What do the rich magnetic structures of iron-based superconductors teach us about their electronic structure?

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Recent discovery of iron-based high temperature superconductors (Fe-SC) has reignited the intense interest in the unresolved relationship of anti-ferromagnetism and high temperature superconductivity. Unlike the well known case of the cuprates, however, the magnetic properties of the Fe-pnictides are much richer, leading to diverse (and mostly inconsistent) descriptions in the field. Here, the puzzling nature of magnetic and lattice phase transitions of Fe-SC is investigated. First, via a first-principles Wannier function analysis of representative parent compound LaOFeAs, a rare ferro-orbital ordering is found to give rise to the recently observed highly anisotropic magnetic coupling[1], and drive both phase transitions — without resorting to widely employed frustration or nesting picture. The revealed necessity of the additional orbital physics leads to a correlated electronic structure fundamentally distinct from that of the cuprates. Second, the rich magnetic correlation across the Fe-based superconducting families are explained via a unified model[2] that encapsulates the essential roles of itinerant and local electrons with double-exchange effects. Interestingly, the ferromagnetic correlation is fond significantly higher in energy, leaving superconductivity the only viable phase to relieve entropy at low temperature upon doping.

[1]C.-C. Lee, W.-G. Yin, and Wei Ku, Phys. Rev. Lett. **103**, 267001 (2009)
[2]W.-G. Yin, C.-C. Lee, and Wei Ku, Phys. Rev. Lett. **105**, 107004 (2010)