

CV

Personal Information

Name: Yilei Wu

Nationality: Chinese

Date/place of birth: 23/11/1996, China

ORCID: 0009-0005-7216-0569

ResearchGate: https://www.researchgate.net/profile/Yilei-Wu-6?ev=hdr_xprf

Google Scholar: <https://scholar.google.com/citations?user=Nfd2T-0AAAAJ&hl=en&oi=ao>

Research Field

I focus on computer simulations (e.g., DFT, AIMD) and machine learning (ML) techniques to understand, design, and assist the synthesis of perovskite materials. I specialize in first-principles calculations, ML project development, quantum chemistry, and solid-state physics.

I have been involved in the following research topics:

- Rational design of perovskites with superior optoelectronic and photovoltaic performance
- ML-guided synthesis for two-dimensional perovskites

Professional Experience

18/02/2025 – to present

Postdoctoral researcher Host: Prof. Bartomeu Monserrat
Department of Materials Science & Metallurgy, University of
Cambridge, Cambridge, United Kingdom
Project: rapid discovery of passivation molecules for perovskite
solar cells by using machine learning

I utilize machine learning techniques and first-principles calculations to efficiently screen passivation molecules for perovskite solar cells. I am responsible for the execution of the entire research, the analysis of results and the writing of paper.

01/02/2024 – 01/02/2025

Postdoctoral researcher Host: Prof. Jinlan Wang
School of physics, Southeast University, Nanjing, P. R. China
Project: data-driven insights into 2D perovskites passivation for
enhancing the performance of 3D perovskite solar cells

I developed a framework that integrates physicochemical insights, ML techniques, and causal inference, to develop an in-depth understanding of stability and photovoltaic performance of 2D/3D perovskites. I am responsible for the execution of the entire research, the analysis of results and the writing of paper.

Education

01/09/2018 – 20/12/2023

Ph.D. in Physics Supervisor: Prof. Jinlan Wang
School of physics, Southeast University, Nanjing, P. R. China
Thesis title: data-driven research in perovskite optoelectronic material design and discovery
I systematically study the synthesis and optoelectronic properties of halide perovskites by utilizing first-principles calculations and ML techniques.
Date of Ph.D. award: 20/12/2023

01/09/2014 – 01/07/2018

B. Sc. in Physics
School of physics, Southeast University, Nanjing, P. R. China

Funding and Grants

- **Post-doctoral Fellowship for Overseas Research Visit**, Southeast University.
Project: Machine Learning-Guided Discovery and Design of Halide Perovskites
Period: February 2025 – February 2028
Role: Postdoctoral Fellow
Total Funding: RMB 930,000

Honors, Awards, and Scholarships

- Marie Skłodowska-Curie Actions (MSCA) Seal of Excellence, European Commission, 2026.
- Outstanding Ph.D. Dissertation Award, Southeast University, China, 2025.
- Good Youth of Southeast University, Southeast University, China, 2023. (1/10 university-wide each year)
- Female Scholar of the Wu Chien-shiung Memorial Fund, Southeast University, China, 2022. (1/10 university-wide each year)
- Merit Student, Southeast University, China, 2022.
- Best Presentation Prize, The 2nd online conference on computational nanoscience and new energy materials, China, 2022.
- Outstanding Student Scholarship, Southeast University, China, 2023, 2022, 2021, 2020.

Publications

* = corresponding author, † = co-first author

- [1] **Yilei Wu,†** Chang-Feng Wang,† Ming-Gang, Ju,†* Qiangqiang Jia, Qionghua Zhou, Shuaihua Lu, Xinying Gao, Yi Zhang,* and Jinlan Wang,* Universal machine learning aided synthesis approach in typical laboratory: a case study of two-dimensional perovskites, *Nat. Commun.* 2024, 15, 138.

The contribution of Wu to this publication is to 1) conceive the project, 2) develop the total framework that integrates ML techniques, DFT calculations, and experiments, 3) train ML

models and proceed further analysis, 4) perform all the calculations, and 5) organize the original manuscript and write the final manuscript.

