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Ferroelectricity driven by zig-zag magnetic chains: orthorhombic HoMnO3 as a multiferroic? SILVIA PICOZZI, KUNIHIKO YAMAUCHI, CNR-INFM CASTI L'Aquila, Italy, BIPLAB SANYAL, Uppsala Univ., Uppsala, Sweden — The search for multiferroic materials showing a coexistence of magnetic and ferroelectric long-range order has recently triggered enormous interests due to their potential use in magnetic recording industry. Based on first-principles density functional calculations including electron-electron correlations explicitly in the framework of Hubbard model, we show that a peculiar arrangement of Mn spins can induce a sizeable ferroelectric polarization in distorted rare-earth manganites. In particular, our calculated ground state magnetic structure of orthorhombic HoMnO3 is AFM-E type in which the zig-zag ferromagnetic chains in the MnO2 planes are antiferromagnetically coupled to their neighboring chains. This unconventional magnetic configuration and the different values of the Mn-O-Mn bond angle for parallel and antiparallel Mn spins lead to a coherent displacement of the O center of mass with respect to the Mn center of mass giving rise to a permanent dipole i.e. ferroelectricity. A quantitative analysis of the ferroelectric polarization, as well as trends in the structural, magnetic and ferroelectric properties as a function of the strength of Coulomb correlation parameter will be presented.

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