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**A Combined Density Functional Theory and Monte Carlo Study of Manganites for Magnetic Refrigeration** ROMI KOROTANA, GIUSEPPE MALLIA, ZSOLT GERCSI, NICHOLAS HARRISON, Imperial College London — Perovskite oxides are considered to be strong candidates for applications in magnetic refrigeration technology, due to their remarkable properties, in addition to low processing costs. Manganites with the general formula $R_{1-x}A_xMnO_3$, particularly for A=Ca and $0.2 < x < 0.5$, undergo a field driven transition from a paramagnetic to ferromagnetic state, which is accompanied by changes in the lattice and electronic structure. Therefore, one may anticipate a large entropy change across the phase transition due to the first order nature. The present work aims to achieve an understanding of the relevant structural, magnetic, and electronic entropy contributions in the doped compound $La_{0.75}Ca_{0.25}MnO_3$. A combination of thermodynamics and first principles theory is applied to determine individual contributions to the total entropy change of the system. Hybrid-exchange density functional (B3LYP) calculations for $La_{0.75}Ca_{0.25}MnO_3$ predict an anti-Jahn-Teller polaron in the localised hole state, which is influenced by long-range cooperative Jahn-Teller distortions. Through the analysis of individual entropy contributions, it is identified that the electronic and vibrational terms have a deleterious effect on the total entropy change.

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