Abstract Submitted
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An experimentally realized 1-D correlated system for which DFT, DFT+U, and DFT+DMFT fall short[1] NADER ZAKI, HYOWON PARK, RICHARD OSGOOD, ANDREW MILLIS, CHRIS MARIANETTI, Columbia University — Density functional theory (DFT) has been immensely successful in its ability to predict physical properties of condensed matter systems, and it is generally qualitatively correct when predicting structural properties. Here, however, we show that DFT qualitatively fails to predict the dimerized structural phase for a monatomic Co wire system that is self-assembled on a vicinal, i.e. stepped, Cu(111) substrate [1]. To elucidate the nature of this failure, we compute the energetics of a Co chain on a Cu surface, step, notch, and embedded in bulk, which demonstrates that increasing coordination and hybridization extinguishes the dimerization. We attribute the failure of DFT for Co on the Cu step to excessive hybridization, which both weakens the ferromagnetic correlations that drive the dimerization and increases the bonding that opposes dimerization. Additionally, we show that accounting for local interactions via DFT+U or DFT+DMFT also fails at predicting the correct structural phase for the step-substrate supported wire, though the Co wire does dimerize in DFT+DMFT for the isolated vacuum case. [1] N. Zaki, et al, Phys. Rev. B **87**, 161406 (2013)

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