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Exchange interaction and bonding in CuO from first-principles ALESSIO FILIPPETTI, VINCENZO FIORENTINI, INFM-SLACS and University of Cagliari, Italy — The understanding of the chemistry of Cu-O interactions is an oustanding open issue in solid state physics in view of its relevance for high-T_c superconductors, whose basic units are Cu-O chains or layers. Despite the clear experimental evidence that Cu-Cu spin coupling is strongly antiferromagnetic in the insulating parent compounds and in the doped superconducting phase, a consistent and realistic picture of bonding and magnetic ordering in real Cu-O compounds is still missing. Here we apply a self-interaction-free density-functional approach to investigate the complex interplay of bonding and magnetism in CuO. The puzzling apparently one-dimensional is explained by the presence of a single, spin-polarized d_x^2 character, which induces an antifferromagnetic ordering built up by ferromagnetic planar chains compensating, with period 2, along the z axis. Despite the apparent one-dimensionality, the analysis of the exchange interactions reveals as many as 5 relevant parameters and shows that only a fully three-dimensional view provides a detailed understanding of magnetic ordering and low-energy excitations.

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