

Introduction of Glassy Thermal Transport in Crystal Solids



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Abstract

Thermal transport in crystals is usually described by particle-like phonon propagation, valid for simple lattices with small unit cells and distinct phonon bands. In complex and modular crystals, however, strong anharmonicity and overlapping linewidths induce glass-like diffusion that dominates heat conduction. Using first-principles and machine-learning-accelerated molecular dynamics, we capture high-order anharmonicity, phonon renormalization, and quantum effects beyond ground-state DFT. The results show that glass-like transport leads to ultra-low and weakly temperature-dependent thermal conductivity, consistent with experiments and underlying the phonon-glass electron-crystal concept. Recognizing this mechanism bridges theory–experiment gaps and guides the design of high-performance thermoelectrics and solid-state electrolytes.

Biography

Prof. Zhen TONG is currently working as an Assistant Professor at the School of Advanced Energy, Faculty of Sun Yat-Sen University. He received his bachelor's degree from Huazhong University of Science and Technology in 2014 and his Ph.D. from Shanghai Jiao Tong University in 2019. He has been a visiting scholar at Purdue University in the United States and a Humboldt Research Fellow in Germany. He is recognized as a Shenzhen Overseas High-Level Talent and a Longhua District Longwu Huazhang High-Level Talent. His research focuses on the fundamental mechanisms of energy carriers including phonons, electrons, photons, and ions in micro/nano-scale energy transport, thermoelectrics, radiative cooling, solid-state battery, and solar-thermal storage, etc. His research has been funded by many sponsors, including the National Science Foundation of China, the Guangdong National Science Foundation, and the Shenzhen Excellent Young Scientist Project.