Abstract Submitted
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Electronic properties of transition metal atoms on Cu2 N/Cu(100): a DFT comparative study[1] ALEJANDRO FERRON, JOSÉ LADO, JOAQUÍN FERNÁNDEZ-ROSSIER, International Iberian Nanotechnology Laboratory — We study the electronic and magnetic properties of individual transition metal atoms (Ti, V, Cr, Mn, Fe, Co and Ni) deposited on a Cu_2N/Cu(100) surface by means of spin-polarized density functional theory (DFT) calculations. We focus our work on a comparative study of the various quantities, such as magnetic moment, orbital occupation, structural properties, hybridization with the substrate and spin polarization of the substrate, paying attention to the trends as the transition metal is changed. In this work we try to go beyond existing theoretical works by providing a comprehensive and comparative study of the electronic, magnetic and structural properties of these seven atoms including also Ni, for which there are no published calculations to the best of our knowledge. In the case of Mn, Fe and Co, we connect our results with the existing scanning tunneling microscope experiments [1,2].

[1] J. Oberg, R. Calvo, F. Delgado, D. Jacob, M. Moro, D. Serrate, J. Fernández-Rossier, C. Hirjibehedin, Nature Nanotechnology, **9**, 64 (2014).
[2] A. Spinelli, B. Bryant, F. Delgado, J. Fernández-Rossier, A. F. Otte, Nature Materials, published online on July 6 (2014). doi:10.1038/nmat4018

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