Novel three-dimensional Fermi surface and electron-correlation-induced charge density wave in FeGe

Xiangang Wan（xgwan@nju.edu.cn）
School of Physics, Nanjing University, China

Abstract: As the first magnetic kagome material to exhibit the charge density wave (CDW) order, FeGe has attracted much attention in recent studies. All the theoretically calculated phonon frequencies in FeGe remain positive. We perform a comprehensive study through first-principles calculations and symmetry analysis. We find that reasonable Heisenberg interactions and magnetic anisotropy cannot explain the double cone magnetic transition, and the DM interactions can result in this small magnetic cone angle. Based on the experimental 2X2X2 supercell, we thus explore the subgroups of the parent phase. Group theoretical analysis reveals that there are 68 different distortions, and only four of them without inversion and mirror symmetry thus can explain the low temperature magnetic structure. We also find that the maximum of nesting function is at K point instead of M point. Considering the effect of local Coulomb interaction, we reveal that the Fermi level eigenstates nested by vector K are mainly distributed from unequal sublattice occupancy, thus the instability at K point is significantly suppressed. Meanwhile, the wave functions nested by vector M have many ingredients located at the same Fe site, thus the instability at M point is enhanced. This indicates that the electron correlation, rather than electron-phonon interaction, plays a key role in the CDW transition at M point.

Bio: Professor Xiangang Wan obtains Ph.D from Nanjing University, China at 2000. After four years Post-doctor at National Institute for Material at Japan and U.C. Davis at US, he back to Nanjing University as Assistant Professor, Associate Professor, and become full Professor at 2010. He had been selected as The Chinese National Science Fund for Distinguished Young Scholars at 2015. He had been awarded the Ye Qisun Prize for Physics at 2019. He had also obtained the XPLORER PRIZE from Tencent Foundation at 2019.