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Chasing a polar catastrophe: *ab-initio* theory of the $LaAlO_3/SrTiO_3$ interface JAEKWANG LEE, A.A. DEMKOV, Department of Physics, UT Ausitn — A polar discontinuity at the abrupt oxide/oxide interface is one of several problems that need to be addressed before we can realize the promise of multiferroic oxide structures. To avoid the so-called polar catastrophe the interface undergrows roughening which renders the structure useless, unless the system finds a mechanism for compensating the interface charges. Recent experiments of Hwang and co-workers (*Nature* **427**, 423-426 (2004) and *Nature* **430**, 657-661 (2004)) suggest that in the case of perovskite oxides two quite different compensatory mechanisms are at play at the heterojunction. For the n-type $LaAlO_3/SrTiO_3$ interface it is purely electronic involving mixed valence Ti ions, while for the p-type it is an actual ionic reconstruction involving oxygen vacancies. We report a first-principles study of both interfaces within density functional theory. We consider the energetics and electronic structure of the interface, including the role of oxygen vacancies and band offsets. In addition we consider the interface stability with respect to inter diffusion of La and Sr across the interface.

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