Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First-principles many-body investigation of δ-doped titanates[1]
FRANK LECHERMANN, MICHAEL OBERMEYER, I. Institute for Theoretical Physics, University of Hamburg — Studying oxide heterostructures provides the possibility for exploring novel composite materials beyond nature's original conception. In this respect, the doping of Mott-insulating distorted-perovskite titanates such as $LaTiO_3$ and $GdTiO_3$ with a single SrO layer gives rise to a very rich correlated electronic structure [1]. A realistic superlattice survey by means of the charge self-consistent combination of density functional theory (DFT) with dynamical mean-field theory (DMFT) reveals layer- and temperature-dependent multi-orbital metal-insulator transitions. In [001] stacking, an orbital-selective metallic layer at the interface dissolves via an orbital-polarized doped-Mott state into an orbital-ordered insulating regime beyond the two conducting TiO_2 layers. We find large differences in the scattering behavior within the latter. Breaking the spin symmetry in δ-doped $GdTiO_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically.

[1] F. Lechermann and M. Obermeyer, arXiv:1411.1637 (2014)

[1]Support from the DFG-FOR1346 is acknowledged.

Frank Lechermann
I. Institute for Theoretical Physics, University of Hamburg

Date submitted: 10 Nov 2014 Electronic form version 1.4