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Importance of oxygen vacancies for the two-dimensional metallic state at the surface of $SrTiO_3$ JUAN SHEN, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt/Main, 60438 Frankfurt, Germany — We analyze by means of density functional theory (DFT) the electronic structure of various oxygen-deficient $SrTiO_3$ surface slabs. We find a significant surface reconstruction after introducing oxygen vacancies and we show that the charges resulting from surface-localized oxygen vacancies –independently of the oxygen concentration– redistribute in the surface region and deplete rapidly within a few layers from the surface suggesting the formation of a two-dimensional electron system (2DES). We also investigate possible oxygen-vacancy clustering effects and discuss our results in the context of recent angle-resolved photoemission spectroscopy observations of a highly metallic 2DES at the (001) vacuum-cleaved surface of $SrTiO_3$.

Roser Valenti
Institut für Theoretische Physik, Goethe-Universität Frankfurt/Main,
60438 Frankfurt, Germany

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