CURRICULUM VITAE

Lijie Ding

Neutron Scattering Division,
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Appointments

May 2024 - present	Postdoctoral Research Associate, Oak Ridge National Laboratory
Jan 2024 - May 2024	Vice President, Quantitative Strategist, Goldman Sachs
Jun 2022 - Dec 2023	Associate, Quantitative Strategist, Goldman Sachs

Education

Sep 2017 - Jun 2022	Ph.D. in Physics, Brown University
	Dissertation: Chiral Liquid Crystal on Deformable Surfaces: A Monte Carlo Study
	Advisor: Robert A. Pelcovits and Thomas R. Powers
Sep 2013 - Jun 2017	B.Sc. in Applied Physics, University of Science and Technology of China
	Thesis: Irreversible Monte Carlo Algorithms
	Advisor: Youjin Deng

Skills

Scientific Computing	Monte Carlo, Molecular Dynamics, LAMMPS, HOOMD-blue, HPC, Slurm
Programming	Python, C/C++, PyTorch, CrewAI, LangChain, NumPy, SciPy, Pandas, Scikit-learn, SQL, Bash
Domain Knowledge	Agentic AI, Computational Physics, Soft Matter Physics, Small-Angle Scattering, Statistical Physics, Polymer Physics, Deep Learning, Machine Learning, Quantitative Finance

Publications

Journal Articles

22. **Lijie Ding**, Jan Michael Y. Carrillo, and Changwoo Do. ToPolyAgent: AI agents for coarse-grained bead-spring topological polymer simulations. *Digital Discovery*, 2026. DOI: 10.1039/D5DD00471C

21. Chi-Huan Tung, Guan-Rong Huang, Ingo Hoffmann, Péter Falus, Bela Farago, Lionel Porcar, Georg Ehlers, Yuya Shinohara, Jan-Michael Carrillo, Yangyang Wang, Sidney Yip, Piotr Zolnierczuk, **Lijie Ding**, Changwoo Do, and Wei-Ren Chen. Bayesian gaussian process inference for neutron spin echo measurement. *The Journal of Chemical Physics*, 163(23):234105, 12 2025. DOI: 10.1063/5.0301962

20. Chi-Huan Tung, Yangyang Wang, Jan-Michael Carrillo, Yuya Shinohara, Chun-Yu Chen, Jhih-Min Lin, Lionel Porcar, Ryan P. Murphy, Guan-Rong Huang, **Lijie Ding**, Changwoo Do, and Wei-Ren Chen.

Bayesian inference of anisotropic 2d small-angle scattering from sparse measurement. *The Journal of Chemical Physics*, 163(15):154103, 10 2025. DOI: 10.1063/5.0291081

19. **Lijie Ding** and Changwoo Do. Deciphering the small-angle scattering of polydisperse hard spheres using deep learning. *APL Machine Learning*, 3(3):036112, 08 2025. DOI: 10.1063/5.0290589

18. Chi-Huan Tung, **Lijie Ding**, Yuya Shinohara, Guan-Rong Huang, Jan-Michael Carrillo, Wei-Ren Chen, and Changwoo Do. A convergence metric for counting statistics in time-resolved small angle neutron scattering. *The Journal of Chemical Physics*, 163(7):074107, 08 2025. DOI: 10.1063/5.0281134

17. **Lijie Ding**, Chi-Huan Tung, Bobby G Sumpter, Wei-Ren Chen, and Changwoo Do. Machine learning inversion from scattering for mechanically driven polymers. *Applied Crystallography*, 58(5):1526–1532, Oct 2025. DOI: 10.1107/S160057672500634X

16. **Lijie Ding**, Chi-Huan Tung, Jan-Michael Y Carrillo, Wei-Ren Chen, and Changwoo Do. Machine learning inversion from small-angle scattering for charged polymers. *Digital Discovery*, 4:2075–2082, 2025. DOI: 10.1039/D5DD00038F

