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Ab initio studies of non-collinear magnetic ordering of Cr dimers on Mo(110) YANG WANG, Pittsburgh Supercomputing Center, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — Small clusters may display innovative properties in ultra small scales, and are very promising for applications in the future. Cr has anti-ferromagnetic ordering in its bulk, described by a spin density wave with a wavelength incommensurate with the lattice constant. In thin films, Cr films are anti-ferromagnetic on most substrates. Here we study magnetic ordering, magnetic anisotropy and spin dynamics of a Cr dimer on Mo (110), smallest possible magnetic recording unit. The locally self-consistent multiple scattering (LSMS) method for spin-dynamics and the full potential linearized augmented plane wave (FLAPW) method for magnetic anisotropy are adopted in the calculations. We found various peculiar features in the free and supported Cr dimers and explained our results from electronic structures.

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