

## EDUCATION

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**Xiamen University** — *Ph.D. in Condensed Matter Physics, GPA 3.91* (EXPECTED) SEP 2022 – JUN 2028

- Research Focus: computational materials, single/dual-atom catalyst design.

**Hangzhou Normal University** — *B.S. in Physics* SEP 2018 – JUN 2022

## WORK EXPERIENCE

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**Deep Principle** — *AI4S Algorithm Intern* JAN 2026 – PRESENT

- Trained and evaluated **MPA**, a materials foundation model bringing LLM-style multi-phase training (pre-/mid-/post-training) to experimental property prediction — **SOTA on 35/40 tasks** and **14.6% lower MAE** than direct fine-tuning under scaffold (OOD) splits, surpassing Uni-Mol2, Suiren, and ChemProp.
- Implemented the **mid-training** (physics-guided alignment on large-scale first-principles data) and **post-training** pipelines — including a **Hybrid Readout** head (attention-pooling + atom-additive) — built the training/evaluation infrastructure and ran all large-scale training.

**Xiamen University** — *Ph.D. Candidate* SEP 2022 – PRESENT

- **Dual-atom catalyst design & mechanism:** designed Si-based dual-atom catalysts for CO<sub>2</sub> reduction (*Appl. Surf. Sci.* 2024); uncovered the p-d orbital-coupling mechanism and screened 360+ candidates with a GBR pipeline (*J. Mater. Chem. A* 2024).
- **Curvature-driven catalysis:** established curvature as an independent activity knob (inverted-volcano relation, interpretable descriptor; *J. Phys. Chem. Lett.* 2026) and generalized it into a unified **geometric-electronic principle** (*ACS Catal.* 2026).

## SELECTED PUBLICATIONS & PATENTS

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Report: **Materials Property Axiom: Adapting Foundation Models to Experimental Property Prediction via Multi-phase Training**

Deep Principle Team, Technical Report, 2026

Paper: **A Geometric-Electronic Principle for Curvature-Driven Catalysis**

M. Wang, Y. Lin, Z. Huang, Y. Sun, Z.-Z. Zhu, S. Wu, X. Cao, *ACS Catal.*, 2026 (Accepted)

Paper: **Curvature Engineering of SiFe Dual-Atom Catalysts for Enhanced CO<sub>2</sub> Electroreduction**

M. Wang, Y. Lin, Y. Xiang, Y. Sun, Z.-Z. Zhu, S. Wu, X. Cao, *J. Phys. Chem. Lett.*, 17, 1227–1234 (2026)

Paper: **p-d Orbital Coupling in Silicon-Based Dual-Atom Catalysts for Enhanced CO<sub>2</sub> Reduction**

M. Wang, Y. Xiang, Y. Lin, Y. Sun, Z.-Z. Zhu, S. Wu, X. Cao, *J. Mater. Chem. A*, 12(46), 31902–31913 (2024)

Paper: **SiFeN<sub>6</sub>-graphene: A Promising Dual-Atom Catalyst for Enhanced CO<sub>2</sub>-to-CH<sub>4</sub> Conversion**

M. Wang, Y. Xiang, W. Chen, S. Wu, Z.-Z. Zhu, X. Cao, *Appl. Surf. Sci.*, 643, 158724 (2024)

Patent: **A Liquid Detection Device**

M. Wang, R. Qin, S. Zhou, W. Ding, Y. Che, **China Invention Patent ZL 2021 1 0042048.9, granted 2024.05**

## SKILLS

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- **Foundation Models:** Foundation models, pre-/mid-/post-training, custom readout heads and loss design, PEFT/LoRA fine-tuning, equivariant GNN potentials.
- **ML Engineering & Evaluation:** Training/evaluation infrastructure, distributed training (DDP), data curation, benchmark design, statistical evaluation.
- **Programming & Computation:** Python, PyTorch, NumPy/Pandas/Matplotlib, Linux, HPC/SLURM, DFT (VASP, JDFTx), ASE, pymatgen, scikit-learn.