

Penghua Lan

👤 Chinese, Male, 30/05/1995

🏛️ Beihang University

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🌐 www.researchgate.net/profile/Penghua-Lan

🌐 [luanshibei.github.io](https://github.com/luanshibei)

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EDUCATION

Beihang University

Master of Engineering

09/2020 - 12/2022

Majoring in Material Science and Engineering

- WAM: 87.6 GPA:3.68/4 RANK:51/149

Xidian University

Bachelor of Engineering

09/2014 - 09/2018

Majoring in Material and Chemical Engineering

- WAM: 80.99 GPA:3.5/4 RANK: 14/62

PUBLICATIONS

- **Penghua Lan**, et al. High-Throughput Computational Design of 2D Ternary Chalcogenides for Sustainable Energy. **Journal of Physical Chemistry Letters**. (under review-minor revision)
- Yu Gan, Naihua Miao, **Penghua Lan**, et al. Robust Design of High-Performance Optoelectronic Chalcogenide Crystals from High-Throughput Computation. **Journal of the American Chemical Society**, 2022, 144(13): 5878-5886.
- Ao Zhang, Zhongqing Jiang, Shaoda Zhang, **Penghua Lan**, Naihua Miao, et al. Coral-Shaped Mn-CuS with Hierarchical Pores and Crystalline Defects for High-Efficiency H₂O₂ Production via Electrocatalytic Two-Electron Reduction. **Applied Catalysis B: Environmental**, 2023, 331: 122721. ((first author in charge of simulation part))
- **Chinese Computer Software Copyright**: Software System for Integrated Computation, Analysis and Design of Cross-Scale Materials and Devices
- **Online Database Website**: 2D Materials Online Database ABX₃

RESEARCH EXPERIENCE

Research on Thermoelectric Properties of Chalcogenides

Graduation Project (Thesis)

2020 - 2023

Supervisor: Prof. Naihua Miao

- Calculated **phonon spectrum**, **exfoliation energy**, and **electrical structure** by using **DFT** theory
- Calculated **Seebeck coefficient**, and **power factor** with BoltzTrap

Programming & Research on Optoelectronic Properties

Software & Research Assist

08/2021 - 01/2022

Partener: Dr. Yu Gan

- Developed a programmer based on the **transform-matrix method** to model the **solar cell device** using data of **first principle calculation** or experiment
- Modeled the generation, diffusion and dissociation of the **photogenerated exciton** in the solar cell
- Realized the **concurrent computation**, **interface visualization**, and **database storage**
- Assisted in drawing and organising data about the optoelectronic properties of chalcogenides ABX₃ for about 3 months

Cooperating with the Experiment group in Electro-Catalytic Research

OER Reaction

09/2021 - 11/2021

Partener: Miss Zhang, Prof. Zhongyu Cai

- Studied the **Mn-CuS catalyst** that oxidizes H₂O to generate H₂O₂
- Calculated **charge density difference**, **adsorption energy**, **charge state**, **ELF**, **-pCOHP**
- Explained experimental phenomena
- Drew the reaction cycle diagram

ANSYS Finite Element Analysis

Computational Material Experiment

09/2021

Teacher: Prof. Jiaxiang Shang

- The temperature distribution of submarine
- The stress and strain distribution of sheet, dam and cooling process of thermal barrier coating
- Analysis of thermoelectric refrigeration

Mathematical Basis in Materials Research

Term Project using **MATLAB**

09/2021 - 12/2021

Teacher: Prof. Yue Zhang, Prof. Chen Si

- Numerical Analysis: Fitting the internal relationship between material properties and factors with bimodal Gaussian function while considering experimental errors
- Solution of **Partial Differential Equation**: Calculating the diffusion coefficients of oxygen vacancy (oxygen ion) in zirconia
- Statistics: Studied the influence that mean and variance of crack length distribution cause to Weibull modulus and mean strength distribution
- **Monte Carlo Simulation**: Simulating the motion state of particles under the action of external one-dimensional potential field
- Optimization: searching for maximum using cubic spline interpolation

Liner Regression Model & Clustering and Discriminant Analysis

Mathematical Statistics Term Project

09/2020 - 12/2020

Teacher: Prof. Haiyan Sun

- Researched for the factors that determinates superconductor critical temperature T_c by using stepwise regression method and **SPSS**
- Clustered the different provinces of china by using k-mean clustering and systematic clustering method and **SPSS**
- Verified the prediction result of clustering model by using cross validation and jackknife

Solution Synthesis of CuInS_2 quantum dots

Graduation Project (Thesis)

12/2017 - 05/2018

Supervisor: Prof. Qiaoying Jia

- Synthesized CuInS_2 by solvothermal method
- Dedispersed the CuInS_2 solution on ITO on the spin coater to synthesize the thin film
- Characterized the cryastallinity and crystal phase with **XRD**, the particle size with **SEM**, optic absorbance and gap with **UV-Vis**

College Students' Innovation and Entrepreneurship Competition

Prepared and characterized thick film photoresistors based on CdS

01/2017 - 05/2018

Supervisor: Dr. Peng Sun

- Preparation of thick film resistors by using screen printing
- Resistance measure by using a luminous flux tester, multimeter and solar simulator

AWARDS

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| • 01/2023: Outstanding Graduates of Beihang University | • 09/2020: The Second Prize Scholarship |
| • 11/2022: National Scholarship for Postgraduates
(RANK:6/587 \approx 1%) | • 09/2016: The Second Prize Scholarship |
| • 09/2022: The Second Prize Scholarship | • 06/2016: The Second Prize of School Level Mathematical
Contest in Modeling |
| • 09/2021: The Second Prize Scholarship | • 09/2015: The Third Prize Scholarship |

TECHNICAL SKILLS

Programming Languages: Python, C, Shell
Frameworks: PyQt5
Applications: Vasp, BoltzTrap, Phonopy, ShengBTE, Lobster

REFEREES

Naihua Miao: Professor, Beihang University & Master Thesis Supervisor	nhmiao@buaa.edu.cn /nhmiao@gmail.com
Linggang Zhu: Associate Professor, Beihang University & Teacher in Our Group	lgzhu7@buaa.edu.cn