

Junke Jiang

School of Physics, Engineering and Technology, University of York

Heslington, York, YO10 5DD, United Kingdom

e-mail: junke.jiang@york.ac.uk

ORCID ID: 0000-0003-2962-766X

Web of Science ResearcherID: F-2187-2018

Education

- **PhD in Physics**, thesis defended on 14 October 2021
Eindhoven University of Technology, 2017–2021
Ph.D. supervisors: Dr. Shuxia Tao, Prof. Peter A. Bobbert
- **M. Sc. in Engineering**, major in Mechatronic Engineering, **First Class Honours**
Guilin University of Electronic Technology, 2014–2017
- **B. Sc. in Engineering**, major in Microelectronics Manufacturing Engineering
Guilin University of Electronic Technology, 2010–2014

Professional Experience

- **Research Associate, March 2026-**
Hybrid semiconductor grain boundary defect dynamics and development of machine learning interatomic potential
Academic advisors: Prof. Keith McKenna
- **Postdoc researcher, November 2022-August 2025**
Institut FOTON, INSA Rennes, Rennes, France
Guest researcher, November 2022-
Institut des Sciences Chimiques de Rennes, Université de Rennes, Rennes, France
Theoretical description of the optoelectronic and dielectric properties of layered perovskite, optimization of perovskite materials and devices based on theoretical studies, semi-empirical methods development, methodology development for large-scale simulation of perovskite.
Academic advisors: Prof. Jacky Even, Dr. Claudine Katan
- **Visiting researcher, April 2023-May 2023**
Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany
Developing the density functional-based tight binding (DFTB) methods for metal-halide perovskite simulation
Academic advisors: Dr. Bálint Aradi
- **Postdoc researcher, November 2021 –November 2022**
Institut des Sciences Chimiques de Rennes, Rennes, France
Theoretical description of the electronic properties of layered perovskite and optimization of perovskite materials and devices (PV, LED) based on theoretical studies.
Academic advisors: Dr. Claudine Katan, Prof. Jacky Even
- **Visiting researcher, October 2021 – November 2021**
Institut des Sciences Chimiques de Rennes, Rennes, France
Optimization of perovskite materials and devices based on theoretical studies
Academic advisors: Dr. Claudine Katan
- **Doctorate, September 2017 – August 2021**
Eindhoven University of Technology, Eindhoven, the Netherlands

Understanding the phase stability of lead halide and lead-free perovskites

Using DFT calculations to provide further insights into the phase transition of lead halide and lead-free perovskites and revealed the mechanism of improved phase stability of mixed perovskites.

The additive effect to the stability and photoluminescence of perovskite quantum dots

Combine density functional theory calculations and *ab initio* molecular dynamics simulations to investigate the surface termination engineering and ligand-surface interaction of the Sn-Pb perovskite quantum dots. Reveal the mechanism of sodium doping and additive iodine in stabilizing perovskite quantum dots.

Solvent-precursor coordination effect on the crystallization process and stability of metal-halide perovskite

Combine density functional theory calculations and *ab initio* molecular dynamics simulations to study several key parameters (e.g., binary solvent effect, solvent category, and reaction pathway) that control the crystallization process and morphology of metal halide perovskites.

Skills

- Theoretical: density functional theory (DFT), DFTB method, molecular dynamics, machine learning interatomic potential (MLIP), DFT-1/2 method, solid-state physics, semiconductor physics, engineering mechanics, mechanical and electrical integration
- Programming: Python, Bash
- Software: VASP, SIESTA, DFTB+, CP2K, PyTorch, GPUMD, AMS, Materials Studio, Hefei-NAMD, Gaussian, QuantumATK, GNUplot, Chemdaw, ChemOffice, VMD

