First-principles many-body investigation of $\delta$-doped titanates\textsuperscript{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 $\delta$-doped GdTiO$_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically.


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