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2D charge confinement in oxide heterostructures: fundaments from First-Principles ALESSIO FILIPPETTI, CNR-IOM UOS Cagliari, c/o Physics Dept. University of Cagliari, Italy — The accurate description of the fundamental properties of complex oxides by First-Principles (FP) is tantamount with the possibility of achieving reliable theoretical design. Here we use the variational pseudo-self-interaction corrected density functional theory (VPSIC) to investigate structural and electronic properties of several exceptionally interesting heterostructures (the STO/LAO interface, the Nb-doped STO superlattice, the SrTiO3/SrZrO3 superlattice, the SrTiO3 surface). The key features which are at the fundament of the 2DEG formation (film polarity, band disalignment, doping, structural and electronic screening, chemistry of 3d orbitals) are described and discussed. Furthermore, we propose a combined VPSIC plus Bloch-Boltzmann approach as reliable and efficient method, applicable to generic doped oxides, to obtain thermoelectric and transport properties in satisfying agreement with the available experimental data. Our theoretical analysis consents to relate the calculated transport properties to the specific features of the band structure at the interface, e.g. on-site and intersite band splitting, which govern the confinement process. This is instrumental to achieve guidelines for the design of interfaces with enhanced transport and thermoelectric functionalities.

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