Title: Experimental and DFT studies on energy storage efficiency of Ag^+ doped barium titanate thin films ($Ba_{1-x}Ag_xTiO_3$ (x = 0.00, 0.10, 0.20))

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Abstract: The current study investigated the energy storage capacity of Ag^+ doped two-dimensional (2D) barium titanate perovskite, using combinations of experimental theoretical techniques. Data from electrochemical impedance spectra and DFT geometrical optimization revealed the existence of +1 valency state by Ag ions. With the obtained parameters, highest efficiency was attributed to 0.10 mol% Ag doped 2D $BaTiO_3$ variant, due to reduced defect and suppressed ferroelectric order. Notably, the piezoelectric response showed slight decreasing trend with Ag^+ content, reaching the lower value of 223 pC/N with 0.20 mol% Ag. Reduction in the values of T_c due to Ag^+ ions indicates reduced polarization and high dielectric permittivity. In all samples used, good relationship existed between recoverable-energy storage and efficiency, owing to remanent polarization, hysteresis loss and dielectric breakdown. Moderate doping improved breakdown strength, leading to reduced P_r which increases Wrec values with relatively 1.12 Jcm^{-3}. The conducted experimental and DFT analysis revealed good alignment between some considered structural and energy storage parameters, such as lattice constants, piezoelectricity, and curie temperature.

Keywords: Barium titanate; Energy storage; Hysteresis; Perovskites; Dielectrics

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