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Orbital ordering in striped phases of $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$: GGA+U versus GGA results NADIA BINGGELI, ICTP and INFN-CNR DEMOCRITOS National Simulation Center, Trieste, Italy, GIANCARLO TRIMARCHI, National Renewable Energy Laboratory — We have investigated the orbital ordering in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$, with $x=2/3$ and $1/2$, within the generalized gradient approximation (GGA) of density functional theory and within the GGA plus onsite Coulomb interaction (GGA+U) approach. The calculations were performed using the pseudopotential plane-waves scheme and include structural relaxation. In the half-doped case, similar results are obtained for the orbital and atomic structure within the two approaches, with structural properties consistent with experiment. For the two-third-doped system, instead, the results differ between the two approaches. Only the GGA+U yields an insulating striped phase with structural properties in agreement with experiment. Our results show the importance of the cooperative effects of the Jahn-Teller distortion, strain modulation, and electronic localization in stabilizing the orbital-ordered striped phases, and provide new insight into the atomic-scale structure of the orbital order in $\text{La}_{1/3}\text{Ca}_{2/3}\text{MnO}_3$.

Nadia Binggeli
ICTP and INFN-CNR DEMOCRITOS

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