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A band theory for magnetic cuprates based on self-interaction free local density approximation VINCENZO FIORENTINI, ALESSIO FILIPPETTI, SLACS and Physics Dept., University of Cagliari — The pseudo-SIC approach is based on an approximate form of self-interaction corrected (SIC) Kohn-Sham Equations. We overview the functionalities of this method applied to cuprates, which are prototypes of difficult materials for standard local-spin density functional theories such as LSDA (or even GGA). Indeed, theories based on local exchange-correlation potentials fail to predict the correct spin-polarized ground-state solution expected for the low-magnetization state (S=1/2) of the Cu(I) ions, thus describing these systems as metallic and nonmagnetic. Here we present our results for a series of relevant cases, including CuO, Cu_2O, $CuGeO_3$, and $YBa_2Cu_3O_{6+x}$, showing that the pseudo-SIC is capable to correct the gross failures of LSDA, restoring the expected S=1/2 electronic ground state and an overall satisfying description of the chemistry and the electronic and magnetic properties of these systems. Furthermore, since the pseudo-SIC is designed to work for metals as well as for insulators we can approach the challenging task of studying by first-principles the insulating-metal transition in doped Mott insulators. We will consider the example of Mn-doped CuO, where Mn-doping induces a simultaneous insulating-to-metal and antiferromagnetic-to-ferromagnetic phase transition.

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