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Atomic structure of the polar $Fe_2O_3(0001)/MgO(111)$ interface¹ K. PANDE, M. GAJDARDZISKA-JOSIFOVSKA, M. WEINERT, U. Wisconsin-Milwaukee — We present a first-principles investigation of the stability and structural properties of layer-by-layer growth of thin films of $Fe_2O_3(0001)$ (hematite) on polar MgO(111). The interface is "oxide-like", atomically abrupt, and stabilized by significant structural relaxations. The electronic and magnetic properties are found to vary as a function of hematite film thickness. In contrast to the insulating and antiferromagnetic nature of bulk hematite, the heterointerface is half-metallic and ferromagnetic. Drastic structural rearrangements of the Fe_2O_3 overlayer are observed at a critical thickness of three Fe bilayers, resulting in an effective expulsion of oxygen from the hematite film. To clarify the effect of the MgO(111) substrate polarity on the nature and growth of the Fe_2O_3 films, comparisons will be made to unsupported hematite slabs and to $Fe_2O_3/Ti(0001)$ interfaces.

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