Strain-induced metal-insulator transitions in $d^1$ perovskites within DFT+DMFT KRZYSZTOF DYMOWSKI, CLAUDE EDERER, Materials Theory, ETH Zürich, Switzerland — We present results of combined density functional theory plus dynamical mean-field theory (DFT+DMFT) calculations, assessing the effect of epitaxial strain on the electronic properties of the Mott insulator LaTiO$_3$ and the correlated metal SrVO$_3$. In particular, we take into account the effect of strain on the collective tilts and rotations of the oxygen octahedra in the orthorhombically distorted $Pbmm$ perovskite structure of LaTiO$_3$. We find that LaTiO$_3$ undergoes an insulator-to-metal transition under a compressive strain of about $-2\%$, consistent with recent experimental observations [1]. We show that this transition is driven mainly by strain-induced changes in the crystal-field splitting between the Ti $t_{2g}$ orbitals, which in turn are related to changes in the octahedral tilt distortion. We compare this with the case of SrVO$_3$, without octahedral tilts, where we find a metal-to-insulator transition under tensile epitaxial strain. Similar to LaTiO$_3$, this metal-insulator transition is linked to the strain-induced change in the crystal-field splitting within the $t_{2g}$ orbitals. [1] Wong et al., Phys. Rev. B 81, 161101 (2010)