北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Weekly Seminar

Thermal and electrical transport from first-principles

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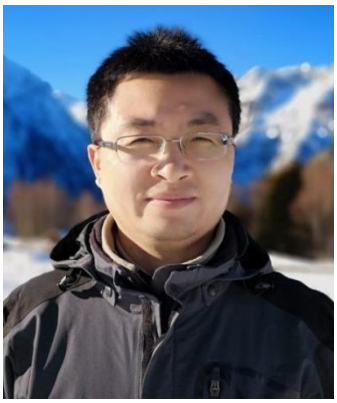

Time: 3:00pm, Mar. 22, 2023 (Wednesday)

时间：2023年3月22日 （周三）下午3:00

Venue: Room W563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

Parameter-free first-principles calculations of thermal and electrical transport in crystals have been made possible with recent advances in solving Boltzmann transport equation and DFT-based calculations of interatomic and electron-phonon interactions. In this talk, I will first review the formalism of phonon Boltzmann transport equation (BTE)[1]. I will then present the advances of our understanding of phonon transport in several systems including elemental tungsten, where the anomalously large phonon thermal conductivity well explains the derivation of measured Lorenz number from the Sommerfeld value[2]. From the relation between the phonon transport and the electronic structure, we identified a high thermal conductivity material q-TaN[3] with a value of ~1000W/m-K. Last, I will show how to realize precise calculations for the phonon-limited mobility based on electronic BTE[4,5]

References

[1] Li, Carrete, Katcho, and Mingo, Comput. Phys. Commun. 185, 1747 (2014) (http://www.shengbte.org/)
[2] Chen, Ma and Li, Phys. Rev. B 99, 020305(R) (2019)
[3] Kundu, Yang, Ma, Ruan, Feng, Carrete, Madsen, and Li, Phys. Rev. Lett. 126, 115901 (2021)
[4] Li, Phys. Rev. B 92, 075405 (2015)
[5] Ma, Nissimagoudar, and Li, Phys. Rev. B 97, 045201 (2018)

About the speaker

Since 2016, Dr. Wu Li has been an Assistant and Associate Professor at Institute for Advanced Study, Shenzhen University. He received his BSc from Zhengzhou University in 2006 and PhD from Institute of Physics, Chinese Academy of Sciences in 2011. During his PhD, he studied in TU Dresden, Germany with a Max-Planck Society Scholarship for two years (2008-2010). He did postdocs at CEA, France (2011-2013) and SCM, Netherlands as a Marie Curie fellow (2013-2015). After that he returned to CEA as a research scientist in 2015. He is a primary developer of the ShengBTE software, routinely used for studying the lattice thermal conductivity. He has been ranked among the World's Top 2% Scientists (2021 and 2022) by citation for “the career long impact”.