

Abstract Submitted
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Termination-specific study of oxygen vacancy transition levels on SrTiO₃(001) surfaces by scanning tunneling spectroscopy¹ WATTAKA SITAPUTRA, NIKHIL SIVADAS, MAREK SKOWRONSKI, DI XIAO, RANDALL FEENSTRA, Carnegie Mellon University — We have studied the surface electronic structure of oxygen vacancies on SrTiO₃(001) surfaces using scanning tunneling spectroscopy and DFT calculations with local spin density approximation (LSDA+U). With high dynamic range measurements, a mid-gap level associated with the surface oxygen vacancies was observed for SrO-terminated surfaces. TiO₂-terminated surfaces, on the other hand, did not exhibit observable mid-gap states (this lack of signal is believed to be due to the nature of defect wavefunction involved, as well as possibly involving transport limitations in the STS measurements). Both vacuum-cleaved and MBE-grown surface have been studied. For the former, the Fermi level is pinned near mid-gap owing to disorder-induced surface states. The amount of surface disorder can be controlled in the case of epitaxially grown surfaces. Rougher MBE-grown surfaces were found to exhibit similar spectral characteristics to the cleaved surfaces, while a shift of the Fermi level toward the conduction band was observed for flatter grown surfaces. Notably, with a decreasing number of disorder-induced surface states, the Fermi level is found to be pinned within the observed band of oxygen vacancy levels.

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