Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Theoretical investigation of oxygen vacancy clustering at $SrTiO_3$ surfaces JUAN SHEN, ROSER VALENTI, HARALD JESCHKE, Goethe Universitaet Frankfurt — Oxygen vacancies have been found, both in experiment and in theory, to create a twodimensional electron gas at $SrTiO_3$ surfaces. We use density functional theory to search for the most stable structural arrangements of multiple oxygen defects. We find that there is a tendency of oxygen defects to cluster. While individual oxygen defects occupy Ti t_{2g} orbitals and contribute to a metallic state, additional defects closeby form localized states in the former $SrTiO_3$ bulk gap. We discuss the relevance of these findings for photoemission experiments.

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Date submitted: 15 Nov 2013 Electronic form version 1.4