

# Lixue Cheng

[Email](#) [Personal Homepage](#) [Lab Website](#) [GitHub](#) [Google Scholar](#)

## EDUCATION

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### California Institute of Technology

Pasadena, CA

Ph.D. in Chemistry, with Prof. Thomas F. Miller III.

August 2017–June 2022

Thesis: Accurate and transferable molecular-orbital-based machine learning for molecular modeling [[Link](#)]

### University of Wisconsin-Madison

Madison, WI

Bachelor of Sciences in Honors, GPA: 3.933/4.0

September 2012–May 2016

Majors: Chemistry (Honor), Mathematics (Honor), Biochemistry, Molecular Biology.

Minor (Certificate): Computer Sciences

## RESEARCH INTERESTS

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I am an AI for science researcher rooted in the fields of quantum and computational chemistry to develop Lego-like AI-powered tools to revolution chemistry research paradigms.

### (1) 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

### (2) AI x quantum computing x quantum chemistry

- Quantum computing for quantum chemistry
- Machine Learning for variational quantum algorithms

### (3) AI for material design

### (4) AI for experimental design

- Bayesian optimization for experimental design

### (5) LLM for science

- Benchmark LLMs in scientific tasks

## RESEARCH AND TEACHING EXPERIENCES

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### The Hong Kong University of Science and Technology

August 2025–Present

*Assistant Professor in Chemistry*

**AI for chemistry 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. The model modules include

- **Simulator:** Generates a small but extremely high-quality dataset of wavefunctions using Deep QMC, AI boost quantum computing and other advanced quantum simulation methods.
- **Emulator:** Uses orbital-representation-based graph neural networks/transformers to learn the Simulator's outputs and expand data volume efficiently.
- **Predictor:** Predict molecular properties directly from structures (molecular graph, SMILES, etc), enabling fast, low-cost end-to-end applications.
- **Evaluator & Agent:** Fine-tune large scientific language models as AI agent + Bayesian optimization to integrate literature data, and guide real-world experiments.

## **Microsoft Research AI4Science Lab (Berlin)**

June 2023–May 2025

*Researcher*

### **AI for quantum chemistry: DeepQMC and MLFF**

- Apply Transformer and other deep learning techniques to develop deep quantum Monte Carlo (DeepQMC) and machine learning force field (MLFF)
- Collect and generate highly accurate quantum simulation data as input data for deep learning model

### **LLMs for Science: ability of GPT-4 in chemistry**

- Assess the ability of GPT-4 in various scientific tasks, such as understanding theoretical chemistry, generating useful simulation inputs, and designing reasonable research plan, with different prompt engineering techniques.
- Participate in the preparation of foundation model for molecular sciences.

## **Tencent Quantum Lab, Tencent**

July 2022–April 2023

*Research scientist*

### **Machine learning assisted quantum computing algorithm design for quantum chemistry**

- Develop AI tools for quantum computing, quantum chemistry and biology
- Develop, implement and test novel Bayesian learning algorithm to optimize quantum computing algorithms running on real quantum devices.
- Design shallow and efficient quantum circuits for VQE to achieve chemical accuracy for molecular systems.

## **Miller Group, California Institute of Technology**

August 2017–Mar 2022

*PhD student*

### **MOB-ML: Molecular Orbital-Based Machine Learning**

- Use the molecular orbital representations to predict the molecular energies via ML tools to give high accuracy as wave function theory method but a low computational cost as density functional theory method.
- Perform electronic structure calculations and quantum simulations for different molecular systems.
- Develop different supervised and unsupervised learning methodologies to model different molecular properties.
- Develop a ML module in open-source quantum chemistry software (*entos*) and build a MOB-ML database.

### **INSPIRE: Computational Parameterization of Nucleic Acid Secondary Structure Models**

- Combine ML tools with molecular dynamics (MD) to derive new thermodynamics and kinetics nucleic acid models with secondary structure information.

