

# JIE HUANG

## PERSONAL DATA

GENDER: Male  
 NATIONALITY: Chinese  
 ADDRESS: Kide 2501, Department of Applied Physics, Aalto University, Finland  
 EMAIL: [jie.huang@aalto.fi](mailto:jie.huang@aalto.fi)  
 WEBSITE: <https://way2ml.github.io>

## EDUCATION

05/2023–now | Doctoral Researcher in **Applied Physics**, **SIN group**  
 Aalto University, Helsinki, Finland, Advisor: **Prof. Adam S. Foster**

09/2018–06/2021 | M.S. in **Condensed Matter Physics**  
 Wenzhou University, Wenzhou, China, Advisor: **Prof. Shibei Li**  
 Thesis: “**Applications of machine learning in hydrogen-bond dynamics in bulk water and polymer chains’ structure factor**”  
**GPA: 3.84/4.0**

09/2012–06/2016 | B.S. in **Electronic Information Engineering**  
 China West Normal University, Nanchong, China  
 Thesis: “**A CCD translation device based on Raspberry Pi**”  
**GPA: 3.22/4.0**

## SCIENTIFIC PUBLICATIONS

1. **Jie Huang**, Niko Oinonen, Fabio Priante, Filippo Federici Canova, Lauri Kurki, Chen Xu, and Adam S. Foster\*, **Improving atomic force microscopy structure discovery via style-translation**, **npj Computational Materials**, 2025
2. Jonas Heggemann, **Jie Huang**, Simon Aeschlimann, Simon Spiller, Adam S. Foster\*, and Philipp Rahe\*, **Sidestepping Intermolecular Hydrogen Bonds: How Single Water Molecules Adsorb and Assemble on the Calcite (104)-(2x1) Surface**, **ACS Nano**, DOI: 10.1021/acsnano.5c05845, 2025
3. Gang Huang and **Jie Huang\***, **Revisiting the Thickness of the Air-Water Interface from Two Extremes of Interface Hydrogen Bond Dynamics**, **Journal of Chemical Theory and Computation**, DOI: 10.1021/acs.jctc.4c00457, 2024
4. **Jie Huang**, Bowen Wang, Hejin Yan, and Yongqing Cai\*, **Mechanism of interaction of water above the methylammonium lead iodide perovskite nanocluster: size effect and water-induced defective states**, **The Journal of Physical Chemistry Letters**, DOI: 10.1021/acs.jpclett.3c02807, 2024
5. **Jie Huang**, Gang Huang\*, and Shibei Li\*, **A machine learning model to classify dynamic processes in liquid water**, **ChemPhysChem**, DOI: 10.1002/cphc.202100599, 2022, **Cover Article**
6. **Jie Huang**, Shibei Li\*, Xinghua Zhang\*, and Gang Huang, **Neural network model for structure factor of polymer systems**, **The Journal of Chemical Physics**, DOI: 10.1063/5.0022464, 2020

## WORK EXPERIENCE

07/2022 - 04/2023 | Research Assistant, Institute of Applied Physics and Materials Engineering, **University of Macau**, Macau, China. Advisor: **Prof. Yongqing Cai**  
 1. Density Functional Theory Study of Perovskite Nanoclusters in Aqueous Environment

09/2016 - 04/2018 | **Software Engineer**, FalconPro Technology Co., Ltd, Shanghai, China  
 1. **Image processing & Barcode decoding**  
 2. **Embedded systems programming**

## AWARDS

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- 2024 | **Third Place** in AI and ML for Microscopy, Hackathon
- 2021 | **Outstanding Graduate** of Wenzhou University
- 2021 | Award for **Excellent Scientific and Technological Innovation**
- 2020 | **National Scholarship**, Ministry of Education of China
- 2015 | **National Undergraduate Electronic Design Contest (TI Cup) Second Prize**
- 2015 | **National Professional Software Engineering Design Contest (Bule Bridge Cup) Second Prize**

## CERTIFICATES

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- 2024 | Coursera certificate from **DeepLearning.AI: Generative Adversarial Networks (GANs)**
- 2018 | MOOC certificate from **Peking University: Artificial Intelligence Practice**
- 2016 | edX certificate from the **University of Texas at Austin: Embedded Systems**
- 2015 | **National Electronics Professionals: Senior Development Engineer of MCU Application**
- 2014 | **National Computer Rank Examination Level 3: Embedded System Development**

## SKILLS

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Machine Learning, Molecular dynamics (MD) simulations, Embedded Systems Programming, Linux, Git

## LANGUAGES

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Chinese (native), English (proficient), Japanese (basic), Python, C

## ACTIVITIES

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- 01/2025 - 06/2026 | **Teaching assistant** for PHYS-E0412 - Computational Physics D, Aalto University
- 2021/11 | Teaching "**Introduction to Deep Learning**" for postgraduates in Physics , Wenzhou University.
- 05/2018 - 11/2019 | **System manager** of the Linux cluster, Beihang University

## HOBBY PROJECTS

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- 2025 | **Sphinx-molview**: A Sphinx extension for interactive 3D molecular visualization
- 2025 | **UP2Git**: A Linux system tray app for uploading files to GitHub
- 2022 | **Guitar Simulations From Wave Equations: Music Demo**
- 2022 | **Huanbu**: A cross-platform and full functional metronome app based on Python
- 2020 | **Adversarial Inverse Reinforcement Learning Implementation** for Mountain Car
- 2019 | **Steady Hand Game Device** Based on **Raspberry Pi**
- 2016 | **Handheld Game Console** Based on **Texas Instruments TM4C123G**

Last updated: January 15, 2026