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Ferroelectric switching pathways in $\text{Ca}_3\text{Ti}_2\text{O}_7$ from first principles ELIZABETH NOWADNICK, ANDREW MULDER, CRAIG FENNIE, Cornell University — Hybrid improper ferroelectricity, where polarization can be induced via a trilinear coupling to two non-polar order parameters (in this case octahedral rotations), has recently been experimentally demonstrated in the $n=2$ Ruddlesden-Popper compound $\text{Ca}_3\text{Ti}_2\text{O}_7$. The observation of an unexpectedly low ferroelectric switching barrier and abundant structural domains suggests that these domains may be critical to the switching process. Key issues that remain to be understood include what are the specific structural properties of $\text{Ca}_3\text{Ti}_2\text{O}_7$ that enable this low-energy switching, and how these properties could be further optimized. To address these questions, we analyze the possible ferroelectric switching pathways that can be facilitated by the presence of orthorhombic twin domains and vertical stacking faults in the $n=2$ Ruddlesden-Popper structure of $\text{Ca}_3\text{Ti}_2\text{O}_7$. Utilizing first principles methods, we calculate the energy barriers of the various switching pathways and study the evolution of the octahedral rotation and polar order parameters during these switching processes. These results offer insight into what is the likely switching mechanism in $\text{Ca}_3\text{Ti}_2\text{O}_7$, and which order parameter is primarily responsible for controlling the energy barriers.

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