Competing electronic reconstruction mechanisms in (111) oriented LaAlO3/SrTiO3 quantum wells: from a ferromagnetic Dirac-point semimetal to a charge ordered flat band insulator

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Abstract

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Remarkably rich electronic behavior has been recently discovered in (001) oriented interfaces between LaAlO3 and SrTiO3 including two-dimensional conductivity, superconductivity and magnetism. However, 111 oriented superlattices promise to host exotic, possibly topologically nontrivial phases. Density functional theory calculations with an on-site Coulomb repulsion term (GGA+U method) reveal competing ground states in M LaAlO3/N SrTiO3(111) superlattices with n-type interfaces, ranging from spin, orbital polarized, Dirac point Fermi surface to charge ordered flat band phases. Orbital selectivity and metal-to-insulator transitions are steered by the interplay of Hubbard U, strain, and the SrTiO3 quantum well thickness. Under tensile strain inversion symmetry breaking drives the honeycomb lattice bilayer (N=2) from a ferromagnetic Dirac-point semimetal to a charge ordered flat band massive insulating phase [1]. An insulator-to-metal transition occurs with increasing SrTiO3 quantum well thickness.

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