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Atomistic Study of Polarization response in 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.
In order to achieve this goal, it is first necessary to understand the atomistic level polarization response of ferroelectric BaTiO3 to the presence of surface ligands used in the material synthesis process. This response is of sufficient magnitude to obscure the energetics of surface and defect chemistry, and is highly sensitive to simulation boundary conditions. In this work, we apply density functional theory to explore the effects of different choices of surface termination and initial starting conditions on the polarization response of the material to the presence of adsorbed molecules and point defects. The examined choices include constrained optimization techniques, preconditioned ferroelectric phases, surface mirroring, and inclusion of compensating electrode layers. The advantages and shortcomings of each option are discussed both in the current context and in relation to previous literature results. Where possible, we place results in the context of our ongoing concurrent experiments.

Authors: Ms DYER, Jessica (Sandia Lational Labs); Dr MONSON, Todd (Sandia National Laboratories); Dr STEVENS, Tyler (Sandia National Laboratories); VAN GINHOVEN, Renee (AFRL)

Presenter: VAN GINHOVEN, Renee (AFRL)

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