15. **Lijie Ding**, Chi-Huan Tung, Zhiqiang Cao, Zekun Ye, Xiaodan Gu, Yan Xia, Wei-Ren Chen, and Changwoo Do. Machine learning-assisted profiling of a kinked ladder polymer structure using scattering. *Digital Discovery*, 4:1570–1577, 2025. DOI: 10.1039/D5DD00051C

14. **Lijie Ding**, Yihao Chen, and Changwoo Do. Machine learning-informed scattering correlation analysis of sheared colloids. *Applied Crystallography*, 58(3):992–999, 2025. DOI: 10.1107/S1600576725003280

13. **Lijie Ding**, Chi-Huan Tung, Bobby G Sumpter, Wei-Ren Chen, and Changwoo Do. Deciphering the scattering of mechanically driven polymers using deep learning. *Journal of Chemical Theory and Computation*, 21(8):4176–4182, 2025. DOI: 10.1021/acs.jctc.5c00409

12. Chi-Huan Tung, Sidney Yip, Guan-Rong Huang, Lionel Porcar, Yuya Shinohara, Bobby G Sumpter, **Lijie Ding**, Changwoo Do, and Wei-Ren Chen. Unlocking hidden information in sparse small-angle neutron scattering measurements. *Journal of Colloid and Interface Science*, page 137554, 2025. DOI: 10.1016/j.jcis.2025.137554

11. Chi-Huan Tung, **Lijie Ding**, G-R Huang, Lionel Porcar, Yuya Shinohara, Bobby G Sumpter, Changwoo Do, and W-R Chen. Insights into distorted lamellar phases with small-angle scattering and machine learning. *Applied Crystallography*, 58(2):523–534, 2025. DOI: 10.1107/S1600576725000317

10. Guan-Rong Huang, Lionel Porcar, Ryan P Murphy, Yuya Shinohara, Yangyang Wang, Jan-Michael Carrillo, Bobby G Sumpter, Chi-Huan Tung, **Lijie Ding**, Changwoo Do, and Wei-Ren Chen. Elongated particles in flow: Commentary on small angle scattering investigations. *Applied Crystallography*, 58(3): 637–658, 2025. DOI: 10.1107/S1600576725002900

9. Chi-Huan Tung, **Lijie Ding**, Ming-Ching Chang, Guan-Rong Huang, Lionel Porcar, Yangyang Wang, Jan-Michael Y Carrillo, Bobby G Sumpter, Yuya Shinohara, Changwoo Do, and Wei-Ren Chen. Scattering-based structural inversion of soft materials via kolmogorov–arnold networks. *The Journal of Chemical Physics*, 162(7), 2025. DOI: 10.1063/5.0253877

8. Chi-Huan Tung, **Lijie Ding**, Guan-Rong Huang, Yangyang Wang, Jan-Michael Y. Carrillo, Bobby G. Sumpter, Yuya Shinohara, Changwoo Do, and Wei-Ren Chen. A discretized representation for monte carlo simulation of deformed semiflexible chains. *The Journal of Chemical Physics*, 161(22):224107, 12 2024. DOI: 10.1063/5.0235798

7. **Lijie Ding**, Chi-Huan Tung, Bobby G Sumpter, Wei-Ren Chen, and Changwoo Do. Off-lattice markov chain monte carlo simulations of mechanically driven polymers. *Journal of Chemical Theory and Computation*, 20(23):10697–10702, 2024. DOI: 10.1021/acs.jctc.4c01260

6. **Lijie Ding**, Robert A Pelcovits, and Thomas R Powers. Chiral fluid membranes with orientational order and multiple edges. *Soft Matter*, 19(43):8453–8464, 2023. DOI: 10.1039/D3SM01158E

5. **Lijie Ding**, Robert A. Pelcovits, and Thomas R. Powers. Deformation and orientational order of chiral membranes with free edges. *Soft Matter*, 17:6580–6588, 2021. DOI: 10.1039/D1SM00629K