- [2] **Yilei Wu**[†], Xiaoyan Li[†], Rong Guo, Ruiqi Xu, Ming-Gang Ju*, Jinlan Wang*, How to accelerate the inorganic materials synthesis: from computational guidelines to data-driven method?, *Nat. Sci. Rev.* 2025, 12, 4, nwaf081.

The contribution of Wu to the publication is to 1) conceive the review and 2) organize the original manuscript and write the final manuscript.

- [3] **Yilei Wu**, Shuaihua Lu, Qionghua Zhou, Ming-Gang Ju,* Xiao Cheng Zeng,* and Jinlan Wang,* Two-dimensional perovskites with tunable room-temperature phosphorescence, *Adv. Funct. Mater.* 2022, 2204579.

The contribution of Wu to this publication is to 1) conceive the project, 2) perform all calculations, 3) proceed data analysis and 4) organize the original manuscript and write the final manuscript.

- [4] **Yilei Wu**, Shuaihua Lu, Ming-Gang Ju,* Qionghua Zhou,* and Jinlan Wang,* Accelerated design of promising mixed lead-free double halide organic-inorganic perovskites for photovoltaics using machine learning, *Nanoscale* 2021, 13, 12250.

The contribution of Wu to this publication is to 1) conceive the project, 2) train ML models and proceed further analysis, 3) perform all DFT calculations, and 4) organize the original manuscript and write the final manuscript.

- [5] Ruikang Dong,[†] **Yilei Wu**,[†] Chunjin Ren, Xiaoshu Gong, Qionghua Zhou,* Jinlan Wang,* and Liang Ma.* A descriptor-driven thermodynamic framework for achieving unidirectional nucleation in 2D material epitaxy. *ACS Nano*, 2025, 19, 37972-37982. (co-first author)

The contribution of Wu to this publication is to 1) write code to calculate the energy difference, 2) co-develop the descriptor for 2D material epitaxy, and (3) prepare and revise the manuscript.

- [6] Jiawei Luo,[†] Qun Ji,[†] **Yilei Wu**,[†] Xinying Gao, Jinlan Wang,* and Ming-Gang Ju,* Eco-friendly inorganic molecular novel antiperovskites for light-emitting application, *Mater. Horiz.* 2023, 10, 1678-1688. (co-first author)

The contribution of Wu to this publication is to 1) co-supervise the project with Prof. Ju, and 2) prepare and revise the manuscript.

- [7] Chang-Feng Wang,[†] Chao Shi,[†] Anyi Zheng,[†] **Yilei Wu**,[†] Le Ye, Na Wang, Heng-Yun Ye, Ming-Gang Ju,* Pengfei Duan,* Jinlan Wang,* and Yi Zhang*, Achieving circularly polarized luminescence and large piezoelectric response in hybrid rare-earth double perovskite by a chirality induction strategy, *Mater. Horiz.* 2022, 9, 2450-2459. (co-first author)

The contribution of Wu to this publication is 1) perform DFT calculation, and 2) investigate the origin of chiroptical properties of hybrid rare-earth double perovskites.

- [8] Xinying Gao,[†] Jiawei Luo,[†] **Yilei Wu**,[†] Aini Lu, Ming-Gang Ju,* and Jinlan Wang*, Toward eco-friendly lead-free low-dimensional perovskites, *Small Struct.* 2022, 2100219. (co-first author)

The contribution of Wu to this publication is 1) perform a portion of DFT calculations, and 2) prepare and revise the manuscript.

