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Electronic states and magnetic structure at the Co_3O_4 (110) surface: a first principles study JIA CHEN, ANNABELLA SELLONI, Princeton University — Tricobalt tetraoxide (Co_3O_4) is an important catalyst and Co_3O_4(110) is a frequently exposed surface in Co_3O_4 nanomaterials. We employed Density-functional theory with on-site Coulomb repulsion U term to study the atomic structures, energetics, magnetic and electronic properties of the two possible terminations, A and B, of this surface. These calculations predict A as the stable termination in a wide range of oxygen chemical potentials, consistent with recent experimental observations. The Co^{3+} ions do not have a magnetic moment in the bulk, but become magnetic at the surface, which leads to surface magnetic orderings different from the one in the bulk. Surface electronic states are present in the lower half of the bulk band gap and cause partial metallization of both surface terminations. These states are responsible for the charge compensation mechanism stabilizing both polar terminations. Furthermore, our calculations predict that the critical thickness for polarity compensation is 4 layers.

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