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Combined Experimental and Theoretical Study of Barium Titanate Nanoparticles: Improving Fundamental Understanding of Pulsed Power Component Materials

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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 non linear 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 difficult to obtain in controlled experiments. The ultimate goal is to improve packing factor and discharge characteristics through design models for capacitors that translate results from the molecular level to macroscopic device level, and incorporate virtual material design models where appropriate.

BaTiO3 particles were created using an alkoxide-hydroxide synthesis in water-ethanol solution. Subsets of the particles were functionalized with octadecylphosphonic acid (ODPA) through addition of ODPA to the suspension. The functionalized particles are characterized with several methods. The species bound to the particles are identified using FT-IR spectroscopy. We also expect to gain insight into ligand-nanoparticle surface interactions using FT-IR. Thermogravimetric analysis (TGA) is used to determine the ligand load in a particular sample and back out particle surface coverage.

In addition, the bonding and arrangement of selected ligands and molecules adsorbed on the surfaces BaTiO3 nanoparticles and thin films is examined theoretically, using density functional theory (DFT). Bond strengths and reaction mechanisms are examined in detail. These results are compared to and combined with experimental data to derive insight into surface characteristics of this material.

Finally, the challenges inherent in characterization and simulation of a reacted composite bulk material are discussed.

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