- [9] Shuaihua Lu,† **Yilei Wu**,† Minggang Ju,* and Jinlan Wang*, Machine learning accelerated insights of perovskite materials, Artificial Intelligence for Materials Science, Springer Series in Materials Science, vol 312. Springer, Cham. (co-first author)
The contribution of Wu to this publication is jointly prepare and revise the manuscript.
- [10] Aini Lu,† **Yilei Wu**,† Qun Ji, Jinlan Wang,* and Ming-Gang Ju,* Toward tunable low-dimensional metal halide perovskites with functional pseudohalides. **Sci. China Mater.** 2024, 67, 2335–2344. (co-first author)
The contribution of Wu to this publication is to 1) co-supervise the project with Prof. Ju, and 2) prepare and revise the manuscript.
- [11] Qun Ji, **Yilei Wu**, Xinying Gao, Tingbo Zhang, Yipeng Zhou, Yehui Zhang, Ming-Gang Ju,* Jinlan Wang,* and Xiao Cheng Zeng,* Influence of organic-cation defects on optoelectronic properties of ASnI₃ perovskites A=HC(NH₂)₂, CH₃NH₃, **Angew. Chem. Int. Ed.** 2023, e202213386.
The contribution of Wu to this publication is to discuss the optoelectronic properties of perovskites.
- [12] Yu Cui, **Yilei Wu**, Chunjin Ren, Qiang Li, Chongyi Ling,* and Jinlan Wang.* Beyond local coordination: how global structure engineers the selectivity of single atom catalysts for CO₂ reduction. **Angew. Chem. Int. Ed.** 2025, e19826.
The contribution of Wu to this publication is discuss the development of the descriptor for single atom catalysts.
- [13] Xinying Gao, **Yilei Wu**, Yehui Zhang, Xinyu Chen, Zhilong Song, Tingbo Zhang, Qianglong Fang, Qun Ji, Ming-Gang Ju*, Jinlan Wang*, How the spacer influence the stability of 2D perovskites? **Small Methods** 2024, 2401172.
The contribution of Wu to this publication is to develop the material descriptors related to organic spacers in 2D perovskites.
- [14] Guangcheng Niu, **Yilei Wu**, Xinyu Chen, Yehui Zhang, Shijun Yuan*, and Jinlan Wang*. Efficient and accurate prediction of double perovskite quasiparticle band gaps via machine learning and a descriptor. **J. Phys. Chem. Lett.** 2025, 16, 4006-4013.
The contribution of Wu to this publication is to 1) construct material descriptions for perovskites, and 2) discuss the development of ML models.
- [15] Chunjin Ren, Shuaihua Lu, **Yilei Wu**, Yixin Ouyang, Yehui Zhang, Qiang Li, Chongyi Ling,* and Jinlan Wang,* A universal descriptor for complicated interfacial effects on electrochemical reduction reactions, **J. Am. Chem. Soc.** 2022, 144, 12874-12883.
The contribution of Wu to this publication is to perform feature engineering for electrochemical reduction reactions.
- [16] Qianglong Fang, Yilv Guo, **Yilei Wu**, Xinying Gao, Ming-Gang Ju,* and Jinlan Wang,* Origins of structural and electronic chirality in the 2D hybrid perovskites, **Adv. Funct. Mater.** 2025, e10580.
The contribution of Wu to this publication is to construct material descriptors related to chiroptical properties of 2D perovskites.
- [17] Qionghua Zhou,† Shuaihua Lu,† **Yilei Wu**, and Jinlan Wang,* Property-oriented material design based on data-driven machine learning technique, **J. Phys. Chem. Lett.** 2020, 11, 3920-3927.

The contribution of Wu to this publication is to discuss the application of ML techniques in material science.

