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Structure and properties of $CaMnO_3/SrMnO_3/BaMnO_3$ superlattices from first principles SHEN LI, SEONGSHIK OH, KARIN RABE, Department of Physics and Astronomy, Rutgers the State University of New Jersey, Piscataway, NJ 08854, USA — Previous theoretical and experimental studies have shown that three-component, or "tri-color" superlattices can exhibit intrinsic electric polarization due to inversion-symmetry breaking in the layer sequence. In ferromagnetic inversion-symmetry-breaking superlattices, controlled symmetry lowering is similarly expected to lead to interesting new and tunable properties. Here, we present results of first-principles density-functional-theory calculations for short-period $CaMnO_3/SrMnO_3/BaMnO_3$ superlattices, using VASP. The ground state structure, magnetic ordering, polarization and dielectric response will be presented. The role of epitaxial strain in the individual layers and the role of layer sequence will be explored. Connections to experimental studies and prospects for future work will be discussed.

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