Xiao Jiang (江筱)

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Research Summary & Interests

I am a recent Ph.D. graduate in condensed matter theory and computational materials science, with a core focus on the fundamental physics of **electron-phonon interactions**. I am passionate about developing and applying unified multi-scale computational frameworks to model how charge carriers couple with lattice vibrations. My work aims to reveal the microscopic mechanisms governing carrier transport, such as polaron formation and dynamics, thereby advancing our fundamental understanding of quantum phenomena in materials.

Building on this expertise, my future research will venture into more complex and emergent quantum phenomena, focusing on three primary directions:

1. **Electron-Phonon Coupling in Strongly Correlated Systems**: Extending and developing first-principles methods to accurately model EPC in strongly correlated materials.
2. **Computational Design of Superconducting Materials**: Applying advanced EPC calculations to the search for new superconductors and investigating phonon-mediated pairing mechanisms.
3. **Non-Equilibrium Carrier Dynamics**: Developing theoretical frameworks to simulate the transport and relaxation of 'hot' carriers under photo-excitation.

Education

Ph.D. in Physics (Condensed Matter Physics) | Lanzhou University | Sept 2018 – June 2025

- **Dissertation**: "First-principles simulation study of carrier transport in transition metal oxide photocatalytic materials"
- **Advisor**: Prof. Weihua Han
- **Co-Advisor**: Prof. Zemin Zhang

B.S. in Physics | Lanzhou University | Sept 2012 – June 2016

Research Experience

Funded Projects

Key Participant | National Natural Science Foundation of China (NSFC) | Jan 2020 – Dec 2023

- **Project**: "Research on the transport behavior of photogenerated carriers in composite semiconductor catalyst heterojunctions" (Grant No. 51972153).
- Contributed significantly to the theoretical and computational aspects of the project, focusing on modeling carrier dynamics at heterojunction interfaces.

Doctoral Research

Doctoral Researcher | School of Physical Science and Technology, Lanzhou University | Sept 2018 – June 2025

- **Multi-Scale Computational Framework Development**
  - Designed and implemented a unified computational framework connecting first-principles calculations (DFT, DFPT) with macroscopic device models (continuity equations).
  - Successfully applied the framework to predict optimal film thickness and guide the rational design of metal oxide photoelectrodes (e.g., p-type $CuFeO_2$ and n-type Fe_2O_3), bridging microscopic theory with experimental device performance.
- **Unveiling Asymmetric Polaron Formation in CeO_2**
  - Revealed the microscopic origins of carrier transport by investigating electron-phonon coupling and polaron formation from first principles.
  - Discovered the novel coexistence of localized Holstein (electron) and delocalized Fröhlich (hole) polarons in CeO_2, elucidating the asymmetric transport mechanisms within a single material.
- **Crystal Symmetry's Role in Polaron Transport**
  - Established a universal link between crystal symmetry, polaron type, and carrier transport anisotropy by systematically analyzing polymorphs of $BiVO_4$ and TiO_2.
  - Resolved the long-standing controversy of polaron types in TiO_2, identifying a unique "crossover" behavior where anatase and rutile phases exhibit completely opposite electron and hole polaron characteristics.

Collaborative Research Projects

DFT Consultant | Catalytic Effects of Gray Gallium Nitride

- **Project**: A collaborative study published in *ACS Nano* (2025) on the catalytic generation of hydrogen peroxide at the GaN-liquid interface under mechanical stimuli.
- **My Contribution**: Served as a DFT consultant, providing theoretical guidance on the simulation of interfacial charge transfer dynamics. Advised on the calculation of adsorption energies, Fermi level shifts, and work function changes to help elucidate the catalytic mechanism.

Computational Contributor | Ferroelectric-Modulated Photoelectrodes

- **Project**: A collaborative study published in *Advanced Functional Materials* (2024, 34, 2316409) on designing high-performance ferroelectric-modulated photocathodes.
- **My Contribution**: I developed the code for the optoelectronic modeling part of this work. My simulations of photocarrier distribution provided the theoretical guidance for the device's structural design.

DFT Consultant | Gas Adsorption Mechanisms on WO_3 Surfaces

- **Project**: A collaborative study published in *The Journal of Physical Chemistry Letters* (2020, 11, 9070-9078) investigating the gas-sensing mechanism of WO_3.
- **My Contribution**: Provided expert guidance on the first-principles DFT calculation section. My advisory role included consulting on the simulation setup and assisting the primary authors in analyzing surface reconstruction, electron localization, and charge transfer mechanisms.

