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Magnetic impurities in Cu nanocontacts: Kondo effect and conductance from first principles DAVID JACOB, Rutgers University, KRISTJAN HAULE, GABRIEL KOTLIAR — We present *ab initio* calculations of the electronic structure and coherent transport properties of Cu nanocontacts hosting a single magnetic impurity (Fe,Co or Ni) in the contact region. The strong electron correlations of the impurity $3d$-electrons are fully taken into account by combining density functional calculations with a dynamical treatment of the impurity $3d$-shell in the so called one-crossing approximation. We find that for all three impurities the strong electron correlations give rise to Kondo resonances at the Fermi level which in turn lead to Fano lineshapes in the coherent transport characteristics of the nanocontact. The exact shape of the Kondo and Fano lineshapes, however, depends strongly on the impurity type and the geometry of the contact. This is in agreement with recent experiments measuring the conductance of magnetic impurities on noble metal surfaces [1-4]. [1] P. Wahl *et al.*, Phys. Rev. Lett. 93, 176603 (2004). [2] N. Néel *et al.*, Phys. Rev. Lett. 98, 016801 (2007). [3] L. Vitali *et al.*, Phys. Rev. Lett. 101, 216802 (2008). [4] N. Néel *et al.*, arXiv:0810.0236 (2008).

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