PINCHEN XIE

50A-2117, Lawrence Berkeley National Lab, CA 94720

Email: PinchenXie@lbl.gov ⋄ Homepage: https://salinelake.github.io/

POSITION

Luis W. Alvarez Postdoctoral Fellow, Lawrence Berkeley National Laboratory   *2024-Present*

EDUCATION

Ph.D. Applied Mathematics, Princeton University   *2018-2024*
Advisor: Roberto Car (Chemistry, Physics) and Weinan E (Mathematics)
B.S. Physics, Fudan University   *2014-2018*

RESEARCH INTERESTS

Methodology and application of machine learning-assisted multi-scale modeling in molecules and condensed matter.

PUBLICATIONS

1. **P. Xie**, Y. Chen, W. E and R. Car. "Thermal disorder and phonon softening in the ferroelectric phase transition of lead titanate" Under review.

2. B. Yang*, **P. Xie***, and R. Car. "Deuteration removes quantum dipolar defects from KDP crystals." npj Comput. Mater. 10.1 (2024): 241

3. **P. Xie** and W. E. "Coarse-graining conformational dynamics with multi-dimensional generalized Langevin equation: how, when, and why." J. Chem. Theory Comput. 20.18 (2024): 7708–7715

4. **P. Xie**, R. Car, and W. E. "Ab Initio Generalized Langevin Equations ." PNAS 121.14 (2024): e2308668121

5. W. E, H. Lei, **P. Xie**, L. Zhang "Machine Learning-Assisted Multi-scale Modeling ." J. Math. Phys. 64.7 (2023): 071101

6. **P. Xie**, and W. E. "Coarse-grained spectral projection: A deep learning assisted approach to quantum unitary dynamics." Phys. Rev. B 103.2 (2021): 024304.

7. R. Wu, X. Cao, **P. Xie**, and Y. Liu. "End-to-end quantum machine learning implemented with controlled quantum dynamics." Phys. Rev. Appl. 14.6 (2020): 064020.

8. **P. Xie**, B. Yang, Z. Zhang and R. F. S. Andrade. "Exact evaluation of the causal spectrum and localization properties of electronic states on a scale-free network " Physica A 502 (2018): 40-48.

9. B. Yang, **P. Xie** and Z. Zhang. "Effects of heterogeneity in site-site couplings for tight-binding models on scale-invariant structures." Phys. Lett. A 381.44 (2017): 3773-3778.

10. **P. Xie**, B. Wu and Z. Zhang. "Exactly solvable tight-binding model on two scale-free networks with identical degree distribution." EPL 116.3 (2016): 38002.

11. **P. Xie**, Z. Zhang and F. Comellas. "The normalized Laplacian spectrum of subdivisions of a graph." Appl. Math. Comput. 286 (2016): 250-256.

12. **P. Xie**, Z. Zhang and F. Comellas. "On the spectrum of the normalized Laplacian of iterated triangulations of graphs." Appl. Math. Comput. 273 (2016): 1123-1129.

13. **P. Xie**, Y. Lin and Z. Zhang. "Spectrum of walk matrix for Koch network and its application." J. Chem. Phys. 142.22 (2015): 224106.

* indicates equal contribution

CONFERENCE PRESENTATIONS

1. APS March Meeting, Anaheim, March 2025

2. 36th Fundamental Physics of Ferroelectrics Workshop, Annapolis, February 2025

3. Simons Symposium: Challenges in Biomolecular Simulations, NYU, New York, May 2024

4. APS March Meeting, Minneapolis, March 2024

5. 35th Fundamental Physics of Ferroelectrics Workshop, Washington, D.C., February 2024

6. Poster, International Workshop on Nuclear Quantum Effects, NYU, New York, June 2023

7. APS March Meeting, Las Vegas, March 2023

8. APS March Meeting, Chicago, March 2022

9. 33rd Fundamental Physics of Ferroelectrics Workshop, Washington, D.C., February 2022

10. U21 Undergraduate Research Conference, University of Edinburgh, Edinburgh, June 2017

SEMINAR TALKS

1. Pitzer Center Theoretical Chemistry Seminar, UC Berkeley, October 2024

2. CS Seminar, Lawrence Berkeley National Lab, January 2024

3. Chemistry in Solution and at Interfaces Seminar, Princeton University, March 2023

4. Invited talk (Virtual), DP Technology, Beijing, January 2023

5. Invited talk, Samsung Semiconductor Advanced Materials Lab, Boston, August 2022

6. PACM Colloquium, Princeton University, February 2022

7. Chemistry in Solution and at Interfaces Seminar, Princeton University, February 2022

PROFESSIONAL SERVICE

Referee for
J. Chem. Theory Comput.; J. Phys. Chem.; Quantum Machine Intelligence; J. Mater. Chem. A
Conference and seminar organization
Tutor, Deep Modeling for Molecular Simulation workshop *2022-2024*

OPEN-SOURCE SOFTWARE DEVELOPMENT

Main contributor
OpenFerro, AIGLETools

TEACHING AND ADVISING

Assistant Instructor - Princeton University
PHY512 Monte Carlo and Molecular Dynamics Simulation *Spring 2022 & 2023*
MAT202 Linear Algebra with Applications *Fall 2021*
MAT199 Math Alive *Spring 2020*
MAT201 Multivariable Calculus *Fall 2019*
Graduate Mentor - Princeton University
Mentoring Möbius Program, Math Department *2020*

HONORS AND AWARDS

Luis W. Alvarez Fellowship *2024-2026*
Lawrence Berkeley National Lab
Chun-Tsung Scholar *2017*
H. C. Chin and T. D. Lee Chinese Undergraduate Research Endowment
SFI Scholarship *2017*
Chinese University of Hong Kong, Shenzhen