Selected Publications #equal contribution *corresponding author

- J. Duan[#], **J. Jiang[#]**, U. Kim, J.W. Lee, Y. Yang, M. Choi, Z. Wu, J. Xi, “Structure and Device-Operando Photostability of Quasi-2D Ruddlesden–Popper Perovskites: Engineering the Spacer Cation Matters”, *ACS Energy Letters*, 2026, 11, 1714–1723. <https://doi.org/10.1021/acsenergylett.5c03228>
- M. Geng[#], **J. Jiang[#]**, X. Ma, J. Li, K. Wang, L. Jiang, D. Lu, B. Li, Y. Gu, T. Xu, “Bidentate Pyridine Passivators Attaching Trifluoromethyl Substitute Groups in Varied Positions for Efficient Carbon-Based Perovskite Solar Cells”, *ACS Applied Materials & Interfaces*, 2025, 17, 64645–64654. <https://doi.org/10.1021/acami.5c18690>
- **J. Jiang**, T. van der Heide, S. Thébaud, C. R. Lien-Medrano, A. Fihey, L. Pedesseau, C. Quarti, M. Zacharias, G. Volonakis, M. Kepenekian, B. Aradi, M. A. Sentef, J. Even, C. Katan, Flexible and Efficient Semi-Empirical DFTB Parameters for Electronic Structure Prediction of 3D, 2D Iodide Perovskites and Heterostructures, *Physical Review Materials.*, 2025, 9, 023803. <https://doi.org/10.1103/PhysRevMaterials.9.023803>
- **J. Jiang[#]**, J. You[#], S. (Frank) Liu, J. Xi, Scale-up solutions of 2D perovskite photovoltaics: insights of multiscale structures, *ACS Energy Letters*, 2024, 9, 17–29. <https://doi.org/10.1021/acsenergylett.3c02009>
- J. Xi[#], **J. Jiang[#]**, H. Duim, L. Chen, J. You, G. Portale, S. (Frank) Liu, S. Tao, M. A. Loi, On the mechanism of solvents catalyzed structural transformation in metal halide perovskites, *Advanced Materials*, 2023, 35, 2302896. <https://doi.org/10.1002/adma.202302896>
- Y. Li[#], **J. Jiang[#]**, D. Wang[#], D. Liu, S. Yajima, H. Li, A. Fuchimoto, H. Li, G. Shi, S. Hayase, S. Tao, J. Shi, Q. Meng, C. Ding, Q. Shen, Electronic Coupling Between Perovskite Nanocrystal and Fullerene Modulates Hot Carrier Capture, *Advanced Functional Materials*, 2024, 2415735. <https://doi.org/10.1002/adfm.202415735>
- N. Ren[#], P. Wang[#], **J. Jiang[#]**, R. Li, W. Han, J. Liu, Z. Zhu, B. Chen, Q. Xu, T. Li, B. Shi, Q. Huang, D. Zhang, S. Apergi, G. Brocks, C. Zhu, S. Tao, Y. Zhao, X. Zhang, Multifunctional additive CdAc₂ for efficient perovskite-based solar cells, *Advanced Materials*, 2023, 35, 2211806. <https://doi.org/10.1002/adma.202211806>

