Hydration phase diagram for BaO terminated BaTiO₃.¹ JOHN
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sylvania — 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 (pH₂O
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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