

Abstract Submitted
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Polarcatrosphy and electronic reconstructions in LaAlO₃/SrMnO₃ (111) digital heterostructures¹ FANG HOU, Department of Mathematics and Physics, Suzhou University of Science and Technology, Suzhou, PR China, SHENG JU, TIAN-YI CAI, Department of Physics, Soochow University, Suzhou, PR China — Based on extensive first-principle density functional theory calculations, we report different electronic phases at the LaAlO₃/SrMnO₃ (111) heterointerfaces. In the *n*-type LaAlO₃/SrMnO₃ (111) superlattices, electrons transferred from LaAlO₃ component distribute unevenly in SrMnO₃ component and occupy Mn's e_g orbital, inducing half-metallic ferromagnetism in the framework of Zener double exchange. With increasing SrMnO₃ layers, the sum of every Mn magmon keep a constant suggesting a fixed number of charge transferred from LaAlO₃ component. For *p*-type superlattices, holes reside almost uniformly at the SrO₃ and LaO₃ plane driven by the polar electric field in the LaAlO₃ and SrMnO₃ component. With absence of the e_g states at the Mn sites, bulk-like G-type AFM ordering were obvious with almost imperceptible octahedron rotation and tilting. But *p*-type superlattices are metallic because of hole transfer. Our studies demonstrate the potential applications of perovskite heterointerfaces in spintronic devices.

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