

Zekun Lou (娄泽坤)

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Education

B.S. in Physics, Fudan University, China 09/2019 - 07/2021 (Expected)

- Cumulative GPA: 3.80/4.0, Major GPA: 3.96/4.0, Department rank: 6/103.
- Selected into Honored student program (top 10% admitted) each year.
- Relevant courses: Computational Physics, Solid State Physics, (Advanced) Quantum Mechanics, C++ / Python Programming.

Research Interests

AI for Materials Science (reversible materials design), AI for Computational Physics (neural network XC functional), Many-body Interaction (excitons and coupling)

Research Projects

Neural network potentials

Shanghai AI Laboratory

Advisor: [Dr. Han-Sen Zhong](#)

09/2022 - Present

- Develop neural network-based exchange-correlation functionals (V_{XC}^{NN}) for KS-DFT.
- Set up datasets consists of volumetric V_{XC} with ρ labels of different chemical accuracies by PySCF, and reconstruct virtual fractional charge/spin samples by Wu-Yang method.
- Build Unet-inspired V_{XC}^{NN} , which is able to capture local density features and long-range interactions. Further improvements are tested, including (steerable/interpolation) CNN and equivariant GCN.
- Deploy V_{XC}^{NN} in SCF procedure.

Reversible bialloy descriptor

Fudan University

Advisor: [Prof. Hongjun Xiang](#)

02/2022 - Present

- Search for "good" descriptors of bialloy structures.
- Perform several reconstruction tests on Fourier transformation coefficients and cluster expansion messages.
- Encode bialloy structures by GNN and build generative models by VAE. The NN is trained by joint learning, and is used for properties optimizing.

Pirani gauge teaching experiment

Fudan University

Advisor: [Prof. Yongkang Le](#)

06/2021 - 08/2022

- Develop a Pirani gauge teaching experiment.
- Everything starts from zero, including circuit designing, SCM programming and PID tuning. Learned lots of techniques and lab skills.
- User instructions and lab handouts are available. The experiment will be open for undergraduate students soon.

Vacuum chamber and puck design

Fudan University

Advisor: [Prof. Yuanbo Zhang](#)

09/2021 - 03/2022

- Design sample pucks and functional vacuum chambers for an ultra-low temperature & strong magnetic field dilution refrigerator.
- Design a tricky and robust mechanism for installing/removing the puck from the cold dock plate.

Course Projects

Invisible cloak

09/2021 - 12/2021

- Course project in *Electrodynamics I*. Advised by [Prof. Lei Zhou](#).
- Design electromagnetic field controlling meta-materials based on transformation optics and conformal mapping respectively. Analysis flux scatter caused by impedance mismatch, and correct it using anisotropic phase-shifting meta-surface.
- Verify the above theoretical results by COMSOL FEA simulation.

Heisenberg model in nano particles

03/2021 - 06/2021

- Course project in *Statistical Physics I*, best two in all 13 projects.
- Research the behaviors of anisotropic Heisenberg model in nanomagnetic particles.
- Implement Monte Carlo Metropolis algorithm in C++.

Drifting Speckles in laser spots

09/2019 - 08/2020

- Course project in *Basic Physics Modeling*, best two in all 17 projects.
- Research the properties of the laser speckle phenomenon, mainly about Fourier optics.
- Experiments, theoretical analysis, and computational simulations (in C language) are conducted.

Skills

Second language: English. IELTS 7.0

Programming Languages: Python (PyTorch, PySCF, NumPy, Pandas, etc.), Wolfram Language ([my lecture video](#)), C/C++, L^AT_EX, PowerShell, bash, microPython/C for SCMs.

Software: VS Code, Mathematica, COMSOL, LAMMPS, VESTA, SOLIDWORKS, Multisim, Arduino, Keil5, Origin, Mathcha Notebook, MikTeX, Overleaf, MS Office.

Honors & Prizes

National undergraduate scholarship (top scholarship, top 2% in Fudan)	2020, 2022
First class scholarship of Fudan University (top 5% in Fudan)	2021
Freshmen scholarship of Fudan University (for outstanding in CPhO 2018)	2019
First prize in China Undergraduate Mathematical Contest in Modeling (Shanghai)	2022
First prize in National Physics Competition for College Students	2019, 2021
First prize in National Physics Experiment Competition for College Students (rank first)	2021
Second prize in China Undergraduate Physics Tournament (CUPT)	2020
Second prize in China Physics Olympiad (CPhO 2018, in high school)	2018
National top student project in basic science (top 10% in physics)	2020, 2021, 2022
Honored student in physics department (top 10% in physics)	2020, 2021, 2022