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Differences in the degree of correlations between Pnictides and Chalcogenides: LaFeAsO vs. FeSe[1]

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The discovery of high-temperature superconductivity in iron-based compounds triggered an enormous amount of research in condensed matter physics. A very intriguing property of these new compounds is the rather high flexibility concerning elemental substitutions, leading to several families of superconductors, termed "1111," "122," "11," and so on, depending on their chemical composition. In this talk we will analyse the single-particle properties of prominent iron-based supercondutors using a combination of density-functional theory with the Dynamical Mean-Field Theory, where also the interaction parameters are calculated ab-initio. This approach enables us to understand also these more complex materials at a first-principle level. We will show that there are significant differences in the electronic properties, when going from more weakly correlated members as LaFeAsO, to more correlated ones like FeSe. For reasonable Coulomb parameters, the properties range from Fermi-liquid like to incoherent bad-metal like.

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