- X. Meng, **J. Jiang**, X. Yang, H. Zhao, Q. Meng, Y. Bai, Q. Wang, J. Song, C. Katan, J. Even, F. Liu, W. W. Yu, Organic-Inorganic Hybrid Cuprous-Based Metal Halides with Unique Two-Dimensional Crystal Structure for White Light-Emitting Diodes, *Angewandte Chemie - International Edition*, 2024, <https://doi.org/10.1002/anie.202411047>
- J. Byeon, S. H. Cho, **J. Jiang**, J. Jang, C. Katan, J. Even, J. Xi, M. Choi, Y. S. Lee, Structural Isomer of Fluorinated Ruddlesden-Popper Perovskites Toward Efficient and Stable 2D/3D Perovskite Solar Cells, *ACS Applied Materials & Interfaces*, 2023, 15, 27853–27864. <https://doi.org/10.1021/acsami.3c01754>
- S. Ji, X. Meng, X. Wang, T. Bai, R. Zhang, B. Yang, K. Han, **J. Jiang***, F. Liu, Colloidal Synthesis of Size-Confined CsAgCl₂ Nanocrystals: Implications for Electroluminescence Applications, *Materials Chemistry Frontiers*, 2022, 6, 3669–3677. <https://doi.org/10.1039/D2QM00997H>
- **J. Jiang**, J. M. Vicent-Luna, S. Tao, The Role of Solvents in the Formation of Methylammonium Lead Triiodide Perovskite, *Journal of Energy Chemistry*, 2022, 68, 393–400. <https://doi.org/10.1016/j.jechem.2021.12.030>
- **J. Jiang**, F. Liu, I. Tranca, Q. Shen, S. Tao, Atomistic and Electronic Origin of Phase Instability of Metal Halide Perovskites, *ACS Applied Energy Materials*, 2020, 3, 11548–11558. <https://doi.org/10.1021/acs.aem.0c00791>
- **J. Jiang**, C. K. Onwudinanti, R. A. Hatton, P. A. Bobbert, S. Tao, Stabilizing Lead-Free All-Inorganic Tin Halide Perovskites by Ion Exchange, *Journal of Physical Chemistry C*, 2018, 122, 17660–17667. <https://doi.org/10.1021/acs.jpcc.8b04013>
- **J. Jiang**[#], F. Liu[#], Q. Shen, S. Tao. The Role of Sodium in Stabilizing Tin-Lead (Sn-Pb) Alloyed Perovskite Quantum Dots, *Journal of Materials Chemistry A*, 2021, 9, 12087–12098. <https://doi.org/10.1039/D1TA00955A>
- F. Liu[#], **J. Jiang**[#], Y. Zhang, C. Ding, T. Toyoda, S. Hayase, R. Wang, S. Tao, Q. Shen, Near-Infrared Emission from Tin - Lead (Sn - Pb) Alloyed Perovskite Quantum Dots by Sodium Doping, *Angewandte Chemie - International Edition*, 2020, 59, 8421–8424. <https://doi.org/10.1002/anie.201916020>
- F. Liu[#], **J. Jiang**[#], T. Toyoda, A. Kamarudin, S. Hayase, R. Wang, S. Tao, Q. Shen, Ultra-Halide-Rich Syntheses Stabilize the Pure Tin-Based Halide Perovskite Quantum Dots, *ACS Applied Nano Materials*, 2021, 4, 3958–3968. <https://doi.org/10.1021/acsanm.1c00324>
- J. Cao[#], **J. Jiang**[#], N. Li[#], Y. Dong, Y. Jia, S. Tao, N. Zhao, Alkali-Cation-Enhanced Benzylammonium Passivation for Efficient and Stable Perovskite Solar Cells Fabricated Through Sequential Deposition, *Journal of Materials Chemistry A*, 2020, 8, 19357–19366. <https://doi.org/10.1039/D0TA04680A>
- Y. H. R. Chang, **J. Jiang**, H. Y. Khong, I. Saad, S. S. Chai, M. M. Mahat, S. Tao, Stretchable AgX (X= Se, Te) for Efficient Thermoelectrics and Photovoltaics, *ACS Applied Materials & Interfaces*, 2021, 13, 25121–25136. <https://doi.org/10.1021/acsami.1c04759>
- A. Caiazzo, K. Datta, **J. Jiang**, M. C. Gélvez-Rueda, J. Li, R. Ollearo, J. M. Vicent-Luna, S. Tao, F. C. Grozema, M. M. Wienk, R. A. J. Janssen, Effect of co-solvents on the crystallization and phase distribution of mixed-dimensional perovskites, *Advanced Energy Materials*, 2021, 11, 2102144. <https://doi.org/10.1002/aenm.202102144>
- D. Bartesaghi, A. Ray, **J. Jiang**, R. K. M. Bouwer, S. Tao, T. J. Savenije, Partially Replacing Pb by Mn in Hybrid Metal Halide Perovskites: Structural and Electronic Properties, *APL Materials*, 2018, 6, 121106. <https://doi.org/10.1063/1.5060953>
- S. Tao, I. Schmidt, G. Brocks, **J. Jiang**, I. Tranca, K. Meerholz, S. Olthof, Absolute Energy Level Positions in Tin-and Lead-Based Halide Perovskites, *Nature communications*, 2019, 10, 2560. <https://doi.org/10.1038/s41467-019-10468-7>
- **J. Jiang**[#], Q. Liang[#], R. Meng, Q. Yang, C. Tan, X. Sun, X. Chen, Exploration of New Ferromagnetic, Semiconducting and Biocompatible Monolayers with Considerable Visible and Infrared Light Absorption, *Nanoscale*, 2016, 9, 2992–3001. (Selected as 2016 Nanoscale Inside Cover) <https://doi.org/10.1039/C6NR07231C>
- **J. Jiang**, Q. Liang, R. Meng, Q. Yang, X. Sun, D. Yang, G. Zhang, X. Chen, The Influence of Tensile Stress on Polyaniline as Strain Sensor, *IEEE Electron Device Letters*, 2016, 37, 1636–1638. <https://ieeexplore.ieee.org/document/7580610>

