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Influence of oxygen defects and lattice distortions on the energy gap formation and magnetic properties of multi-ferroic materials JIJI PULIKKOTIL, VLADIMIR ANTROPOV, Ames Laboratory — Full potential density functional calculations are performed to study the effects of O-vacancies on the structural parameters and electronic properties of $RMnO_{3-\delta}$, (R=Y, rare-earths). We find that vacancies at the 2a-position of the hexagonal unit cell can introduce a small gap of magnitude 0.2eV. Although significantly lower than the experimentally observed value of 2.5eV, we claim that already such defects, which in general are inevitable in oxides, can introduce the energy gap in addition to the most commonly accepted Coulomb correlation mechanism. Besides, the off-plane O-vacancies modify the magnetic properties of the system and induce small magnetic polarization on the in-plane O-sites and at the interstitials. The electronic structure and magnetic properties modifications as a function of several lattice distortions have been analyzed. We also discuss the mechanisms of the exchange coupling and its most effective path. In addition we compare previously known results of the electronic structure calculations for these systems.

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