4. **Lijie Ding**, Robert A Pelcovits, and Thomas R Powers. Shapes of fluid membranes with chiral edges. *Physical Review E*, 102(3):032608, 2020. DOI: 10.1103/PhysRevE.102.032608

3. Shayan Lameh, **Lijie Ding**, and Derek Stein. Controlled Amplification of DNA Brownian Motion Using Electrokinetic Noise. *Physical Review Applied*, 14(5):054042, 2020. DOI: 10.1103/PhysRevApplied.14.054042

2. Sherjeel M Khan, Nadeem Qaiser, Sohail F Shaikh, **Lijie Ding**, and Muhammad M Hussain. Do-it-yourself integration of a paper sensor in a smart lid for medication adherence. *Flexible and Printed Electronics*, 4(2):025001, 2019. DOI: 10.1088/2058-8585/ab10f5

1. Eren Metin Elçi, Jens Grimm, **Lijie Ding**, Abrahim Nasrawi, Timothy M Garoni, and Youjin Deng. Lifted worm algorithm for the Ising model. *Physical Review E*, 97(4):042126, 2018. DOI: 10.1103/PhysRevE.97.042126

Preprints

6. **Lijie Ding**, Janell Thomson, Jon Taylor, and Changwoo Do. LLMs can assist with proposal selection at large user facilities. *arXiv preprint arXiv:2512.10895*, 2025. arXiv: 2512.10895

5. Hongyi Du, Jiaqi Su, Jisen Li, **Lijie Ding**, Yingxuan Yang, Peixuan Han, Xiangru Tang, Kunlun Zhu, and Jiaxuan You. Which LLM multi-agent protocol to choose? *arXiv preprint arXiv:2510.17149*, 2025. arXiv: 2510.17149

4. **Lijie Ding**, Egang Lu, and Kin Cheung. Deep learning option pricing with market implied volatility surfaces. *arXiv preprint arXiv:2509.05911*, 2025. arXiv: 2509.05911

3. **Lijie Ding** and Changwoo Do. SasAgent: Multi-agent ai system for small-angle scattering data analysis. *arXiv preprint arXiv:2509.05363*, 2025. arXiv: 2509.05363

2. **Lijie Ding**, Egang Lu, and Kin Cheung. Fast derivative valuation from volatility surfaces using machine learning. *arXiv preprint arXiv:2505.22957*, 2025. arXiv: 2505.22957

1. **Lijie Ding**, Robert A Pelcovits, and Thomas R Powers. Brownian dynamics simulations of inclusions in an active fluid bath. *arXiv preprint arXiv:2505.09744*, 2025. arXiv: 2505.09744

In preparation

1. **Lijie Ding** and Changwoo Do. Deep learning the small-angle scattering of polydisperse rods. 2025. (in preparation)

Presentations

Invited Talks

8. LLMs Can Assist with Proposal Selection at Large User Facilities. Neutron Day 2026, Oak Ridge National Laboratory (Jan. 2026)

7. Machine Learning for Scattering Analysis and Derivative Valuation. Condensed Matter and Biophysics Seminar. Brown University (Sep. 2025)

6. Machine Learning for Derivative Valuation with Volatility Surfaces. Large Scale Structures Seminar Series, Neutron Scattering Division, Oak Ridge National Laboratory. (Sep. 2025)

5. Examples of Machine Learning for Small-Angle Scattering. Joint Nanoscience and Neutron Scattering User Meeting. Knoxville. (Aug. 2025)

4. Mechanically Driven Polymers: Monte Carlo Simulation and Machine Learning-Assisted Scattering Analysis. SMART forum. Oak Ridge National Laboratory (Apr. 2025)

3. Machine Learning-Assisted Inference of Sheared Suspension using Scattering. Neutron Scattering Day, Oak Ridge National Laboratory. (Jan. 2025)

