Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Spin polarized electronic states and spin textures at the surface of oxygen-deficient $SrTiO_3$[1] HARALD O. JESCHKE, MICHAELA ALTMEYER, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany, MARCELO ROZENBERG, MARC GABAY, Laboratoire de Physique des Solides, Université Paris-Sud, France, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany — We investigate the electronic structure and spin texture at the (001) surface of $SrTiO_3$ in the presence of oxygen vacancies by means of *ab initio* density functional theory (DFT) calculations of slabs. Relativistic non-magnetic DFT calculations exhibit Rashba-like spin winding with a characteristic energy scale ~ 10 meV. However, when surface magnetism on the Ti ions is included, bands become spin-split with an energy difference ~ 100 meV at the Γ point. This energy scale is comparable to the observations in SARPES experiments performed on the two-dimensional electronic states confined near the (001) surface of $SrTiO_3$. We find the spin polarized state to be the ground state of the system, and while magnetism tends to suppress the effects of the relativistic Rashba interaction, signatures of it are still clearly visible in terms of complex spin textures.

[1]We gratefully acknowledge financial support from the Deutsche Forschungsgemeinschaft through grants SFB/TR 49 and FOR 1346.

Harald O. Jeschke
Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany

Date submitted: 05 Nov 2015 Electronic form version 1.4