

# 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 IrO<sub>2</sub> Nano-Array Electrochemical Sensor
- Adviser: Professor Huimin Meng
- Develop a new method of the synthesis of the one-dimensional IrO<sub>2</sub> 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<sup>A</sup>T<sub>E</sub>X, 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  $\delta$ -phase  $\text{UZr}_2$ . *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*)