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Institute of Applied Physics and Computational Mathematics, Huayuan Road, 100088 Beijing, China

Education

2021.9–present **Ph.D. Candidate in Fundamental Mathematics**, Institute of Applied Physics and Computational Mathematics, China.

Advisors: Prof. Han Wang, Prof. Wengu Chen.

2020.1–2020.7 **Exchange Student**, Georgia Institute of Technology, USA.

2017.9–2021.6 **B.S. in Mathematics and Applied Mathematics**, Taishan College, Shandong University, China.

Research Interests and Experience

My research focuses on machine learning methods for multi-scale modeling, especially in quantum many-body physics and ultrafast dynamics.

- Developed machine learning potentials to simulate dynamic mechanical response of materials under extreme conditions.
- Proposed a neural network framework for solving the time-dependent Schrödinger equation in real space.
- Familiar with deep learning techniques such as physics-informed neural networks (PINNs), graph neural networks (GNNs), and generative models.
- Familiar with quantum chemistry simulation methods, including traditional methods like Hartree-Fock (HF), Full Configuration Interaction (FCI), and machine learning based methods like FermiNet.
- Current research: machine learning modeling of ultrafast dynamics in quantum many-body systems.
- Broader interests: Monte Carlo methods, scientific computing, uncertainty quantification.

Publications and Preprints

- 2025 [Enze, Hou](#), Yuzhi Liu, Lei Wang*, Han Wang*
A Global Spacetime Optimization Approach to the Real-Space Time-Dependent Schrödinger Equation [\[Preprint\]](#)
arXiv preprint. [arXiv:2511.12983](https://arxiv.org/abs/2511.12983).
- 2025 [Enze, Hou](#), Xiaoyang Wang, Han Wang*
Revealing the dynamic responses of Pb under shock loading based on DFT-accuracy machine learning potential [\[Preprint\]](#)
arXiv preprint. [arXiv:2507.03456](https://arxiv.org/abs/2507.03456).
- 2025 Xiaoyang Wang, [Enze, Hou](#), Han Wang*
A Machine Learning Potential Model for Simulating Dynamic Mechanical Response of Pb-Sn Alloy [\[Published\]](#)
Chinese Journal of High Pressure Physics. doi:[10.11858/gywlb.20251151](https://doi.org/10.11858/gywlb.20251151).

Presentations

- 2025.8 **2025 Beijing-Tianjin-Hebei+ Computational Mathematics Academic Exchange Conference**.
Jinan, China. [Enze, Hou](#).

Awards and Honors

- 2023 Outstanding Graduate Student Cadre, IAPCM
- 2022 Outstanding Graduate Student, IAPCM

2018	First-Class Specialty Scholarship, Shandong University
2018	Outstanding Student Cadre, Shandong University

Skills

- Programming Languages: Python, C, MATLAB.
- Scientific Computing: Quantum chemistry packages (PySCF), Machine learning frameworks (PyTorch, JAX), DFT software (VASP, ABACUS), Visualization tools (OVITO).
- Computing Environment: Linux, Git, HPC clusters, Shell scripting.
- Tools: LaTeX, Markdown.
- Languages: Mandarin (native), Cantonese, English (fluent).