PINCHEN XIE

Program in Applied and Computational Mathematics, Princeton University , NJ 08544
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EDUCATION

Ph.D. Applied Mathematics, Princeton University *2018 - June 2024 (expected)*
Advisors: Roberto Car and Weinan E
B.S. Physics, Fudan University *2014 - 2018*
Advisors: Xiaopeng Li and Zhongzhi Zhang
Visiting student, University of California, Berkeley *2016*

RESEARCH INTERESTS

Methodology and application of machine learning-assisted, dynamically consistent, multi-scale modeling in biomolecules (protein dynamics) and condensed matter (microstructure evolution).

WORKS IN PROGRESS

1. **P. Xie**, R. Car, and W. E. "Ab Initio Generalized Langevin Equations ." submitted to Proceedings of the National Academy of Sciences (Under review)
2. B. Yang*, **P. Xie***, and R. Car. "First-principles path-integral molecular dynamics study of ferroelectricity and isotope effects in KDP crystals with deep neural networks." Manuscript in progress, to be submitted for publication in spring 2024.
3. **P. Xie**, Y. Chen, W. E, and R. Car. "Ab initio multi-scale modeling of ferroelectrics: The case of $PbTiO_3$." arXiv:2205.11839 (2022) Manuscript in progress, to be submitted for publication in spring 2024.

PUBLICATIONS

1. W. E, H. Lei, **P. Xie**, L. Zhang "Machine Learning-Assisted Multi-scale Modeling ."J. Math. Phys. 64.7 (2023): 071101
2. **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.
3. 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.
4. **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.
5. 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.
6. **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.
7. **P. Xie**, Z. Zhang and F. Comellas. "The normalized Laplacian spectrum of subdivisions of a graph." Appl. Math. Comput. 286 (2016): 250-256.
8. **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.
9. **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

1. APS March Meeting, Minneapolis, March 2024
2. 35th Fundamental Physics of Ferroelectrics Workshop, Washington, D.C., February 2024
3. Poster, International Workshop on Nuclear Quantum Effects, NYU, New York, June 2023
4. APS March Meeting, Las Vegas, March 2023
5. APS March Meeting, Chicago, March 2022
6. 33rd Fundamental Physics of Ferroelectrics Workshop, Washington, D.C., February 2022
7. 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, July 2023
Tutor, Deep Modeling for Molecular Simulation workshop, July 2022 (virtual)

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*

TECHNICAL STRENGTH

- High-performance programming with Python (PyTorch, JAX) for scientific computing and deep learning
- Familiar with LAMMPS, OPENMM, GROMACS, i-PI, PLUMED, Quantum Espresso, VASP, DeePMD, DeepChem, and relevant softwares

HONORS AND AWARDS

Azure Cloud Computing Grant 2022
Center for Statistics and Machine Learning, Princeton University
Chun-Tsung Scholar 2017
H. C. Chin and T. D. Lee Chinese Undergraduate Research Endowment
SFI Scholarship 2017
Chinese University of Hong Kong, Shenzhen