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Experimental and Theoretical Characterization of Functionalized Barium Titanate Nanoparticles

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To further the goal of optimized material design for pulsed power components, we aim to achieve a fundamental understanding of the model nonlinear dielectric material BaTiO3, through concurrent experimental and theoretical study. This effort is intended to lead to improved synthesis and design control, and a validated model to enable material predictions. The ultimate goal is to improve energy storage and discharge characteristics through design models for dielectric materials that translate results from the molecular level to macroscopic device level.

We examined the bonding and arrangement of selected ligands and molecules adsorbed on BaTiO3 surfaces using both density functional theory (DFT) and experimental techniques. Bond strengths and reaction mechanisms were examined in detail. Initial DFT results showed that the energy involved in the polarization response in a ferroelectric BaTiO3 slab is similar to or greater than the local adsorption or reaction energy of the molecule with the top layer of the slab. Several approaches are applied for systematically distinguishing these effects and extracting molecular desorption barriers, including thermogravimetric analysis (TGA) and Fourier-transform infrared spectroscopy (FTIR) experiments.

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