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Atomic and electronic structure of $\text{Fe}_2\text{O}_3(0001)$ films on polar and non-polar substrates K. PANDE, M. GAJDARDZISKA-JOSIFOVSKA, M. WEINERT, U. Wisconsin - Milwaukee — To address the role of polarity on the growth and stability of heterointerfaces, we present a first-principles study of the structural, electronic, and magnetic properties of the layer-by-layer growth of $\text{Fe}_2\text{O}_3(0001)$ thin films on polar $\text{MgO}(111)$ and metallic $\text{Ti}(0001)$ substrates. The films show thickness-dependent properties, including metallic interface states even at the polar “oxide-like” interface between Fe_2O_3 and MgO . Drastic structural relaxations are, especially at thicknesses of three Fe-bilayers on both the polar and metallic substrates. The stability of the Fe and O surface terminations as a function of the chemical potential will also be discussed.

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