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Hydration phase diagram for BaO terminated BaTiO₃¹ JOHN MARK MARTIREZ, Department of Chemistry, University of Pennsylvania, WISSAM AL-SAIDI, Department of Chemical and Petroleum Engineering, University of Pittsburgh, ANDREW RAPPE, Department of Chemistry, University of Pennsylvania — This study reveals geometries H₂O adopts upon adsorption on BaO terminated BaTiO₃(BTO) at low to high saturation. A hydration phase diagram for the aforementioned termination is presented, for moderate temperatures, and moderate to ultra high vacuum H₂O pressures. Calculations suggest a very stable H₂O adsorption for wide range of pressures, including high vacuum conditions (p_{H_2O} 10⁻¹² bar). This opens venues for mechanistic studies and hopefully will serve as a guide to condition that might suppress H₂O adsorption on BTO for applications where it is undesired.

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