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Electrostatic doping in oxide heterostructures JAEKWANG LEE, ALEXANDER A. DEMKOV, Department of Physics, The University of Texas at Austin — Recent experiments on perovskite heterostructures grown by molecular beam epitaxy or pulsed laser deposition suggest the possibility of creating high mobility two dimensional electron gas at the oxide/oxide interface. However, the origin of charge in these insulating materials is still not clear and deemed controversial. We report a first-principles study of SrTiO₃/LaAlO₃ heterostructures using density functional theory at the LDA+U level. We consider the energetics and electronic structure of the junction, while focusing on the role of electrostatics. Our results suggest that a complex balance of the crystal field, Jahn-Teller effect, lattice dynamics and internal electric field result in the robust electrostatic doping for carefully chosen thickness of the polar oxide. We explore the possible uses of this effect in other oxide-based heterostructures.

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