

Abstract Submitted
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Trends in $(\text{LaMnO}_3)_n/(\text{SrTiO}_3)_m$ superlattices with varying layer thicknesses¹ JILILI JIWUER, FABRIZIO COSSU, UDO SCHWINGENSCHLÖGL, KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia — We investigate the thickness dependence of the structural, electronic, and magnetic properties of $(\text{LaMnO}_3)_n/(\text{SrTiO}_3)_m$ ($n, m = 2, 4, 6, 8$) superlattices using density functional theory. The structure relaxation turns out to be highly sensitive to the onsite Coulomb interaction. In contrast to bulk SrTiO_3 , strongly distorted O octahedra are observed in the SrTiO_3 layers with a systematic off centering of the Ti atoms. The systems favour ferromagnetic spin ordering rather than the antiferromagnetic spin ordering of bulk LaMnO_3 and all show half-metallicity, while a systematic reduction of the minority spin band gaps as a function of the LaMnO_3 and SrTiO_3 layer thicknesses originates from modifications of the Ti d_{xy} states.

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