JIAXUAN GUO

Department of Physics, Fudan University
220 Handan Rd., Shanghai, China
Phone: (+86) 187-3604-1701
E-mail: jiaxuanguo20@gmail.com
Website: https://jgcompu.github.io/

EDUCATION

Fudan University Shanghai, China
Bachelor of Science in Physics Aug. 2020-July 2024(Expected)

- Overall GPA: **3.75/4.00** Ranking: **8/131**
- Selected into *Mentor Program for Top Undergraduate* (**top 10** admitted every year)
- Relevant courses: Thermodynamics and Statistical Physics, Quantum Mechanics, Quantum Field Theory, Solid State Physics, Solid State Theory, Electrodynamics, C Programming, Methods of Mathematical Physics.

RESEARCH INTEREST

- *Ab Initio* Methods for Electronic and Optical Properties of Real Materials (DFT, GW+BSE)
- Twisted 2D Bilayer Materials
- Artificial Intelligence for Science (Physics, Materials Science)

RESEARCH EXPERIENCE

Yale University New Haven, CT
Project: **First-Principles Study of Time-Resolved ARPES on t-MoSe2/WS2 Bilayer** May 2023-Present
Supervisor: **Prof. Diana Qiu**

Part I: Density Functional Theory (DFT) Level Study

- Employed the Quantum ESPRESSO package to analyze electronic orbital-projected band structures, wavefunctions, and density of states (DOS) of the twisted MoSe2/WS2 heterostructure.
- Developed a theoretical model to predict the oscillation period resulting from the interference between electrons in the top and bottom layers.
- Computed the K point matrix elements in ARPES via the free electron approximation, thereby simulating the photoemission (PE) intensity and validating the theoretical model.

Part II: Exciton Level Study

- Utilized the BerkeleyGW package to perform a one-shot G0W0 calculation and applied the Bethe-Salpeter equation (BSE) approach to characterize excitonic properties, including exciton binding energy and exciton wavefunction.
- Developed scripts to visualize the distribution of excitons within momentum space and computed the band-to-band transition matrix term (no free electron approximation) at each k-point.
- Simulated the PE intensity from the exciton level and put forward an explanation for the oscillations observed in the experiment.
- Discovered discrepancies between experimental results and literature regarding the band alignment, challenging the computational accuracy of prior research on MoSe2/WS2 heterostructure.

Fudan University Shanghai, China

Project: **Deep Learning Approach to Novel Topological Materials** Dec. 2022-Apr. 2023

Supervisor: **Prof. Jing Wang**

- Learned some machine learning (ML) methods, including Convolutional Neural Networks (CNN), Support Vector Machine (SVM), HDBSCAN, and t-SNE.
- Applied CNN algorithms to streamline the exploration of materials exhibiting notably clean Fermi surfaces, achieving an accuracy rate exceeding 90%.
- Identified 210 prospective material candidates from a pool of 1781 entries, significantly accelerating the process of seeking novel topological materials.

Project: **Crystal Graph Convolutional Neural Networks for Prediction of Superconductors**

Supervisor: **Prof. Jing Wang** Sept. 2023-Present

- Constructed a training dataset comprising 1120 CIF structure files of superconducting materials along with their corresponding transition temperatures T_c, and this dataset is continuously expanding.
- Based on Atomistic Line Graph Neural Networks (ALIGNN), currently enhancing the input node features and model framework to improve prediction accuracy.

COURSE PROJECT

➢ **Fundamentals of Computational Physics** Sept. 2022-Nov. 2022

Supervisor: **Hongjun Xiang**

- Developed algorithms to solve ordinary differential equations (ODEs) through the implementation of the shooting method and partial differential equations (PDEs) using the Crank-Nicolson scheme.
- Utilized Monte Carlo (MC) simulations as a computational tool to estimate the Curie temperature for ferromagnetic systems within the framework of the Heisenberg spin model.

HONORS & PRIZES

FUMEI Research Scholarship (**top 3/131** students in Department of Physics, **$7000**)	2023
Outstanding Undergraduate Scholarship of Fudan University (**top 8%**)	2021, 2022
Professional Scholarship (Department of Physics)	2022, 2023

SKILLS

Programming Languages: Python (NumPy, Pymatgen, h5py, etc.), C, Linux (Shell), LaTex, Wolfram Language.

Software: Quantum ESPRESSO, BerkeleyGW, Mathematica, MATLAB, TensorFlow, Origin, Mathcha, Overleaf.

Language Skills: TOEFL iBT 105 (Reading 26/30 + Listening 29/30 + Speaking 24/30 + Writing 26/30)