Correlations and effects of pressure in Fe-pnictides

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In this talk we will explore the effects of correlations and pressure in Fe-based superconductors by considering a combination of density functional theory calculations and dynamical mean field theory and compare our results with recent ARPES and de Haas van Alphen experiments. We will discuss the importance of orbital-selective correlations in the 111 (LiFeAs, LiFeP) and 122 families (BaFe$_2$As$_2$, CaFe$_2$As$_2$, KFe$_2$As$_2$) [1,2] and indicate how the topology of the Fermi surface, specially in KFe$_2$As$_2$, is influenced by these effects. In this context, we will show why MgFeGe, an isostructural and isoelectronic system to LiFeAs, doesn’t superconduct [3]. In the case of the 122 systems, we will predict and analyze changes in the electronic and magnetic properties under hydrostatic, tensile and compressive pressure and will discuss our results in relation to (i) superconductivity, (ii) magnetism and (iii) the mechanisms involved in the detwinning process of an orthorhombic iron-pnictide crystal a [4].


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