Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

The failure of DFT computations for a stepped-substrate-supported monatomic highly-correlated wire system[1] NADER ZAKI, RICHARD M. OSGOOD, ANDREW J. MILLIS, CHRIS A. MARIANETTI, Columbia University — The ab-initio method, density functional theory (DFT), has been immensely successful in its ability to predict physical properties of condensed matter systems. In particular, DFT calculations have proven to be quantitatively accurate in predicting structural properties in a wide range of materials and qualitative failures are rare. Here, however, we show that DFT can fail qualitatively to correctly predict the dimerized structural phase for a recently reported experimentally realized monatomic Co wire system that is self-assembled on a vicinal, i.e. stepped, Cu(111) substrate [1]. We attribute this failure to DFT's over-prediction of hybridization of the Co wire with the underlying Cu substrate. We demonstrate that this over-hybridization leads to weakening of the magnetic coupling along the wire, which is responsible for dimerization, while increasing the stiffness of the wire due to strengthening of the non-magnetic elastic term. Additionally, we show that accounting for local interactions via DFT+U also fails at predicting the correct structural phase. [1] N. Zaki et al, arXiv:1208.0612 (2012)

[1]Department of Energy Contract No. DE-FG 02-04-ER-46157

Nader Zaki
Columbia University

Date submitted: 08 Nov 2012 Electronic form version 1.4