

Abstract Submitted  
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**Spin fluctuations-corrected DFT for Fe-based superconductors**

LUCIANO ORTENZI, Institute for Complex Systems (ISC), CNR, U.O.S. Sapienza, v. dei Taurini 19, 00185 Rome, Italy, HLYNUR GRETARSSON, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany, S. KASAHARA, Y. MATSUDA, Department of Physics, Kyoto University, Kyoto 606-8502, Japan, T. SHIBAUCHI, Department of Advanced Materials Science, The University of Tokyo, Japan, K.D. FINKELSTEIN, Cornell High Energy Synchrotron Source, Cornell University, Ithaca, New York 14853, USA, W. WU, S.R. JULIAN, YOUNG-JUNE KIM, Department of Physics, University of Toronto, 60 St. George St., Toronto, Ontario, M5S 1A7, Canada, I.I. MAZIN, code 6390, Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, DC 20375, USA, LILIA BOERI, Institute for Theoretical and Computational Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria — Albeit density functional theory (DFT) is, at the moment, the most appropriate tool for treating itinerant magnetism, its mean field implementations -local spin density approximation (LSDA) with or without gradient corrections- underestimate the effect of non local spin fluctuations. As a result DFT fails in reproducing, at the same time, the crystal structure and the amplitude of local moment in near critical systems. In this talk I will present a simple method for correcting the magnetic properties of itinerant systems in LSDA. The method is called reduced Stoner theory (RST). I will apply this method to study the ferromagnetic-paramagnetic transition under pressure in  $\text{Ni}_3\text{Al}$  itinerant ferromagnet and for describing the puzzling temperature behavior of the local moment found in doped- $\text{CaFe}_2\text{As}_2$  pnictides.

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