

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 (Department rank: 6/104), Major GPA: 3.96/4.0.
- Selected into Honored Student Program (top 10% admitted) each year.
- Relevant courses: Computational Physics, Solid State Physics, (Advanced) Quantum Mechanics, (Advanced) Electrodynamics, C++/Python Programming, Machine Learning (via Coursera).

Research Interests

AI for Science (Materials Science, Computational Physics, Chemistry), Many-body Interaction (excitons and coupling)

Research Projects

Neural network XC potentials

Shanghai AI Laboratory

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

09/2022 - Present

- Develop neural network-based exchange-correlation functionals (V_{XC}^{NN}) for Kohn-Sham density functional theory.
- Set up datasets consists of V_{XC} with ρ labels of different chemical accuracies by PySCF. Reconstruct virtual fractional charge/spin samples by Wu-Yang method.
- Build Unet-inspired V_{XC}^{NN} on rasterized grids and quadrature grids. Build graph-based V_{XC}^{NN} with atom-centered electron descriptors. Deploy above V_{XC}^{NN} s in PySCF self-consistent field calculation.

Reversible bialloy descriptor

Fudan University

Advisor: [Prof. Hongjun Xiang](#)

02/2022 - Present

- Search for "good" descriptors of bialloy structures. Perform reconstruction tests on Fourier transformation coefficients and cluster expansion messages.
- Encode bialloy structures by Graph Neural Networks and build generative models by Variational Autoencoder for property optimization.

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, microcontroller programming, and PID tuning. Learned lots of techniques and lab skills. User instructions and lab handouts are available for undergraduate students.

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

Electrodynamics I. Advised by [Prof. Lei Zhou](#).

- Design electromagnetic field controlling meta-structures based on transformation optics and conformal mapping. Analyse energy scattering caused by impedance mismatch, and correct it using gradient-index meta-surfaces.
- Verify the above theoretical results by COMSOL FEA simulation.

Heisenberg model in nano particles

03/2021 - 06/2021

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

Basic Physics Modeling, best two in all 17 projects.

- Research the properties of the laser speckle phenomenon, mainly about Fourier optics.
- Conducted experiments, theoretical analysis, and computational simulations (in C and OpenMP).

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, C/microPython 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 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