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Electronic structure of iron-based superconductors from DFT+DMFT: the important role of Hund's coupling and correlations
ZHIPING YIN, KRISTJAN HAULE, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University — The iron pnictide and chalcogenide compounds are a subject of intensive investigations due to their surprisingly high temperature superconductivity. Density functional theory (DFT) has been widely used in the theoretical study but often suffers from significant discrepancy with experimental observations. The fundamental reason is that the low energy electrons in many iron-based superconductors, while displaying nice Fermi-liquid behavior, form quasiparticles and acquire sizable masses. Thus the actual low energy electronic states are strongly renormalized compared to DFT bands. We show that the combination of DFT and dynamic mean field theory (DFT+DMFT), which incorporates the detail electronic structure and local electronic correlations, overcomes most of DFT limitations and describe well the trends in all the physical properties such as the ordered moments, effective masses, Fermi surfaces, x-ray spectroscopy, optical conductivity, magnetic excitations and so on across all families of iron-based compounds, and find them in good agreement with various different experiments. We stress that Hund's blocking mechanism and electronic correlations are crucial in determining the electronic structures of iron-based superconductors.

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