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 LaVO$_3$/SrTiO$_3$ heterostructures with varying superlattice periodicities and substrate terminations. Our aim is to assess whether the metallicity observed at the LaVO$_3$/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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