

Abstract Submitted
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DFT+DMFT study of strain and interface effects in d^1 and d^2 t_{2g} -perovskites GABRIELE SCLAUZERO, KRZYSZTOF DYMKOWSKI, CLAUDE EDERER, Materials Theory, ETH Zurich — Metal-insulator transitions in thin films of early-transition metal correlated oxides are linked to both epitaxial strain and electronic reconstruction at the film/substrate interface. We separately address these two key factors for LaTiO_3 and LaVO_3 through density functional theory plus dynamical mean-field theory (DFT+DMFT). We find that mere epitaxial strain suffices to induce an insulator-to-metal transition in LaTiO_3 [1], but not in LaVO_3 , in agreement with recent experiments [2]. We show that this difference can be explained by the combined effect of strain-induced changes in the crystal field splitting of t_{2g} orbitals and different orbital filling in these two materials. The role of the interface is investigated through DFT+DMFT simulations of $\text{LaVO}_3/\text{SrTiO}_3$ heterostructures with varying superlattice periodicities and substrate terminations. Our aim is to assess whether the metallicity observed at the $\text{LaVO}_3/\text{SrTiO}_3$ interface could be driven by pure electronic reconstruction effects, rather than structural or stoichiometric reasons (such as, e.g., O-related defects). [1] Dymkowski and Ederer, Phys. Rev. B **89**, 161109 (2014). [2] He *et al.*, Phys. Rev. B **86**, 081401 (2012).

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