- **J. Jiang**[#], Q. Liang[#], S. Zhang[#], R. Meng, C. Tan, Q. Yang, X. Sun, H. Ye, X. Chen, Tuning the electronic and optical properties of graphane/silicane and fhBN/silicane nanosheets via interfacial dihydrogen bonding and electrical field control, *Journal of Materials Chemistry C*, 2016, 4, 8962-8972. <https://doi.org/10.1039/C6TC02343F>
- R. Meng[#], **J. Jiang**[#], Q. Liang, Q. Yang, C. Tan, X. Sun, X. Chen, Design of graphene-like gallium nitride and WS₂/WSe₂ nanocomposites for photocatalyst applications, *Science China Materials*, 2016, 59, 1027-1036. <https://doi.org/10.1007/s40843-016-5122-3>
- X. Chen, **J. Jiang**^{*}, Q. Liang^{*}, R. Meng, Q. Yang, C. Tan, X. Sun, The electronic and optical properties of silicene/g-ZnS heterobilayer: a theoretical study, *Journal of Materials Chemistry C*, 2016, 4, 7004 -7012. <https://doi.org/10.1039/C6TC01468B>
- X. Chen, **J. Jiang**, Q. Liang, R. Meng, C. Tan, Q. Yang, S. Zhang, H. Zeng, Tunable electronic structure and enhanced optical properties in quasi-metallic hydrogenated/fluorinated SiC heterobilayer, *Journal of Materials Chemistry C*, 2016, 4, 7406 -7414. (Selected as 2016 Journal of Materials Chemistry C Hot Paper) <https://doi.org/10.1039/C6TC01988A>
- Q. Liang[#], **J. Jiang**[#], H. Ye, N. Yang, M. Cai, J. Xiao, X. Chen, Sorption and diffusion of water vapor and carbon dioxide in sulfonated polyaniline as chemical sensing materials, *Sensors*, 2016, 16, 606. <https://doi.org/10.3390/s16050606>
- Q. Liang[#], **J. Jiang**[#], R. Meng, H. Ye, C. Tan, Q. Yang, X. Sun, D. Yang, X. Chen, Tuning electronic properties and work functions of graphane/fully hydrogenated h-BN heterobilayer via heteronuclear dihydrogen bonding and electric field control, *Physical Chemistry Chemical Physics*, 2016, 18, 16386-16395. <https://doi.org/10.1039/C6CP01541G>
- X. Chen, **J. Jiang**, Q. Liang, N. Yang, H. Ye, M. Cai, L. Shen, D. Yang, T. Ren, First-principles study of the effect of functional groups on polyaniline backbone, *Scientific Reports*, 2015, 5, 16907. <https://doi.org/10.1038/srep16907>