- Develop and revise ML algorithms that can improve the efficiency of the strategy.
- Perform MD simulations for different nucleic acid reaction systems as a source of data for ML model.

**Record Group, University of Wisconsin-Madison**

January 2013–July 2017

*Undergraduate researcher*

**Interpreting and predicting Hofmeister salt ion, polyol, PEG and sugar effects on biopolymer processes using solubility assay and solute-partitioning model**

- Design and lead projects using solubility experiments to measure different solutes-biomolecule interactions.
- Recruit and mentor other undergraduate students to collect solute–nucleobase thermodynamics data.
- Develop mathematical models and analyze the data to interpret functional group chemical interactions.
- Determine interaction constants between different bases and different solutes and apply them to predict and interpret solute-biopolymer interaction and drug solubility data.

**Math studies supervised by Qin Li, University of Wisconsin-Madison**

August 2015–May 2016

*Undergraduate researcher*

**Randomized Singular Value Decomposition algorithm for low rank matrices & its numerical applications**

- Reprove and improve the theorems in the literature as a mathematical exercise.
- Develop MATLAB codes to implement the algorithm studied in the literature and perform numerical tests.
- Compare and analyze the numerical test results and explain the mathematical origins in different cases.

**Grader/TA for Chem/Biochem 565/665 Biophysical Chemistry**

University of Wisconsin-Madison

2015 Fall & 2016 Fall

**Grader/TA for Math 341 Linear Algebra (Honor) and Math 561 Differential Geometry**

University of Wisconsin-Madison

2016 Spring

## VOLUNTEERING, TEACHING & COMMUNITY EXPERIENCES

I'm an active volunteer & organizer for “[AI for science](#)” research community to bridge scientists from different backgrounds, a practitioner for “AI for science” education to cultivate the next generation talents, and a part-time open-source software developer to break the knowledge barrier in research.

**AI for Science community & workshops**

May 2023–Present

*Core member & Organizer*

- Organize the AI for science workshops in top conferences
- Start the AI for Edu and AI for science paper collection initiatives
- Participate in the proposal and review report writing

**AI for Science education for high school students**

Jan 2021–Present

*Instructor*

- Introduce cutting-edge AI for science contents to high school students all over the world  
[Link][An example course page]
- Introduction to AI for protein 3D structure predictions for high school students [Link]
- Introduction to Methodologies in Scientific Research for High School Students [Link]

**AI for Science paper collection (over 100 stars) [GitHub]**

June 2024–Present

*Organizer & Core maintainer*

**MathTranslate (over 1300 stars) [GitHub][YouTube][Bilibili]**

April 2023–Present

*Core developer*

- A core developer for this free open-source software to provide high quality translation of scientific papers with heavy math symbols.
- Maintain social media & user discussion groups.

**Department of Mathematics, University of Wisconsin–Madison**

*Administrative Office and Front Desk Student Help*

August 2015–May 2016

**Sonoco Products Co., 455 Science Drive, Madison, WI**

*Research Project Assistant*

September 2014–January 2015

- Measure geometries and properties of different materials and perform mathematical modeling of products.
- Analyzing data using various software, for example, Excel, Auto CAD, FEA.
- Develop test devices and search the literature to support our own research projects.

**Department of Chemistry and Mathematics, University of Wisconsin–Madison**

*Private Tutor*

August 2014–May 2017

**College Library, University of Wisconsin–Madison**

*Circulation Student Assistant*

August 2013–May 2015

**Greater University Tutoring Service (GUTS), University of Wisconsin–Madison**

*Academic Tutor (Chemistry and Mathematics)*

September 2012–August 2013

## HONORS AND AWARDS

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- 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
  - 2015 Eugene and Patricia Kreger Herscher Undergraduate Scholarship for the 2015–16 Academic Year, Department of Chemistry, UW-Madison
  - 2015 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
  - 2014 Gerald W. and Tui G. Hedstrom Scholarship, College of Letters & Science, UW-Madison
  - 2014 Martha Gunhild Weeks Undergraduate Scholarship for the 2014-15 Academic Year, Department of Chemistry, UW-Madison
  - 2014 The Honor Society of Phi Kappa Phi Member, University of Wisconsin-Madison Chapter

