Abstract Submitted
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Zero bias STS Kondo anomalies of Co impurities on Cu surfaces: do ab initio calculations work? PIER PAOLO BARUSELLI, SISSA, Via Bonomea 265, Trieste 34136, Italy, ALEXANDER SMOGUNOV, SISSA, Via Bonomea 265, Trieste 34136, Italy, CEA Saclay, MICHELE FABRIZIO, SISSA, Via Bonomea 265, Trieste 34136, Italy, ICTP Trieste, RYAN REQUIST, SISSA, Via Bonomea 265, Trieste 34136, Italy, ERIO TOSATTI, SISSA, Via Bonomea 265, Trieste 34136, Italy, ICTP Trieste — Transition metal atoms such as Co on Cu (111), (100), and (110) surfaces produce STS I-V spectra showing different zero bias Kondo anomalies [1] but these differences have been neither quantitatively predicted nor fully explained theoretically. We apply to this problem the DFT+NRG scheme of Lucignano et al [2], where one solves by NRG an Anderson model built from ab initio phase shifts provided by DFT. For Co/Cu(100) and Co/Cu(110) our calculations describe correctly the experimental trend of Kondo temperatures, and fairly the lineshapes too. By contrast, they fail to describe Co/Cu(111) where in particular the anti-lorentzian lineshape found in experiment remains unexplained. This failure underscores the role of surface states, probably relevant for Co/Cu(111) [3] but not correctly described by our thin slab calculations. Future efforts to quantitatively include Kondo screening by surface states are therefore called for. 1. N. Knorr et al PRL 88, 096804 (2002); M. Ternes et al 2009 J. Phys.: Cond. Matt. 21, 053001 (2009); A. Gumbsch et al PRB81, 165420 (2010). 2. P. Lucignano et al Nature Mat. 8, 563 (2009); P.P. Baruselli et al, Physica E, doi:10.1016/j.physe.2011.05.005. 3. C. Lin et al. PRB 71, 035417 (2005).

Pier Paolo Baruselli
SISSA, Via Bonomea 265, Trieste 34136, Italy

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