

Lyuwen Fu

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EDUCATION

Columbia University, New York, New York

Ph.D. in Materials Science

Jan 2017 – Oct 2021

- Advisor: Professor Chris Marianetti
- Research Focus: Generic first-principle computation on phonons and phonon-phonon interactions
- Thesis: Thermodynamics of Interacting Phonons

Columbia University, New York, New York

Master of Science in Materials Science

Sep 2015 – Dec 2016

- Cumulative GPA: 3.81 / 4.00
- Coursework: Solid State Physics, Computing Electronic Structure of Complex Materials, Theory of Crystalline Materials, Mechanical Behavior of Materials, etc.

University of Science and Technology Beijing, Beijing, China

Bachelor of Engineering in Materials Physics

Sep 2011 – Jun 2015

- Adviser: Professor Jiao Teng
- Thesis: Research on the Quantum Transport Properties of Resistive RAM
- Cumulative GPA: 3.46 / 4.00

RESEARCH

Columbia University, New York, New York

Department of Applied Physics and Applied Mathematics

May 2016 – Oct 2021

- Project: Thermodynamics of interacting phonons
- Adviser: Professor Chris Marianetti
- Develop group theoretical approach to extract arbitrary order phonons and their interactions in terms of space group *irreducible derivatives*.
- Develop finite difference algorithm which extracts all irreducible derivatives in the smallest possible supercells with the fewest possible calculations.
- Develop software to compute thermal dynamic properties using the extracted phonon interaction data.
- Perform high-throughput computations on HPC clusters.
- Manage an in-house cluster of more than 80 nodes.

University of Science and Technology Beijing, Beijing, China

Undergraduate Thesis, Department of Materials Physics and Chemistry

Feb 2015 – Jun 2015

- Project: Research on the Quantum Transport Properties of Resistive RAM
- Adviser: Professor Jiao Teng
- Design the synthesis process and the pattern of ReRAM thin film. Realized the resistive switch phenomenon in ReRAM.
- Research on the theoretical background of ReRAM and the mechanism and conditions for the Quantized Anisotropic Magnetoresistance.
- Study the resistive switch properties and electron transport properties of the ReRAM samples.

Undergraduate Student Research, Institute for Advanced Materials and Technology Oct 2013 – May 2014

- Project: Research on the Performance Study of One-dimensional IrO₂ Nano-Array Electrochemical Sensor
- Adviser: Professor Huimin Meng
- Develop a new method of the synthesis of the one-dimensional IrO₂ nanometer array electrodes and studied electrochemistry properties of the electrode.

SKILLS

- Programming Languages: Proficient in Python, C/C++, Familiar with Objective-C, Java, C#, Fortran.
- First-principle Computation: VASP, Quantum ESSRESSO, Abinit.
- Other Softwares: L^AT_EX, Docker, MATLAB, Mathematica, Blender, Adobe Photoshop.

RESEARCH INTERESTS

First-principle computation and simulation, Computational materials science. Phonon and phonon interactions. Materials thermodynamics and thermal transport.

PUBLICATIONS

1. Fu, L., Kornbluth, M., Cheng, Z., & Marianetti, C. A. (2019). Group theoretical approach to computing phonons and their interactions. *Physical Review B*, 100(1), 014303.
2. Bryan, M. S., Fu, L., et al. (2020). Nonlinear propagating modes beyond the phonons in fluorite-structured crystals. *Communications Physics*, 3(1), 1-7.
3. Ding, X., Yao, T., Fu, L., et al. (2020). Magnetic, transport and thermal properties of δ -phase UZr_2 . *Philosophical Magazine Letters*, 1-11.
4. C.A. Dennett, ..., L. Fu, et al. (2021). An Integrated Experimental and Computational Investigation of Defect and Microstructural Effects on Thermal Transport in Thorium Dioxide, *Acta Mater.*, 213, 116934.

SUBMITTED FOR PUBLICATIONS

1. E. Xiao, H. Ma, M. S. Bryan, L. Fu, et al. (2022). Validating First-Principles Phonon Lifetimes via Inelastic Neutron Scattering, arXiv:2202.11041.
2. M. A. Mathis, A. Khanolkar, L. Fu, et al. (2022). The Generalized Quasiharmonic Approximation via Space Group Irreducible Derivatives, arXiv:2202.14016.

CONFERENCES

1. Fu, L., Kornbluth, M., & Marianetti, C. A. (2018). An optimal approach to computing phonons and their interactions via finite difference. APS March Meeting 2018, X29.00006.
2. Fu, L., Kornbluth, M., Cheng, Z., & Marianetti, C. A. (2019). An optimal approach to computing phonons and their interactions via finite displacements. APS March Meeting 2019, H22.00003.
3. Fu, L., Mathis, M., Xiao, E., & Marianetti, C. A. (2020). Phonon interactions in rock salt and fluorite structures. APS March Meeting 2020, P44.00009. (*Meeting canceled due to COVID-19 pandemic*)