

Abstract Submitted  
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**Role of covalency in “Charge Ordering” perovskite ferrates<sup>1</sup>** ANTONIO CAMMARATA, JAMES RONDINELLI, Drexel University — Transition-metal oxides (TMO) with the perovskite crystal structure exhibit strong electron–electron correlation effects and complex structural distortions. The balance of those factors determines the stability of charge ordered states in chemistries susceptible to valence instabilities. We use first-principles density functional calculations to investigate the role of symmetry-unique structural distortions on covalent bonding in the “charge-ordered” insulator  $\text{CaFeO}_3$ . We evaluate the electronic density distribution along the Fe–O bonds to assess the ground state stability by tracing the evolution in the oxygen environment, which appears as octahedral expansion/contractions and rotations. We show that nearly zero charge transfer occurs; the insulating phase results from a complex interplay of symmetry-lowering structural distortions and enhanced covalent interactions. Finally, we discuss possible routes to control the metal–insulator transition by fine-tuning the covalency.

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