

# Yongxin Lyu

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[Google Scholar](#)

[ORCID](#)

[GitHub](#)

## Education

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**Ph.D., Materials Science and Engineering**

June 2021 – Present

University of New South Wales, Sydney

**M.Phil., Applied Physics**

Sep 2017 – May 2020

The Hong Kong Polytechnic University, Hong Kong SAR

**GPA: 4.0/4.0**

**B.Sc. (Hons), Engineering Physics**

Sep 2013 – May 2017

The Hong Kong Polytechnic University, Hong Kong SAR

**GPA: 3.73/4.0**

## Research Interests

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- 2D perovskite solar cells
- First principles simulation
- Making Academic Memes

## Research Experience

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**Ph.D. Researcher**

June 2021 - Present

Prof. Tom Wu's Group

School of Materials Science and Engineering, University of New South Wales

- Atomic scale simulation of 2D perovskites
- Machine learning, high throughput DFT

**M.Phil. Researcher**

Sep 2017 – June 2021

Prof. Jianhua Hao's Group

Department of Applied Physics, The Hong Kong Polytechnic University

- First principles simulation of the luminescence mechanism of lanthanide dopant in 2D transition metal dichalcogenides.
- Molecular dynamics simulations of the growth mechanism of black phosphorus in pulsed laser deposition under different laser influence.

## Publications

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1. [Yongxin Lyu](#), Zehan Wu, Weng Fu Io, and Jianhua Hao\*, "Observation and theoretical analysis of near-infrared luminescence from CVD grown lanthanide Er doped monolayer MoS<sub>2</sub> triangles", *Appl. Phys. Lett.*, 2019, 115, 153105.

2. Zehan Wu, Yongxin Lyu, Yi Zhang, Ran Ding, Beining Zheng, Zhibin Yang, Shu Ping Lau, Xianhui Chen\*, and Jianhua Hao\*, “Large-scale growth of few-layer two-dimensional black phosphorus”, *Nat. Mater.*, 2021, 20 (9), 1203-1209.
3. Ran Ding, Yongxin Lyu, Zehan Wu, Feng Guo, Weng Fu Io, Sin-Yi Pang, Yuqian Zhao, Jianfeng Mao, Man-Chung Wong, Jianhua Hao\*, “Effective piezo-phototronic enhancement of flexible photodetectors based on 2D hybrid perovskite ferroelectric single-crystalline thin-films”, *Adv. Mater.*, 2021, 33, 2101263.

## **Outreach Activities**

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### **Fantastic perovskites and where to find them**

Speaker at Pint of Science Australia

May 2023

## **Awards and Honors**

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### **UNSW Women in Maths and Science Champions Program 2023**

Faculty of Science, University of New South Wales

Feb 2023 – Jan 2024

- Selected as one of 20 PhD students from Faculty of science to participate in an exclusive program designed to promote and support women in STEM fields.
- Engaged in a series of workshops, seminars, and networking events to develop leadership skills and enhance professional development.
- Organized and contributed to outreach efforts to promote STEM education and encourage diversity in the field.

### **Third Place in 2022 APAC HPC-AI Competition**

HPC-AI Advisory Council, NSCC Singapore, NCI Australia

March – Nov 2022

### **Australian Government Research Training Program (RTP) Scholarship**

Faculty of Science, University of New South Wales

June 2021 – Dec 2024

### **Dean’s Honours List 2016**

Faculty of Applied Sciences and Textiles, The Hong Kong Polytechnic University

## **References**

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### **Prof. Tom Wu**

School of Materials Science and Engineering

University of New South Wales

(02) 9385 6559, [tom.wu@unsw.edu.au](mailto:tom.wu@unsw.edu.au)

### **Prof. Jianhua Hao**

Department of Applied Physics

The Hong Kong Polytechnic University

(852) 2766 4098, [jh.hao@polyu.edu.hk](mailto:jh.hao@polyu.edu.hk)

## **Skills**

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- Proficiency in simulation software such as VASP, Quantum Espresso, Gaussian, LAMMPS
- Proficiency in programming languages such as Python, Bash
- Familiar with simulation result analysis tools such as numpy, pandas, matplotlib, rdkit, pymatgen, scikit-learn
- Experience with high-performance computing (HPC) and command line environment

## **Mentoring experience**

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### **Graduate Mentor, Personalised English Language Enhancement Program**

Faculty of Arts, Design and Architecture, University of New South Wales. 2022 - 2023

- Assisted students in improving their English language skills by providing support during lectures and tutorials.
- Developed communication and interpersonal skills through collaborative peer mentoring with students from diverse cultural and linguistic backgrounds.
- Received positive feedback from students and faculty for providing valuable support and enhancing the learning experience.