JIAXUAN GUO

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EDUCATION

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

- Overall GPA: **3.75/4.00** Ranking: **8/131**
- FUMEI Research Scholarship (**top 3/131** students in Department of Physics, **$7000**)
- 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, Material 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: **Diana Qiu**

Part I: Density Functional Theory (DFT) Level Study

- Utilized Quantum ESPRESSO to perform Density Functional Theory (DFT) calculations, investigating electronic band structures and k-resolved orbital projected Density of States (DOS) for the MoSe2/WS2 heterostructure with a twist angle of 60 degrees.
- Formulated and implemented post-processing scripts to calculate matrix elements in ARPES via the free electron final state approximation, thereby describing the intensity distribution in ARPES experiments.
- Discovered the interference of wavefunction originating from the upper and lower layers of the heterostructure, thus establishing a theoretical explanation for the oscillation of photoemission (PE) intensity as a function of photon energy.

Part II: Exciton Level Study

- Utilized BerkeleyGW package to conduct one-shot G0W0 calculation based on DFT ground state for MoSe2/WS2 heterostructure. Employed Bethe-Salpeter equation (BSE) approach to characterize excitonic properties (e.g. exciton binding energy and exciton wavefunction).
- Developed custom scripts to visualize the distribution of excitons within momentum space and calculate the band-to-band transition matrix term, revealing the combined influence of these factors on both the quantity and positioning of intensity peaks observed in experimental results.
- Conducted simulations of PE intensity in tr-ARPES experiments from the exciton level and put forward an explanation for the varying PE intensities observed in t-MoSe2/WS2 at different temperatures.

Fudan University Shanghai, China

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

Supervisor: **Jing Wang**

- Learned some machine learning (ML) methods, including Convolutional Neural Network (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 approximately 150 prospective material candidates from a pool of 2,000 entries within the 2Dmatpedia database, significantly accelerating the process of seeking novel topological materials.

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

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

- Constructed a training dataset comprising 1120 CIF structure files of superconducting materials along with their corresponding transition temperatures Tc , and this dataset is continuously expanding.
- Based on Atomistic Line Graph Neural Network (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

Outstanding Undergraduate Scholarship of Fudan University (**top 8%**) 2021, 2022

Professional Scholarship (Department of Physics) 2022

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)