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An empirical method to account for spin-fluctuation suppression of magnetism in Fe pnictides PETER BLAHA, TU Wien, IGOR MAZIN, MICHELLE JOHANNES, Naval Research Laboratory — Parent materials of Fe-based superconductors, such as BaFe_2As_2 , are itinerant antiferromagnets, and as such should be better described by LDA calculations than are strongly-correlated cuprates. To an extent, this is true, but LDA, being a mean-field approximation, underestimates the suppression of the long-range magnetism due to spin fluctuations. These can be accounted for within Moria’s self-consistent renormalization theory, which, however, includes unknown parameters such as the mean amplitude of the spin-fluctuations. We propose to include Moria’s renormalization empirically, through a scaling of the LDA exchange-correlation magnetic field by a uniform constant factor, tuned so as to reproduce the observed phase diagram. This is a much more physical method to produce electronic bands with a proper exchange splitting, than adding an artificial “negative-U” term within an LDA+U formalism, a technique used now. We will report the results of such renormalized calculations for BaFe_2As_2 and, for comparison, for a prototypical itinerant magnet, ZrZn_2 .

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