First-principles dynamical mean-field perspective on electron correlation and magnetism in oxide heterostructures

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The investigation of oxide heterostructures provides the possibility for exploring novel composite materials beyond nature's original conception (see [1] for a recent review). Emerging electronic phases within the interface region between e.g. bulk compounds of band- and/or Mott-insulating character pose a formidable problem beyond the scope of either conventional density functional theory (DFT) or minimal model-Hamiltonian approaches. By means of the charge self-consistent combination of DFT with dynamical mean-field theory (DMFT) an advanced realistic many-body methodology is available that may tackle this challenge. In this talk the theoretical framework will be presented and the application to intricate heterostructure problems discussed.

I thereby mainly focus on two concrete problems. First, the δ-doping of distorted-perovskite Mott-insulating titanates with a single SrO layer along the [001] direction gives rise to a rich correlated electronic structure [2]. From a realistic superlattice study, layer- and temperature-dependent multi-orbital metal-insulator transitions are revealed. Furthermore, breaking the spin symmetry in δ-doped $GdTiO_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically. Second, DFT+DMFT insight [3] into the metallic state and the key mechanism for itinerant ferromagnetism at the band-band insulating $LaAlO_3/SrTiO_3$ interface will be provided.

[1] J. Chakhalian, J. W. Freeland, A. J. Millis, C. Panagopoulos and J. M. Rondinelli, RMP 86, 1189 (2014) [2] F. Lechermann and M. Obermeyer, arXiv:1411.1637 (2014) [3] F. Lechermann, L. Boehnke, D. Grieger and C. Piefke, PRB 90, 085125 (2014)