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Role of cooperative structural distortions in the metal–insulator transitions of perovskite ferrates[1] ANTONIO CAMMARATA, JAMES RONDINELLI, Drexel University — Transition-metal oxides within the perovskite crystal family exhibit strong electron–electron correlation effects that coexist with complex structural distortions, leading to metal-insulator (MI) transitions. Using first-principles density functional calculations, we investigate the effects of cooperative octahedral rotations and dilations/contractions on the charge-ordering MI-transition in $CaFeO_3$. By calculating the evolution in the lattice phonons, which describe the different octahedral distortions present in the low-symmetry monoclinic phase of $CaFeO_3$ with increasing electron correlation, we show that the MI-transition results from a complex interplay between these modes and correlation effects. We combine this study with group theoretical tools to disentangle the electron–lattice interactions by computing the evolution in the low-energy electronic band structure with the lattice phonons, demonstrating the MI-transition in $CaFeO_3$ proceeds through a symmetry-lowering transition driven by a cooperative three-dimensional octahedral dilation/contraction pattern. Finally, we suggest a possible route by which to control the charge ordering by fine-tuning the electron–lattice coupling.

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