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Theoretical study on the diffusion of hydroxyl radical on BaO terminated $BaTiO_3$ (001) surface[1] JOHN MARK MARTIREZ, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, WISSAM AL-SAIDI, Department of Chemical and Petroleum Engineering , University of Pittsburgh, Pittsburgh, PA 15261, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323 — In this study, the role of surface adsorbed hydroxyl radical (OH) in stabilizing ferroelectricity in $BaTiO_3$ thin films was investigated using first-principles density functional theory (DFT). The stable adsorption sites for OH adsorption and the low-energy pathways for OH diffusion were explored. Thin film $BaTiO_3$ was simulated using a five-layer supercell slab model and the plane-wave pseudopotential DFT method. The diffusion pathways were identified using the nudged elastic band (NEB) method. Diffusion barriers and pathways were calculated for different OH coverages and polarization directions, elucidating the relationship between OH diffusion and depolarization of nanoscale ferroelectric materials.

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