北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

Kagome materials in SG 191: LEGO building block of band structure, soft flat phonons, and CDW formation

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Venue: Room w563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

Kagome materials with flat bands exhibit wildly different physical properties depending on symmetry group, and electron number. Their complicated physics and even the one-particle “spaghetti” of electron/phonon bands are so far amenable only to phenomenological interpretation. In this work, we advance the understanding of the Kagome materials in SG 191 by combining ab-initio calculations and analytical approach.

Firstly, we show that the “spaghetti” electron bands observed in the 11 material (FeGe class) can be decomposed into three distinct groups [1]. This decomposition provides an analytical framework for understanding the presence of flat bands in these materials. Additionally, we observe the band structure of 166 material (MgFe6Ge6 class) can be constructed by treating the 11 material as a fundamental "LEGO"-like building block enabling further insights into its electronic properties [1].

Secondly, we focus on the formation of charge density waves (CDWs) of a specific 166 material, ScV6Sn6 [2]. Our analysis reveals that a flat and soft phonon band collapses at (1/3, 1/3, 1/2) as the temperature decreases. This collapse is attributed to the coupling between the mirror-even phonon orbital and mirror-even electron orbital, where the phonon and electron orbitals share the same Wannier center. Moreover, we highlight that the flatness of the soft phonon band induces strong fluctuations, ultimately stabilizing a CDW phase at a different wave vector (1/3, 1/3, 1/3) through a first-order transition.

[1] To be published

[2] H. Hu, Y. Jiang, et al, arXiv:2305.15469 (2023).

About the speaker

Hu Haoyu is currently working with Prof. Andrei Bernevig as a postdoc at Donostia international physics center, Spain. He received his B.S. degree from the University of Science and Technology of China in 2016, and his Ph.D. degree from Rice University in 2022 under the supervision of Prof. Qimiao Si. He is currently working on the flat band system including twisted bilayer graphene and kagome materials, and the interplay between correlation effect and topology.