Confinement-induced electronic reconstruction in (001) and (111) oriented perovskite superlattices

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Oxide interfaces exhibit a broad spectrum of functional properties that are not available in the respective bulk compounds, such as two-dimensional conductivity, superconductivity and magnetism. In this talk I will compare the mechanisms of electronic and orbital reconstruction in oxide quantum wells with (001) and (111) crystallographic orientation. The latter promise to host even more exotic electronic states compared to the much studied (001)-oriented systems due to their distinct topology [1]. Material-specific density functional theory calculations with an on-site Coulomb repulsion term are used to explore the role of confinement, symmetry breaking, polarity mismatch and strain in the emergence of novel electronic phases. The results illuminate a rich set of competing ground states in polar $(LaAlO_3)_M/(SrTiO_3)_N(111)$ [2] and non-polar $(LaNiO_3)_M/(LaAlO_3)_N(111)$ [3,4] superlattices, ranging from spin-polarized, Dirac-point Fermi surfaces protected by lattice symmetry to charge-ordered Mott or Peierls insulating phases. Analogous to the (001) counterparts [5,6], orbital reconstructions and metal-to-insulator transitions depend critically on the thickness of the quantum well and in-plane strain, thus opening avenues for engineering properties at the nanoscale.
Research in collaboration with D. Doennig, A. Blanca-Romero and W.E. Pickett; supported by the DFG, SFB/TR80.

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