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Atomic and Electronic structure of Fe_2O_3 films on MgO(111) K. PANDE, University of Wisconsin-Milwaukee, A. CELIK-AKTAS, M. GAJDARDZISKA-JOSIFOVSKA, M. WEINERT — Polar oxide surfaces have interesting properties due to the strong ionic character of the metal-oxygen bonds and the layering of metal and oxygen planes parallel to the surface. In this first-principles study we investigate the effect of MgO(111) surface polarity on the structure of iron oxide films. The calculated energetics of different surface terminations on the unreconstructed MgO(111) surface suggest that the interface has a Mg-O-Fe stacking with no intermixing of O and Fe atoms at the interface. The magnetic ordering of Fe atoms both within the layers and between neighboring (bi)layers will be described. The calculated structural and electronic properties will be compared to the results of high-resolution transmission electron microscopy (HRTEM) and selective area diffraction (SAD) experiments of Fe_2O_3 films on MgO(111) surface.

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