- 2014 Trewartha Senior Thesis Grant, Letters & Science Honors Program, UW-Madison
- 2014 Wisconsin Hilldale Undergraduate/Faculty Research Fellowship, UW-Madison
- 2013 John & Elizabeth Moore Awards for Excellence, Department of Chemistry, UW-Madison: Excellence for Chem109 Advanced General Chemistry, 1/350

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## PATENTS, PUBLICATIONS AND THESES

[Google Scholar Citation](#): 973; h-index: 12; i10-index: 15

### Publications

19. Foster, A.\*; Schatzle, Z.\*; Szabo, P. B.\*; **Cheng, L.\***; Kohler, J.; Cassella, G.; Gao, N.; Li, J. ; Noe, F.; Hermann, J. A Wavefunction Foundation Model that Accurately Describes Bond Breaking. arXiv:2506.19960. (2025). (\*co-first author) [\[Link\]](#)[\[Repo\]](#)
18. Sun, J.; **Cheng, L.**; Zhang, S.X. Stabilizer ground state: Theory, algorithms and applications. *Quantum*, 2025.[\[Link\]](#)[\[Repo\]](#)
17. Jacobson, G.\*; **Cheng, L.\***; Bhethanabotla, V; Sun, J; McCoy, A. B., Machine Learning Approaches for Developing Potential Surfaces: Applications to OH<sup>-</sup>(H<sub>2</sub>O)<sub>n</sub> (n=1-3) Complexes, *J. Phys. Chem. A.*, **2025** [\[Link\]](#)[\[Repo\]](#)
16. **Cheng, L.**; Szabó, P.B.; Schätzle, Z.; Kooi, D.; Köhler, J.; Noé, F.; Gori-Giorgi, P.; Foster, A. Highly Accurate Real-space Electron Densities with Neural Networks, *J. Chem. Phys.*, **2025** [\[Link\]](#)
15. **Cheng, L.\***; Chen, Y.Q.\*; Zhang, S.X.; Zhang, S. Quantum approximate optimization via learning-based adaptive optimization. *Commun. Phys.*, **2024** (\*co-first author) [\[Link\]](#) [\[Repo\]](#)
14. Sun, J.; **Cheng, L.**; Li, W. Towards chemical accuracy with shallow quantum circuits: A Clifford-based Hamiltonian engineering approach. *J. Chem. Theory Comput.*, **2024**.[\[Link\]](#)[\[Repo\]](#)
13. MR AI4Science\*, MA Quantum. The Impact of Large Language Models on Scientific Discovery: a Preliminary Study using GPT-4. arXiv:2311.07361 (2023). [\[Link\]](#) (**\*Major contributor to Chap 4**)
12. Li, W.; Allcock, J.; **Cheng, L.**; Zhang, S.X.; Chen, Y.Q.; Mailoa, J.P.; Zhang, S. TenCirChem: An efficient quantum computational chemistry package for the NISQ era. *J. Chem. Theory Comput.*, **2023**. [\[Link\]](#)[\[Repo\]](#)
11. **Cheng, L.**; Yang, Z.; Liao, B.; Hsieh, C.; Zhang, S. ODBO: Bayesian Optimization with prescreening for directed protein evolution. arXiv:2205.09548 (2022). [\[Link\]](#)[\[Repo\]](#)
10. **Cheng, L.**; Sun, J.; Deustua, J. E.; Bhethanabotla, V.C; Miller III, T.F. Molecular-orbital-based machine learning for open-shell and multi-reference systems with kernel addition Gaussian process regression. *J. Chem. Phys.*, **2022**. [\[Link\]](#)
9. Sun, J.; **Cheng, L.**; Miller III, T. F. Molecular dipole moment learning via rotationally equivariant Gaussian process regression with derivatives in molecular-orbital-based machine learning. *J. Chem. Phys.* **2022**. [\[Link\]](#)
8. **Cheng, L.**; Sun, J.; Miller III, T.F. Accurate molecular-orbital-based machine learning energies via unsupervised clustering of chemical space. *J. Chem. Theory Comput.*, **2022**. [\[Link\]](#)
7. Sun, J.; **Cheng, L.**; Miller III, T.F. Molecular energy learning using alternative blackbox matrix-matrix multiplication algorithm for exact Gaussian process. arXiv: 2109.09817 (2022). Appears in NeurIPS 2021 AI for Science Workshop [\[Link\]](#).
6. Lu, F.\*; **Cheng, L.\***; DiRisio, R. J.\*; Finney, J. M.; Boyer, M. A.; Sun, J.; Lee, S. J. R.; Deustua, J. E.; Miller III, T. F.; McCoy, A. B. Fast near *ab initio* potential energy surfaces using machine learning. *J. Phys. Chem. A*, **2022**. (\*co-first author) [\[Link\]](#)
5. Husch, T.; Sun, J.; **Cheng, L.**; Lee, S. J. R.; Miller III, T.F. Improved accuracy and transferability of molecular- orbital-based machine learning: Organics, transition-metal complexes, non-covalent interactions, and transition states. *J. Chem. Phys.*, **2021**. [\[Link\]](#)
4. **Cheng, L.**; Kovachki, N; Welborn, M.; Miller III, T. F. Regression clustering for improved accuracy and training costs with molecular-orbital-based machine learning. *J. Chem. Theory*

