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Oxygen vacancies at the surface of $SrTiO_3$ thin films[1] ALEXANDRE R. SILVA, GUSTAVO M. DALPIAN, Universidade Federal do ABC — The 2-D electron gas at the interface between $LaAlO_3$ (LAO) and $SrTiO_3$ (STO), two band insulators, has been the subject of intense research owing to the fact that this interface can show metallic, superconducting, and magnetic effects, properties that are absent in the bulk counterparts. The metallic behavior has also been observed at the STO surface, without the need of the oxides' interface. Although the reason of this behavior is not well defined, there are three hypotheses for this: the polar catastrophe; the oxygen vacancies produced in the experiment, and cations intermixing. In this work, first principles calculations based on the density functional theory and using hybrid functionals were performed to reveal the atomic and the electronic structure of vacancies at the (001) surface of STO films. We have analyzed both the TiO_2 and SrO-terminated surfaces. For pure surfaces, we observed atomic relaxations up to the 5^{th} atomic layer. The surface band structure of ideal STO slabs shows that the STO thin films are insulating in both terminations, but insert surface levels in the gap of bulk STO. Defective STO slabs are observed to be metallic, and we observe a strong tendency for the oxygen vacancies to migrate into the surface.

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