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Microscopic Origin of Polarization Switching in Zr-Doped HfO2: Real-Space Charge Redistribution and Berry-Phase Branch Analysis

Ferroelectric Hafnium Oxide (HfO2) is a leading candidate for scalable nonvolatile devices, yet the microscopic origin of polarization switching in isovalently doped HfO2 remains incompletely understood. Here, we investigate Zr-doped HfO2 using first-principles density-functional theory by constructing ±P polarization endpoints and analyzing the real-space charge density ρ(+P), ρ(-P), and their difference Δρ=ρ(+P)-ρ(-P) in the xz-plane (averaged along y) for 3.125%, 6.25%, and 9.375% Zr concentrations. The charge density maps show oxygen-centered electron localization in both polarization states, confirming that the material remains insulating and predominantly ionic across all dopings. The Δρ distributions exhibit clear dipolar charge rearrangements around the anion sublattice, indicating that polarization reversal is governed by collective Hf/Zr–O displacement patterns rather than metallic charge transfer. Despite the persistence of a coherent switching-induced charge redistribution, the magnitude and spatial uniformity of Δρ evolve with Zr content, revealing a doping-dependent modulation of the local polar distortion network. In parallel, Berry-phase polarization analysis demonstrates that experimentally relevant switching polarization corresponds to a physically connected branch of the polarization lattice; a consistent branch correction (n=+1) is required to obtain meaningful switched polarization values for the calculated Zr-doped structures.

Academic or Professional Status

Graduate Student

Authors: Dr LIU, Jinjie (Delaware State State University); Mr DÍAZ-APONTE, Kevin (Delaware State State University); MOODY, Malachi (Delaware State State University); Dr RANA, Mukti (Delaware State State University); SULTANA, Nurunnesa (Delaware State State University); Dr XU, Yanan (Delaware State State University)

Presenter: MOODY, Malachi (Delaware State State University)

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