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Localized vs. Itinerant Magnetism in Fe-based Superconductors

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Since the discovery of a high temperature superconducting transition in ferropnictides approximately two years ago, the highly magnetic character of these compounds and the close relationship between superconductivity and magnetism has been widely recognized and intensely studied. Initially, debate about the nature of the magnetism was split into two camps: localized moments (as in cuprates) and pure itineracy (a spin-peierls type transition). We argue that the magnetism in pnictides and in the related chalcogenides is between these two extremes, consisting of Hund's rule (or Stoner) derived moments on the Fe atoms. Using density functional theory (DFT) calculations, we show that the ordering mechanism is not Fermi surface driven and is also unlikely to be of superexchange origin. We explain, from a computational perspective, how the magnetic and structural transitions are related and compare calculated doping and pressure dependent quantities to experiment. We discuss which quantities are well reproduced and explainable using DFT and what remaining questions need to be answered before magnetism, superconductivity and their relationship can be considered as understood. We argue that spin fluctuations are the driving force behind the superconductivity and that magnetic order is a competing, and therefore detrimental, phase. We propose a particular spin fluctuation scheme that could explain why the structural transition appears either in conjunction with or before the magnetic transition.