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Correlation, magnetization and conduction in iron pnictides and iron chalcogenides ZHIPING YIN, Department of Physics, Rutgers and Stony Brook University, KRISTJAN HAULE, GABRIEL KOTLIAR, Department of Physics, Rutgers University — By combining density functional theory (DFT) and dynamical mean field theory (DMFT), we study the electronic properties of iron pnictides and iron chalcogenides in both the paramagnetic and magnetic states. With ab initio derived realistic Coulomb interaction U and Hund's exchange coupling J, we find detailed agreements bewtween our calculations and many experimental observations in these compounds, including ARPES, magnetic properties, optical conductivity and anisotropy, and so on, WITHOUT any adjustment such as shifting of atomic positions, Fermi level and bands and renormalizations of bands which are commonly needed in DFT calculations in order to compare with experiments. Our theory explains the origin of the different magnetizations in FeTe and other iron pnictides and provides a unique physical picture. We find that in the magnetic phase of the iron pnictides, both the spin and the orbital polarization are strongly energy dependent. The spin polarization becomes weaker around Fermi level when the orbital polarization is stronger and vice verse at high energies. We stress on the role of the Hund's J rather than the Coulomb U and show how the iron pnictides and iron chalcogenides differ from other compounds.

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