Teaching and Mentoring

- **Teaching Assistant**, *General Physics* (Undergraduate Course), Lanzhou University.
- **Mentor for Undergraduate Students**, advised students on final year thesis projects and scientific innovation projects.

Conference Presentations

- **Jiang, X.**, et al. (2021). Poster presentation at the Chinese Physical Society (CPS) Fall Meeting.

Honors and Awards

- **University-level Graduate Scholarship**, Lanzhou University (Multiple Awards during Ph.D. studies)

Skills

- **Programming Languages**: Python, C++, Julia
- **Scientific Software**: Quantum ESPRESSO, VASP, Wannier90, EPW, Yambo, Elk, **TRIQS** (Contributor to the `dft_tools` submodule, including bug fixes).
- **Theoretical Models**: Density Functional Theory (DFT), Density Functional Perturbation Theory (DFPT), Dynamical Mean-Field Theory (DMFT), Many-Body Perturbation Theory (GW/BSE), Boltzmann Transport Equation, Polaron Theory.
- **Languages**: Chinese (Native), English (Fluent)

Publications

*(*Corresponding author)*

First-Author:

1. **Jiang, X.**, Cheng, X., Liu, Z., Ding, L., Han, W.* "First-Principles Study of Polarons in Multiple Crystal Phases of Bismuth Vanadate." *The Journal of Physical Chemistry C* 129.42, 19190-19198 (2025).
2. **Jiang, X.**, Cheng, X., Liu, Z., Ding, L., Han, W.* "Understanding Polaron Dynamics in CeO_2 for Advanced Catalytic Material Design." *Physical Chemistry Chemical Physics* 27, 21673-21682 (2025).
3. **Jiang, X.**, Cheng, X., Zhang, Z.*, et al. "Computation-assisted performance optimization for photoelectrochemical photoelectrodes." *Applied Physics Letters* 120, 063901 (2022).
4. **Jiang, X.**, Zhang, Z., Mei, J., et al. "Carbon quantum dots based charge bridge between photoanode and electrocatalysts for efficiency water oxidation performance." *Electrochimica Acta* 273, 208-215 (2018).

Co-authored:

5. Liu, Z., **Jiang, X.**, Cheng, X., et al. "Catalytic Effect of Gray Gallium Nitride for Hydrogen Peroxide Generation: Insights into Mechanical Stimuli-Driven Semiconductor–Liquid Interface Alteration" *ACS Nano* 19.37, 33361–33371 (2025).
6. Shao, J., Liu, H., **Jiang, X.**, et al. "High Performance Ferroelectric-modulated Photoelectrodes by Using Grid Charge Collector." *Advanced Functional Materials* 34.32, 2316409 (2024).
7. Sun, M., Chen, W., **Jiang, X.**, et al. "Optoelectrical Regulation of CuBi2O4 Photocathode via Photonic Crystal Structure for Solar-Fuel Conversion." *ACS Applied Materials & Interfaces* 14.38, 43946-43954 (2022).

8. Liu, B., **Jiang, X.**, Jiang, X., et al. "Z-Scheme Photocarrier Transfer Realized in Tungsten Oxide-Based Photocatalysts by Combining with Bismuth Vanadate Quantum Dots" *Inorganic Chemistry* 60.5, 3057-3064 (2021).
9. Ma, Y., **Jiang, X.**, Sun, R., et al. "Z-scheme $Bi_2O_{2.33}$/Bi_2S_3 heterojunction nanostructures for photocatalytic overall water splitting." *Chemical Engineering Journal* 382, 123020 (2020).
10. Cheng, X., **Jiang, X.**, Tao, K., et al. "Microscopic Nature of Gas Adsorption on WO_3 Surfaces: Electron Interaction and Localization." *The Journal of Physical Chemistry Letters* 11.21, 9070-9078 (2020).
11. Zhang, Z., **Jiang, X.**, Mei, J., et al. "Improved photoelectrocatalytic hydrogen generation through $BiVO_4$ quantum-dots loaded on nano-structured SnO_2 and modified with carbon quantum-dots" *Chemical Engineering Journal* 331, 48-53 (2018).

References

Available upon request.