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Ferroelectricity and magnetism in the hexagonal manganite $YMnO_3$ from first principles CRAIG FENNIE, KARIN RABE, Rutgers University — The hexagonal manganites are a class of multiferroic materials that are simultaneously ferroelectric and antiferromagnetic. Here, we describe a first-principles study of the structural energetics and polarization in magnetic $YMnO_3$, with the LSDA+U as implemented in VASP. For selected collinear magnetically ordered structures, the lowest symmetry-allowed terms in the Taylor expansion of the energy as a function of zone-center and zone-boundary distortions are identified and computed. The implications for the phase transitions in $YMnO_3$ will be discussed.

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