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DFT and STM studies of magnetism in single Co(TCNE) complexes on an ultrathin insulating film[1] M. BADAL, T. CHOI, D. STROUD, J.A. GUPTA, Ohio State U. — We present results from large-scale ab initio DFT calculations for geometry and electronic structure of Co(TCNE) complexes on a $c(2 \times 2)Cu_2N$ substrate. The long-term aim is to study charge and spin transport in molecular systems. The work is done in concert with STM experiments. In particular, we perform calculations to help explain STM observations indicating that the electronic and magnetic properties of Co(TCNE) complexes vary with apparent molecular orientation. Using plane wave DFT with a GGA functional and spin polarization, we perform geometry optimization to identify the most commonly seen orientations of Co(TCNE). We further study the resulting electronic structure, using calculated LDOS and simulated STM images, to compare with observations. To study the strong in-plane magnetic anisotropy suggestd by spin-flip spectroscopy, we do noncollinear magnetic calculations on the relaxed structure, including spin-orbit coupling effects.

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