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Strain-induced metal-insulator transitions in d^1 perovskites within DFT+DMFT KRZYSZTOF DYMKOWSKI, 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 *Pbnm* 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)

Krzysztof Dymkowski
Materials Theory, ETH Zürich, Switzerland

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