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Electrostatic doping in oxide heterostructures.[1] ALEXANDER A. DEMKOV, JAEKWANG LEE, NA SAI, The University of Texas — Recent experiments on perovskite heterostructures grown by methods ranging from molecular beam epitaxy to pulsed laser deposition suggest the existence of two dimensional electron gas of high mobility at the oxide/oxide interface, and even a possibility of a superconducting state. Both p-type and n-type interfaces have been reported. However, the origin of charge in these insulating materials is still under debate. We report a first-principles study of several heterostructures where we employ the internal filed in a polar oxide $LaAlO_3$ to demonstrate the possibility of the electrostatic doping, an effect similar to a well known polar catastrophe in e.g., III-V semiconductors. We use density functional theory at the LDA+U level. We mainly focus on the electronic structure of the oxide/oxide junctions. The results of our calculations suggest that once the critical thickness of the aluminate layer is reached the internal electric field is sufficient to produce the electrostatic doping. We will discuss simple estimates for the temperature of the superconducting transition and the role of oxygen-related defects such as vacancies in the electronic structure and thermodynamic stability of these fascinating oxide structures.

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