

# Zekun Lou (娄泽坤)

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## Education

B.S. in Physics, Fudan University, China

09/2019 - 07/2021 (Expected)

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

Pre-college Education, in Henan, China

Born - 07/2019

## Publications

Not yet. Wait and see.

## Research Projects

### Neural network potentials

Shanghai AI Laboratory

Advisor: [Dr. Hansen Zhong](#)

09/2022 - Present

- Develop neural network-based exchange-correlation functionals for KS-DFT.
- Set up datasets containing  $V_{XC}$  with  $\rho$  labels of different chemical accuracy by PySCF, and reconstruct virtual fractional charge/spin samples by Wu-Yang method.
- Pretrain neural networks and refine weights based on specified prediction tasks.
- Deploy  $V_{XC}^{NN}$  in SCF procedure for molecular dynamics simulations.

### Reversible bialloy descriptor

Fudan University

Advisor: [Prof. Hongjun Xiang](#)

02/2022 - Present

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

### 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.

## Course Projects

### Invisible cloak

09/2021 - 12/2021

- Course project in *Electrodynamics I*.
- Design electromagnetic field controlling meta-materials based on transformation optics and conformal mapping.
- Correct scatter in conformal mapping approach by well-designed anisotropic 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++. Use Python to automate simulations and data mining.

### 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 are conducted.

## Skills

**Second language:** English. IELTS 7.0, CET6 617 (top 4% in undergraduates)

**Programming Languages:** Python (PyTorch, PySCF, NumPy, etc.), Wolfram Language ([my lecture video](#)), C/C++, L<sup>A</sup>T<sub>E</sub>X, 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
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
First prize in National Undergraduate Physics Experiment Competition (rank first)	2021
Second prize in China Undergraduate Physics Tournament (CUPT)	2020
Second prize in China Physics Olympiad (CPhO)	2018

## Interests

**Academic:** Solid state physics, computational chemistry, quantum computing, machine learning (especially deep learning and AI4science).

**Sports:** Badminton, swimming.

**Musical:** Accordion.