Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**Kondo anomalies in magnetic nanocontacts from first principles** PROCOLO LUCIGNANO, SISSA, Trieste; and CNR-INFM Coherentia, Naples, Italy , PIERPAOLO BARUSELLI, SISSA, and CNR-Democritos, Trieste, Italy, MICHELE FABRIZIO, SISSA, ICTP, and CNR-Democritos, Trieste, Italy, RICCARDO MAZZARELLO, SISSA, Trieste, Italy; and ETH Zurich, USI Campus, Lugano, Switzerland, ALEXANDER SMOGUNOV, ICTP, SISSA, and CNR-Democritos, Trieste, Italy, ERIO TOSATTI, SISSA, ICTP, and CNR-Democritos, Trieste, Italy — A realistic calculation of electron transport through magnetic nanocontacts should connect together DFT based electronic structure with many body methods like NRG. We recently moved a first step in this direction [1,2]. Identifying symmetry-dictated conduction channels, we calculate first the DFT channel- and spin-dependent impurity scattering phase shifts; then build an Anderson model whose symmetry and parameters are forced to reproduce at the Hartree Fock level the phase shifts; and finally solve the Anderson model by NRG. This yields much more than just the Kondo temperature. As exemplified by a Ni impurity in a Au nanocontact, we uncover the orbital origin the Fano interference in the predicted zero bias Kondo anomalies; the origin of their large structural dependence; and the likely occurrence of the so far ignored "ferro" Kondo effect. We are presently extending calculations to other nanocontacts including magnetic impurities on surfaces and nanotubes.

[1] P. Lucignano et al., Nat. Mat. 8, 563 (2009).

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Date submitted: 29 Dec 2009 Electronic form version 1.4