2. Characterizing structure of ladder polymer using machine learning assisted scattering data analysis. AI for Neutrons Workshop, Oak Ridge National Laboratory (Oct. 2024)

1. Shapes and orientational order of colloidal membrane. Oak Ridge National Laboratories (Apr. 2022), Johns Hopkins University (Apr. 2022), Instituto Gulbenkian de Ciência (Apr. 2022), Merck (Mar. 2022), Rice University (Feb. 2022), Sandia National Laboratories (Dec. 2021)

Contributed Talks

9. Extracting properties of charged polymers from scattering using Machine Learning. AI4Science Workshop, ORNL (Apr. 2025)

8. Characterizing structure of ladder polymer using machine learning assisted scattering data analysis. ACS Spring meeting, session on General Topics: New Synthesis and Characterization of Polymers. San Diego (Mar. 2025)

7. Monte Carlo Simulation and Machine Learning-Assisted Scattering Analysis of Mechanically Driven Polymers. APS Global Physics Summit, session on Machine Learning and Optimization for Accelerating Polymer Physics. Anaheim (Mar. 2025)

6. Characterizing structure of ladder polymer using machine learning assisted scattering data analysis. 99th New England Complex Fluids Meeting Brown University (Jun. 2024)

5. Three-dimensional structures of chiral membrane with edges, APS March Meeting, Session on Membranes, Micelles and Vesicles. Chicago (Mar. 2022)

4. 3D structures of chiral membrane with edges. 89th New England Complex Fluids Meeting. Harvard University (Dec. 2021)

3. Chiral membranes with orientational order and free edges, APS March Meeting, Session on Membranes, Micelles and Vesicles. Online (Mar. 2021)

2. Membranes with orientational order and free edges. 86th New England Complex Fluids Meeting. Online (Mar. 2021)

1. Shapes of fluid membrane with chiral edges. 81st New England Complex Fluids Meeting. Harvard University (Dec. 2019)

Posters

7. Mechanically Driven Polymers: Monte Carlo Simulation and Machine Learning Scattering Analysis (and more). Southeast Polymer Forum, University of Georgia (May. 2025)

6. Characterizing structure of ladder polymer using machine learning assisted scattering data analysis. Southeast Polymer Forum, Oak Ridge National Laboratory (Oct. 2024)

5. 3D structures of chiral membranes with free edges. Mechanics of Life workshop, Flatiron Institute (May. 2022)

4. 3D structures of chiral membranes with free edges. Physics Department Poster Session. Brown University(Nov. 2021)

3. Membranes with orientational order and free edges. Physics Department Poster Session. Brown University(Nov. 2020)

2. Shapes of fluid membrane with chiral edges. Physics Department Poster Session. Brown University (Nov. 2019)

1. Membranes with edges. Materials Research Science and Engineering Centers Retreat. Brandeis University (Nov. 2018)

Mentoring

Simon Nirenberg (Brown 2028)   Research student internship program, (Summer 2025)

Teaching

Teaching Assistant   Basic Physics B, Brown University (Spring 2018)
Teaching Assistant   Basic Physics A, Brown University (Fall 2017)
Teaching Assistant   Mechanics and Thermal Physics, USTC (Fall 2016)

Professional Activities
- Reviewer, Computational Economy (Dec 2025)
- Reviewer, Machine Learning with Application (Aug. 2025)
- Presider, ACS Spring Meeting, Session on General Topics: New Synthesis and Characterization of Polymers. San Diego (Mar. 2025)
- Reviewer, Scientific Reports. (Jun. 2024)

Awards and Honors

2025   Faculty Poster Award, Southeast Polymer Forum, University of Georgia, U.S.
2021   Physics Dissertation Fellowship, Brown University, U.S.
2016   National Scholarship, Ministry of Education, China
2015   Grand Prize, China Undergraduate Physics Tournament, China
2015   National Scholarship, Ministry of Education, China
2012   Bronze Medal, Chinese Physics Olympiad, China

VITA Prepared January 27, 2026