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First-principles modeling of $Pt/LaAlO_3/SrTiO_3$ nanocapacitors under an external bias potential CLAUDIO CAZORLA, MASSIMILIANO STENGEL, Institute of Materials Science of Barcelona — We study the electronic, structural and electrical properties of $Pt/LaAlO_3/SrTiO_3$ nanocapacitors under the action of an external applied bias, using first-principles calculations performed at fixed electric displacement D. In particular, we deduce a complete set of *ab initio* band diagrams and a simple analytical expression for the electric field within the $LaAlO_3$ (LAO) film as a function of thickness and applied potential. In addition, we investigate the capacitance of the metal-oxide heterostructure in a field-effect transistor setup. We find that the electric field within LAO is a non-intrinsic quantity that monotonically decreases with increasing LAO thickness. The occurrence of spontaneous Zener tunneling in this system, therefore, is ruled out. We discuss the implications of our results in the light of recent experimental observations involving biased LAO/STO junctions and metallic top electrodes.

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