Formation of orbital-selective electron states in $LaTiO_3/SrTiO_3$ superlattices

F. Lechermann, L. Boehnke and D. Grieger
I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

The interface electronic structure of correlated $LaTiO_3/SrTiO_3$ superlattices is investigated by means of the charge self-consistent combination of the local density approximation (LDA) to density functional theory (DFT) with dynamical mean-field theory (DMFT), i.e. the DFT+DMFT approach. Utilizing a pseudopotential technique together with a continuous-time quantum Monte-Carlo framework [1], the complex multi-orbital electron states in unit cells with up to 100 atoms are addressed in a coherent fashion beyond static mean-field. General structural relaxations are taken into account on the LDA level and eventually cooperate with the strong electronic correlation driving forces. This alliance leads to an d_{xy} dominated low-energy quasiparticle peak and a lower Hubbard peak in line with photoemission studies. Furthermore correlation effects close to the band-insulating bulk $SrTiO_3$ limit as well as the Mott-insulating bulk $LaTiO_3$ limit are studied via embedded singe-layer architectures. Metallicity with varying correlation strength is obtained in these limiting cases. This research paves the road for novel first-principles many-body investigations of engineered correlated materials systems.

[1] D. Grieger, C. Piefke, O. E. Peil and F. Lechermann, Phys. Rev. B **86**, 155121 (2012).