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Domain walls and ferroelectric reversal in corundum derivatives[1]
MENG YE, Institute for Molecular Engineering, University of Chicago, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — Domain walls are the topological defects that mediate polarization reversal in ferroelectrics, and they may exhibit quite different geometric and electronic structures compared to the bulk. Therefore, a detailed atomic-scale understanding of the static and dynamic properties of domain walls is of pressing interest. In this work, we use first-principles methods to study the structures of 180° domain walls, both in their relaxed state and along the ferroelectric reversal pathway, in ferroelectrics belonging to the family of corundum derivatives. Our calculations predict their orientation, formation energy, and migration energy, and also identify important couplings between polarization, magnetization, and chirality at the domain walls. Finally, we point out a strong empirical correlation between the height of the domain-wall mediated polarization reversal barrier and the local bonding environment of the mobile A cations as measured by bond valence sums. Our results thus provide both theoretical and empirical guidance to further search for ferroelectric candidates in materials of the corundum derivative family.

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