- Comput.*, **2019**. [\[Link\]](#)
3. **Cheng, L.**; Welborn, M.; Miller III, T. F. A universal density matrix functional from molecular orbital- based machine learning: Transferability across organic molecules. *J. Chem. Phys.*, **2019**. [\[Link\]](#)
  2. Welborn, M.; **Cheng, L.**; Miller III, T. F. Transferability in machine learning for electronic structure via the molecular orbital basis. *J. Chem. Theory Comput.* **2018**.[\[Link\]](#) (Highlighted with commentary in [C&EN](#) and [Caltech News](#))
  1. Knowles, D. B.; Shkel, I. A.; Phan, N. M.; Sternke, M.; Lingeman, E.; Cheng, X.; **Cheng, L.**; O'Connor, K.; Record, M. T. Chemical interactions of polyethylene glycols (PEGs) and glycerol with protein functional groups: Applications to effects of PEG and glycerol on protein processes. *Biochemistry* **2015**, *54* (22), 3528– 3542. [\[Link\]](#)

## Patents

3. **Cheng, L.**; Yang, Z.; Liao, B.; Zhang S. Object determining method and apparatus, computer device, and storage medium. 2024/10/10 US, 18745916 程立雪; 杨子翊; 廖奔彝; 张胜誉. 对象确定方法、装置、计算机设备和存储介质), 2022-05-09, 中国, 2022104986847 [\[Link\]](#)
2. **Cheng, L.**; Mailoa, J.P.; Zhang S. Molecular energy prediction method and apparatus, device, and storage medium 2024/7/18 US, 18619052 程立雪; 赖炫尧; 张胜誉; 分子能量的预测方法、装置、设备及存储介质, 2022-10-18, 中国, 2022112749576 [\[Link\]](#)
1. Patent: Miller III, T.F.; Welborn, M.; **Cheng, L.**; Husch, T.; Song, J.; Kovachiki, N.; Burov, D.; Teh, Y.S.; Anandkumar, A.; Ding, F.; Lee, S.J.R.; Qiao, Z.; Lale, A.S. Systems and methods for determining molecular structures with molecular-orbital-based features. U.S. Patent 16817489, 2020 [\[Link\]](#)