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Polar catastrophe, electron leakage, and magnetic ordering at the LaMnO₃/SrMnO₃ interface¹ BIRABAR NANDA, SASHI SATPATHY, University of Missouri-Columbia — Issues such as polar catastrophe, two-dimensional electron gas, etc., which are well studied for the prototypical LaAlO₃/SrTiO₃ interface also arise at the (100) interface between LaMnO₃ (LMO) and SrMnO₃ (SMO). We have studied the nature of electronic reconstruction and its effect on the polar discontinuity and magnetic ordering for the latter interface from density-functional calculations and model studies. We show that the polar catastrophe, originating from the charged LMO layers, is avoided by the accumulation of extra 0.5 electrons at the interface just like the LaAlO₃/SrTiO₃ interface. In addition, the Mn e_a electrons leak out from the LMO side to the SMO side, the extent of the leakage being controlled by the interfacial potential barrier and the substrate induced epitaxial strain. The leaked electrons mediate a ferromagnetic Zener double exchange, making the interfacial layers ferromagnetic, while the two bulks retain their original type A or G antiferromagnetic structures. The interfacial electrons form a half-metallic conduction band, while both bulks remain insulating, resulting in an interesting interface system.

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