

# 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-MoSe<sub>2</sub>/WS<sub>2</sub> 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 MoSe<sub>2</sub>/WS<sub>2</sub> 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 G<sub>0</sub>W<sub>0</sub> calculation based on DFT ground state for MoSe<sub>2</sub>/WS<sub>2</sub> 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-MoSe<sub>2</sub>/WS<sub>2</sub> 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.

## **COURSE PROJECT**

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➤ **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**

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

2021, 2022

Professional Scholarship (Department of Physics)

2022

## **SKILLS**

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**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)