Conferences and Workshops

- Two talks at E-MRS Spring meeting, Strasbourg, France, 2025
- Talk at the Journées Pérovskites Halogénées (JPH), Erquy, France, 2025
- Invited talk at the HNU Yuelu International Young Scholar Forum, Changsha, China, 2024
- Invited talk at the 12th Young Scholars Forum, Nanjing/Suzhou, China, 2024
- Invited talk at the 10th Silk Road International Autumn Symposium for Distinguished Young Scholars (SRIS), Xi'an, China, 2024
- Talk at the Materials for Sustainable Development Conference (MATSUS24), Barcelona, Spain, 2024
- Invited talk at the 12th East Lake International Forum for Outstanding Overseas Young Scholars, Wuhan, China, 2023
- Talk at French National Conference of GDG NANOmaterials for Energy applications (NAME), Rennes, France, 2023
- Talk at E-MRS fall meeting, Warsaw, Poland, 2023
- Talk at PeroCUBE workshop Rennes, France, 2023
- Talk at Dutch National Conference of Physics@Veldhoven, the Netherlands, 2021
- Poster presentation at MRS Spring/Fall Meeting & Exhibit, 2020
- Talk at Internet Conference on Theory and Computation of Halide Perovskites, 2020
- Poster presentation at Applied Computational Science (ACOS) Symposium, Eindhoven, the Netherlands, 2020
- Talk at nanoGe Fall Meeting, 2020
- Poster presentation at International Conference on Hybrid and Organic Photovoltaics, 2020
- Poster presentation at Applied Computational Science (ACOS) Symposium, Eindhoven, the Netherlands, 2019
- Poster presentation at Next-Gen IV PV Materials, Groningen, the Netherlands, 2019

- Poster presentation at Applied Computational Science (ACOS) Symposium, Eindhoven, the Netherlands, 2018
- Poster presentation at E-MRS Fall Meeting, Warsaw, Poland, 2018
- Poster presentation at 4th Dutch Perovskite Workshop, Eindhoven, the Netherlands, 2018
- Poster presentation at International Conference on Perovskite Thin Film Photovoltaics, Photonics and Optoelectronics, Rennes, France, 2018
- Talk at 17th International Conference on Electronic Packaging Technology (ICEPT), 16-19, August 2016, Wuhan, China
- Poster presentation at the 16th International Conference on Electronic Packaging Technology (ICEPT), 11-14, August 2015, Changsha, China

Awards and Scholarships

- Best paper award: awarded to top 10 papers in the years 2016-2017, Science China Materials, 2019
- Best master thesis award: awarded to top 1-2%, Guilin University of Electronic Technology, China, 2017
- Best master graduate award: awarded to top 1%, Guangxi Province, China, 2017
- Awarded the National Scholarship from the Ministry of Education of China, 2016
- Awarded the Graduate Student Scholarship (first class) from the Guilin University of Electronic Technology, 2014-2017
- Honored the third prize in the National Multimedia Courseware Design Competition, China, 2015

Funding

- Research Grant from Guangxi Provincial Department of Education, China, 2014 - 2017
- Computational Resources Grant from the Dutch National Supercomputer, Netherlands, 2019-2020
- Participated in the EU Horizon 2020 project "High-Performance Large-Area Organic Perovskite Devices for Lighting, Energy and Li-F (PeroCUBE)", CNRS of France is responsible for some sub-topics as the main executive, 2020-2024
- Participated in the EU Horizon 2020 project "Polaronic Logic (Polloc)", CNRS of France is responsible for some sub-topics as the main executive, 2020-2024
- Participated in the European M-ERA.NET project "Physical and Data-Driven Multiscale Modeling Design of Layered Lead Halide Perovskite Materials (Phantastic)", National Institute of Applied Sciences of Rennes, France is responsible for some sub-topics as the main executive, 2022-2025
- Participated in the Netherlands National Research Council (NWO) project "Computational Science for Energy Research (CSER)" as the main executive, 2016-2021

Academic Activity

- Early Career Editorial Members of Nanomaterials
- Guest editor of journals including Nanomaterials, Micromachines, Frontiers in Materials
- Reviewer of more than 50 journals including Advanced Materials, Physical Review Letters, Advanced Energy Materials, Nano Letters, Physical Review B, etc.

Teaching Experience

- Fall 2018, Computational Materials Science, Teaching Assistant
- Spring 2019, Finite Element Modeling, Lecturer

Languages

- English, advanced
- Chinese (Mandarin), native