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Coulomb Catastrophe and the Origin of the Sheet Carrier Density at the n-type LaAlO₃/SrTiO₃ interface: What do band calculations tell us?¹ ZORAN POPOVIC, Institute for Nuclear Sciences, Belgrade, SASHI SATPATHY, University of Missouri, Columbia, RICHARD MARTIN, University of Illinois, Urbana — Transport measurements of the two-dimensional electron gas (2DEG) at the intrinsic n-type LaAlO₃/SrTiO₃ interface have found a density of carriers much lower than expected from the "Coulomb catastrophe" arguments. From a detail density-functional study, we suggest how this discrepancy may be reconciled. We find that electrons occupy multiple subbands at the interface leading to a rich array of transport properties. Some electrons are confined to a single interfacial layer and susceptible to localization, while others with small masses and extended over several layers are expected to contribute to transport.

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