

PINCHEN XIE

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POSITION

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

EDUCATION

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

RESEARCH INTERESTS

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

PUBLICATIONS

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1. **P. Xie**, R. Car, and W. E. “Ab Initio Generalized Langevin Equations .” [PNAS 121.14 \(2024\): e2308668121](#)
 2. W. E, H. Lei, **P. Xie**, L. Zhang “Machine Learning-Assisted Multi-scale Modeling .”[J. Math. Phys. 64.7 \(2023\): 071101](#)
 3. **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](#).
 4. 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](#).
 5. **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](#).
 6. 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](#).
 7. **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](#).
 8. **P. Xie**, Z. Zhang and F. Comellas. “The normalized Laplacian spectrum of subdivisions of a graph.” [Appl. Math. Comput. 286 \(2016\): 250-256](#).
 9. **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](#).
 10. **P. Xie**, Y. Lin and Z. Zhang. “Spectrum of walk matrix for Koch network and its application.” [J. Chem. Phys. 142.22 \(2015\): 224106](#).

CONFERENCE PRESENTATIONS

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1. Simons Symposium: Challenges in Biomolecular Simulations, NYU, New York, May 2024
 2. APS March Meeting, Minneapolis, March 2024
 3. 35th Fundamental Physics of Ferroelectrics Workshop, Washington, D.C., February 2024
 4. Poster, International Workshop on Nuclear Quantum Effects, NYU, New York, June 2023
 5. APS March Meeting, Las Vegas, March 2023
 6. APS March Meeting, Chicago, March 2022

7. 33rd Fundamental Physics of Ferroelectrics Workshop, Washington, D.C., February 2022
8. U21 Undergraduate Research Conference, University of Edinburgh, Edinburgh, June 2017

SEMINAR TALKS

1. CS Seminar, Lawrence Berkeley National Lab, January 2024
2. Chemistry in Solution and at Interfaces Seminar, Princeton University, March 2023
3. Invited talk (Virtual), DP Technology, Beijing, January 2023
4. Invited talk, Samsung Semiconductor Advanced Materials Lab, Boston, August 2022
5. PACM Colloquium, Princeton University, February 2022
6. 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

Conference and seminar organization

Tutor, Deep Modeling for Molecular Simulation workshop,

2022-2024

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