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First-principles calculations of water-based surfactant-assisted growth of polar CaO(111) oxide film XIN TAN, PETER ZAPOL, Materials Science Division, Argonne National Laboratory, USA — Despite many attempts to grow rocksalt (111) oxide surfaces, the growth of an atomically flat polar oxide film with an arbitrary thickness still remains challenging because of surface roughening during the growth process, such as faceting into neutral {100} surface planes. This seemingly unavoidable behavior leads to a grainy morphology and diminished functionality. Here, we present a first-principles investigation of the surfactant-assisted growth of polar CaO(111) film in the presence of a water-based surfactant, both from thermodynamic and kinetic points of view. We show that water molecules not only supply a surfactant by depositing hydrogen on the surface throughout the growth process, but also supply oxygen atoms as an elemental constituent in the film growth, i.e. water oxygen atoms are easily inserted into the top surface layer of the growing film. We suggest that adding water surfactants to conventional synthesis techniques leads to the continuous presence of hydrogen atoms in the surface region during the growth process, which efficiently quenches polarity and dynamically stabilizes the growth of the polar surface, and thus facilitates the growth of defect-free CaO(111) films with arbitrary thickness.

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