First principles investigation of surface dynamics involving OH on thin-film $BaTiO_3$ surfaces

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Abstract

Several experimental and theoretical evidences concerning ultra-thin ferroelectric materials have closely tied polarization state and surface morphology. OH, a chemical species believed to be ubiquitous on surfaces of oxides, has been proven to help stabilize polarization in thin-film $BaTiO_3$ (BTO). In this study, ab-initio calculations for surface processes concerning OH will be used to attempt to explain depolarization kinetics observed for poled ultra-thin BTO. DFT calculations, done in concert with nudged elastic band method, revealed that the depolarization in the domain of ultrathin thickness can be closely associated to the effective diffusion of OH on the surface, at temperatures where finite decay time is observed. The study was able to achieve a potential explanation for the relatively slow depolarization rate and as a consequence, further strengthened the hypothesis that the polarization of these materials are induced by surface adsorbates.