phys.*, vol. 7, no. 1, p. 83, 2024.

14 J. Sun, **L. Cheng**, and W. Li, "Toward chemical accuracy with shallow quantum circuits: A Clifford-based Hamiltonian engineering approach," *J. Chem. Theory Comput.*, vol. 20, no. 2, pp. 695–707, 2024.

13 M. AI4Science and M. Quantum, The impact of large language models on scientific discovery: A preliminary study using gpt-4, 2023. arXiv: 2311.07361.

12 W. Li, J. Allcock, **L. Cheng**, S.-X. Zhang, Y.-Q. Chen, J. P. Mailoa, Z. Shuai, and S. Zhang, "Tencirchem: An efficient quantum computational chemistry package for the nisq era," *J. Chem. Theory Comput.*, vol. 19, no. 13, pp. 3966–3981, 2023.

11 **L. Cheng**, J. Sun, J. E. Deustua, V. C. Bhethanabotla, and T. F. Miller III, "Molecular-orbital-based machine learning for open-shell and multi-reference systems with kernel addition gaussian process regression," *J. Chem. Phys.*, vol. 157, no. 15, p. 154 105, 2022. DOI: 10.1063/5.0110886.

10 J. Sun, **L. Cheng**, and T. F. Miller, "Molecular dipole moment learning via rotationally equivariant derivative kernels in molecular-orbital-based machine learning," *J. Chem. Phys.*, vol. 157, no. 10, p. 104 109, 2022.

9 **L. Cheng**, Z. Yang, B. Liao, C. Hsieh, and S. Zhang, "Odbo: Bayesian optimization with search space prescreening for directed protein evolution," *Preprint at https://arXiv.org/abs/2205.09548*, 2022.

8 **L. Cheng**, J. Sun, and T. F. Miller III, "Accurate molecular-orbital-based machine learning energies via unsupervised clustering of chemical space," *J. Chem. Theory Comput.*, vol. 18, no. 8, pp. 4826–4835, 2022.

7 F. Lu, **L. Cheng**, R. J. DiRisio, J. M. Finney, M. A. Boyer, P. Moonkaen, J. Sun, S. J. Lee, J. E. Deustua, T. F. Miller III, et al., "Fast near ab initio potential energy surfaces using machine learning," *J. Phys. Chem. A*, vol. 126, no. 25, pp. 4013–4024, 2022.

6 J. Sun, **L. Cheng**, and T. F. Miller III, "Molecular energy learning using alternative blackbox matrix-matrix multiplication algorithm for exact gaussian process," in *NeurIPS 2021 AI for Science Workshop*, 2021.

5 T. Husch, J. Sun, **L. Cheng**, S. J. Lee, and T. F. Miller III, "Improved accuracy and transferability of molecular-orbital-based machine learning: Organics, transition-metal complexes, non-covalent interactions, and transition states," *J. Chem. Phys.*, vol. 154, no. 6, p. 064 108, 2021.

4 **L. Cheng**, N. B. Kovachki, M. Welborn, and T. F. Miller III, "Regression clustering for improved accuracy and training costs with molecular-orbital-based machine learning," *J. Chem. Theory Comput.*, vol. 15, no. 12, pp. 6668–6677, 2019.

3 **L. Cheng**, M. Welborn, A. S. Christensen, and T. F. Miller III, "A Universal Density Matrix Functional from Molecular Orbital-based Machine Learning: Transferability across Organic Molecules," *J. Chem. Phys.*, vol. 150, no. 13, p. 131 103, Apr. 2019, ISSN: 0021-9606. DOI: 10.1063/1.5088393.

2 M. Welborn, **L. Cheng**, and T. F. Miller III, "Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis," *J. Chem. Theory Comput.*, vol. 14, no. 9, pp. 4772–4779, Sep. 2018. DOI: 10.1021/acs.jctc.8b00636.

1 D. Knowles, I. A. Shkel, N. M. Phan, M. Sternke, E. Lingeman, X. Cheng, **L. Cheng**, K. O'Connor, and M. T. Record, "Chemical interactions of polyethylene glycols (pegs) and glycerol with protein functional groups: Applications to effects of peg and glycerol on protein processes," *Biochemistry*, vol. 54, no. 22, pp. 3528–3542, 2015.

Research Interests

- **AI for quantum chemistry:** Orbital-based machine learning for highly accurate ground and excited state wavefunction theory emulation; Ab initio wavefunction learning via Deep Quantum Monte Carlo.
- **AI x quantum computing x quantum chemistry:** Quantum computing for quantum chemistry; Machine Learning for variational quantum algorithms.
- **AI for material design**
- **AI for experimental design:** Bayesian optimization for experimental design.
- **LLM for science:** Benchmark LLMs in scientific tasks.

Honors & Awards

2017 **Caltech General Fellowship**, Division of Chemistry and Chemical Engineering, Caltech.

2016 **Mary Ellen Rudin Foundation Scholarship Award**, Department of Mathematics, UW-Madison.

2015 **David H. Durra Scholarship**, College of Letters & Sciences, UW-Madison.

Honors & Awards (continued)

- **Eugene and Patricia Kreger Herscher Undergraduate Scholarship**, Department of Chemistry, UW-Madison.
- **Walter W. & Young-Ja C. Toy Summer Research Fellowship**, Department of Chemistry, UW-Madison.

2014
- **Biochemistry Undergraduate Summer Research Scholarship**, Department of Biochemistry, UW-Madison.
- **Gerald W. and Tui G. Hedstrom Scholarship**, College of Letters & Science, UW-Madison.
- **Martha Gunhild Weeks Undergraduate Scholarship**, Department of Chemistry, UW-Madison.
- **The Honor Society of Phi Kappa Phi Member**, University of Wisconsin-Madison Chapter.
- **Trewartha Senior Thesis Grant**, Letters & Science Honors Program, UW-Madison.
- **Wisconsin Hilldale Undergraduate/Faculty Research Fellowship**, UW-Madison.

2013
- **John & Elizabeth Moore Awards for Excellence**, Department of Chemistry, UW-Madison.

Patents

2024
- **Object determining method and apparatus, computer device, and storage medium.** US Patent 18745916. [Link]
- **Molecular energy prediction method and apparatus, device, and storage medium.** US Patent 18619052. [Link]

2020
- **Systems and methods for determining molecular structures with molecular-orbital-based features.** US Patent 16817489. [Link]