Zhenyao Fang

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Research Interests

My research interest is to combine first-principles methods and machine learning techniques to advance the prediction of physical properties of materials and gain insights into complex phenomenon, such as disorder, defects, and light-matter interactions. By developing physics-inspired machine learning models, my current work seeks to develop computational framework for understanding the disorder effect in materials and unravel how it impacts other functional properties such as optical conductivity and carrier transport. My research goal is to build scalable high-throughput workflows for material databases, develop data-driven machine learning architectures for efficient predictions of material properties, and inversely design materials with target functionalities, accelerating future discovery and development of next-generation optoelectronic materials and devices.

Education

2019-2023 **Ph. D in Chemistry,** Department of Chemistry, University of Pennsylvania, USA
Supervisor: Prof. Andrew M. Rappe
Thesis: First-Principles Study on Properties of Low-Energy Electrons in Solid States

2017-2019 **Master of Chemical Sciences,** Department of Chemistry, University of Pennsylvania, USA

2013-2017 **B. S. in Chemistry,** Zhejiang University, China

Professional Experience

2023-Present Post-doctoral researcher, Department of Physics, Northeastern University, USA
Supervisor: Prof. Qimin Yan

Teaching and Mentoring Experience

2024 QuESO workshop, Northeastern University
Topic: Machine learning for quantum materials

2020 Teaching assistant, Honors General Chemistry II, University of Pennsylvania

2019 Teaching assistant, Honors General Chemistry I, University of Pennsylvania

Awards

2024 Best Oral Presentation Award of 2024 MRS Fall Meeting

2020 Chemistry Teaching Assistant Commendation Award for Honors General Chemistry II

2019 Chemistry Teaching Assistant Commendation Award for Honors General Chemistry I

2017 Excellent Report Award of the 4th National Science and Technology Conference for Chemistry Majors

Contributed Presentations

2025 Penn Conference on Theoretical Chemistry, Philadelphia, PA, USA
Approaching Disorder Effects in Materials Using Graph Neural Networks

2025 American Physical Society March Meeting, Anaheim, CA, USA
Towards Accurate Prediction of Configurational Disorder Properties Using Graph Neural Networks

2024 Materials Research Society Fall Meeting, Boston, MA, USA

Towards Accurate Prediction of Configurational Disorder Properties Using Graph Neural Networks

2024 American Physical Society March Meeting, Minneapolis, MN, USA
Controllable Topological Insulator Phases in Square-Net Litharge-Phase InBi Monolayer

Publications

1) **Zhenyao Fang**, Ting-Wei Hsu, Qimin Yan. Dataset of tensorial optical and transport properties of materials from the Wannier function method. ***Sci. Data*** 2025, 12, 1092.
2) Zhongxuan Wang, Ti Xie, **Zhenyao Fang**, Jun Zhang, Cheng Gong, Qimin Yan, Shenqiang Ren. Chiral Molecular Magnet Superstructures with Light Control. ***Nano Letters*** 2025, 25, 2502-2508.
3) **Zhenyao Fang**, Qimin Yan. Leveraging Persistent Homology Features for Accurate Defect Formation Energy Predictions via Graph Neural Networks. ***Chem. Mat.*** 2025, 37, 1531-1540.
4) Hui Fang, Anupma Thakur, Amirhossein Zahmatkeshsaredorah, **Zhenyao Fang**, Vahid Rad, Ahmad A. Shamsabadi, Claudia Pereyra, Masoud Soroush, Andrew M. Rappe, Xiaoji G. Xu, Babak Anasori, and Zahra Fakhraai. Stabilizing $Ti_3C_2T_x$ MXene flakes in air by removing confined water. ***Proc. Natl. Acad. Sci.*** 2024, *121*, (28), e2400084121.
5) **Zhenyao Fang**, Qimin Yan. Towards accurate prediction of configurational disorder properties in materials using graph neural networks. ***npj Computational Materials*** 2024 10, No. 9.
6) Young-Chul Leem*, **Zhenyao Fang***, Yun-Kyung Lee, Na-Yeong Kim, Arvin Kakekhani, Wenjing Liu, Sung-Pyo Cho, Cheolsu Kim, Yuhui Wang, Zhurun Ji, Abhirup Patra, Leeor Kronik, Andrew M. Rappe, Sang-Youp Yim, and Ritesh Agarwal. Optically Triggered Emergent Mesostructures in Monolayer WS_2. ***Nano Letters*** 2024 *24* (18), 5436-5443.
7) **Zhenyao Fang**, Andrew M. Rappe. Controllable topological insulator phases in litharge-phase InBi monolayer. ***Phys. Rev. Mater.*** 2023, *7*, No. 074202.
8) Bing Xu*, **Zhenyao Fang***, Miguel-Ángel Sánchez-Martínez*, Jorn W. F. Venderbos, Zhuoliang Ni, Tian Qiu, Kaustuv Manna, Kefeng Wang, Johnpierre Paglione, Christian Bernhard, Claudia Felser, Eugene J. Mele, Adolfo G. Grushin, Andrew M. Rappe, Liang Wu. Optical signatures of multifold fermions in the chiral topological semimetal CoSi. ***Proc. Natl. Acad. Sci.*** 2020 *117* (44), pp 27104-27110.
9) **Zhenyao Fang**, Heng Gao, Jorn W. F. Venderbos, Andrew M. Rappe. Ideal near-Dirac triple point semimetal in III-V semiconductor alloys. ***Phys. Rev. B*** 2020, *101*, No. 125202.