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A tight-binding LDA+DMFT study of manganite superlattices

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— The combination of *ab initio* density functional theory with model “many-body” calculations provides a very promising way for a realistic theoretical treatment of surface and interface effects of strongly correlated electron materials. Here we show in detail how the electronic structure of LaMnO_3 calculated within the local density approximation (LDA) can be efficiently parametrized using a physically transparent tight binding model and considering both nearest and next nearest neighbor hoppings. In particular, we address effects due to rotations of the oxygen octahedra surrounding the Mn cations. The resulting two-band model is then applied to study LaMnO_3 - SrMnO_3 superlattices using dynamical mean-field theory (DMFT) and the predicted ground state phases for superlattices with a small number of individual LaMnO_3 and SrMnO_3 layers are compared with the results obtained by density functional theory.

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