# Seminar

# Electron-correlation-induced charge order in Kagome magnet FeGe

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**Time: 3:00 pm, Sept. 14, 2023 (Thursday)**

**时间：2023年9月14日 （周四）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

A 2 × 2 × 2 charge density wave (CDW) order was recently observed deep inside the antiferromagnetic phase of a Kagome metal FeGe, which significantly enhances its spin-polarization. A key question is whether the CDW in FeGe is driven by its electronic correlation and magnetism. Here, we address this problem using density functional theory and its combination with *U* as well as dynamical mean-field theory. Our calculations show that large dimerization (~1.3 Å) of Ge1-sites along c-axis will enhance electronic correlation of the Fe-3d orbitals and, as a result, it enhances the spin-polarization and saves more magnetic exchange energies. We demonstrate that the balance between magnetic energy saving and structural energy cost via partially dimerizing Ge1-sites in an enlarged superstructure could induce a new ground state, in which the charge ordering is induced naturally to respond the large partial Ge1-dimerization. We thus reveal a novel unconventional CDW mechanism driven by primarily saving magnetic energies, instead of charge via the interplay of structure, electronic correlation and magnetism [1,2]. Recent experiments [3,4,5] have provided strong support to our theoretical predications.

Refs:
[1] Hu Miao*, Yilin Wang*, *et al.*, arXiv: 2210.06359 (2022)
[2] Yilin Wang, arXiv:2304.01604 (2023)
[3] Ziyuan Chen *et al.*, arXiv, 2307.07990 (2023)
[4] Ziyuan Chen *et al.*, arXiv:2302.04490 (2023)
[5] Zhisheng Zhao *et al.*, arXiv, 2308.08336 (2023)

## About the speaker

王义林，2016年在中国科学院物理研究所获得博士学位，2016-2020年在美国布鲁克海文国家实验室从事博士后研究，2020年加入中国科学技术大学，任特聘研究员。王义林主要从事强关联电子材料的第一性原理计算以及X-射线谱学的模拟，使用的方法包括：DFT+DMFT、DFT+Gutzwiller、NRG，ED等；在强关联诱导的量子反常霍尔效应、多极矩序、固体材料中分子轨道的RIXS谱模拟、三通道的近藤模型的精确求解等体系的研究方面发表SCI论文30余篇。目前主要研究兴趣是通过第一性原理计算揭示强关联材料中晶格自由度和电子关联相互作用导致的新奇物理现象。