Polarcatrosphysy and electronic reconstructions in LaAlO$_3$/SrMnO$_3$ (111) digital heterostructures$^1$ 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 LaAlO$_3$/SrMnO$_3$ (111) heterointerfaces. In the $n$-type LaAlO$_3$/SrMnO$_3$ (111) superlattices, electrons transferred from LaAlO$_3$ component distribute unevenly in SrMnO$_3$ component and occupy Mn’s $e_g$ orbital, inducing half-metallic ferromagnetism in the framework of Zener double exchange. With increasing SrMnO$_3$ layers, the sum of every Mn magnon keep a constant suggesting a fixed number of charge transferred from LaAlO$_3$ component. For $p$-type superlattices, holes reside almost uniformly at the SrO$_3$ and LaO$_3$ plane driven by the polar electric field in the LaAlO$_3$ and SrMnO$_3$ 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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