Oxygen vacancy driven structural and orbital reconstruction on SrTiO$_3$ surface and subsurface

CHANDRIMA MITRA, CHUNGWEI LIN, ALEXANDER A. DEMKOV, University of Texas at Austin — The role played by oxygen vacancies in bringing about important structural and electronic changes on oxide surfaces and interfaces have been a subject of intense scientific study. From two-dimensional electronic conductivity to the formation of magnetic states, oxygen vacancies have been suggested to be responsible for introducing a variety of interesting physical effects in bulk oxides and their surfaces. In this work, we employ Density Functional theory to perform first principles calculations of oxygen vacancy defects on SrTiO$_3$ surface and subsurface. In a defect free SrTiO$_3$ surface, the surface Ti atoms have conduction bands whose lower end comprises of split $t_{2g}$ states (lower lying degenerate $d_{xz}$ and $d_{yz}$ states and the upper lying $d_{xy}$ state). The upper conduction bands consist of split $e_g$ states where the $d_{z^2}$ orbital is shifted lower in energy with respect to the $d_{x^2-y^2}$ orbital. In the presence of an oxygen vacancy, orbitals reorder and the Ti $d_{z^2}$ orbitals, (which also hybridizes itself with Ti $4s$ state and the neighboring oxygen $p$ states) gets pushed down and occupied leading to the formation of a defect state. Formation energies of oxygen vacancies on the surface and subsurface of SrTiO$_3$ will be presented and the possibility of vacancy induced magnetic states on SrTiO$_3$ surface will be discussed.

Chandrima Mitra
University of Texas at Austin

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