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Interaction of water with Barium Titanate thin films and nanoparticles: Oxygen-deficient defects and hydrogen decorated surfaces

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To understand effects of processing and surface chemistry on nanodielectric material properties, we study interaction of molecular species used in synthesis, functionalization, and suspension of BaTiO3 particles in solution. We investigate interaction of water with BaTiO3 using density functional theory (DFT) applied to slab configurations. Slabs meant to represent the environment of a nanoparticle surface are constructed of sufficient size to approach convergence for defect and surface-reacted molecules while remaining computationally tractable. We investigate the dissociation/formation of H2O on stoichiometric and O-deficient surfaces, including successive placement of hydrogen to form H-decorated surfaces.

H2O adsorption, H-decoration, and Oxygen vacancies all lead to significant relaxation and notable polarization effects in the surrounding material. We pay particular attention to the oxygen vacancy, as it can significantly alter the electrical properties of the material, and is an expected defect when processing or functionalizing under acidic conditions. Given ligands used to functionalize particles are often acidic, a thorough understanding of this defect is important. Oxygen deficiency can cause particles to have a reduced band gap, or to become metallic. Macroscopic materials made with these particles will show effects such as changes in overall conductivity, breakdown, and dielectric properties. The oxygen vacancy is significantly lower energy a few layers into the slab than at the surface, likely due screening on a charged defect. We discuss this result and the required level of theory for accurate description of formation and selected properties of the oxygen vacancy.

DFT-derived results and interpretation are compared with concurrent experiments using solvated BaTiO3 nanoparticles.
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