- [18] Cai Ning, Qun Ji, **Yilei Wu**, Jinlan Wang,* and Ming-Gang Ju,* Disorder on mixed cation halide perovskite for photovoltaic applications, **J. Phys. Chem. Lett.** 2023, 14, 8034–8042.
The contribution of Wu to this publication is to discuss the optoelectronic properties of mixed cation halide perovskites.
- [19] Qianglong Fang, Mingao Hu, Xinying Gao, **Yilei Wu**, Qun Ji, Ming-Gang Ju,* and Jinlan Wang,* Orbital-level engineering of bonding networks to modulate halogen migration in lead-free double perovskites, **Mater. Horiz.** 2026, Advanced Article.
The contribution of Wu to this publication is to discuss fundamental properties of lead-free double perovskites.
- [20] Shuaihua Lu,† Qionghua Zhou,† Yilv Guo, Yehui Zhang, **Yilei Wu**, and Jinlan Wang,* Coupling a crystal graph multilayer descriptor to active learning for rapid discovery of 2D ferromagnetic semiconductors/half-metals/metals, **Adv. Mater.** 2020, 32, 2002658.
The contribution of Wu to this publication is to discuss the development of ML models.
- [21] Xinying Gao, Yehui Zhang, Tingbo Zhang, **Yilei Wu**, Qun Ji, Ming-Gang Ju*, and Jinlan Wang,* Coupled dynamic characteristics of mobile ions in halide perovskites. **J. Phys. Chem. Lett.** 2024, 15, 21, 5779–5787
The contribution of Wu to this publication is to discuss the electronic properties of perovskites.
- [22] Xinyu Chen, Zhilong Song, Shuaihua Lu, **Yilei Wu**, Ming-Gang Ju, Qionghua Zhou*, and Jinlan Wang*. AI-driven materials design: paradigm shift from small data to big data. **Sci. Sin. Chim.** 2025, 55, 6, 1648-1659.
The contribution of Wu to this publication is to discuss and revise the manuscript.
- [23] Qun Ji, Qianglong Fang, Xiaoli Wei, Yehui Zhang, **Yilei Wu**, Xinying Gao, Xiaoyan Li, Cai Ning, and Ming-Gang Ju*. Origin and suppression of nonradiative recombination in inorganic halide perovskites. **Nano Lett.** 2025, 25, 5875-5880.
The contribution of Wu to this publication is to discuss the electronic properties of perovskites.
- [24] Xinyang Wan, Yehui Zhang, Shuaihua Lu, **Yilei Wu**, Qionghua Zhou,* and Jinlan Wang,* Machine learning accelerated search for new double perovskite oxide photocatalysis, **Acta Phys. Sin.** 2022, 71, 17, 177101.
The contribution of Wu to this publication is to discuss the development of ML models.

Presentations

- 1) 12/01/2026
Title: Data-driven material discovery and synthesis of perovskite optoelectronic materials.
Molecular & Materials Modelling: Learning, Exchange & Collaboration, London, UK.
- 2) 12/05/2025 – 12/05/2025
Title: Data-driven material discovery and synthesis for perovskite optoelectronic materials
Lennard-Jones Centre Discussion Group, Cambridge, UK.
- 3) 21/08/2022 – 23/04/2021
Title: Accelerated design of promising mixed lead-free double halide organic-inorganic perovskites for photovoltaics using machine learning

ACS Fall 2022 meeting, Chicago, USA.

4) 21/07/2022 – 25/07/2022

Title: Two-dimensional perovskites with tunable room-temperature phosphorescence

2022 CNEM online meeting, Xi'an, China.

Organisation of conferences/workshops

06/09/2024 – 08/09/2024

Volunteer of Strategy workshop on multiscale materials simulation and calculation: bridging the gap between theory and experiments, Nanjing, China

Teaching experiences

1) 17/09/2018 – 20/01/2019

Teaching assistant for the course of Atomic Physics

2) 16/09/2019 – 14/01/2020

Teaching assistant for the course of Atomic Physics

3) 29/09/2020 – 31/01/2021

Teaching assistant for the course of Atomic Physics

4) 06/09/2021 – 09/01/2022

Teaching assistant for the course of Atomic Physics

Supervising and mentoring activities

1) 06/09/2021 – 03/07/2022

Co-supervision of postgraduate for the project - Eco-friendly inorganic molecular novel antiperovskites for light-emitting application.

2) 30/08/2022 – 25/06/2023

Co-supervision of postgraduate for the project - Toward tunable low-dimensional metal halide perovskites with functional pseudohalides.

Public outreach activities

1) 06/06/2023

Organize and lead a guided tour of the Chien-Shiung Wu Memorial Hall.

Aim: Honor Dr. Chien-shiung Wu and embody her spirit.

2) 01/10/2014 – 08/06/2017

Organize and participate in a series of talks covering culture, literature, traditional Chinese opera, and science (over 100 talks, with a total audience of over 50K). Host a portion of these talks, including Dr. Samuel C. C. Ting's talk (Nobel laureate in Physics) and Xiaoxia Li's talk (Olympic champion).

Aim: Improve the cultural literacy of students and elevate the cultural atmosphere of the university.