Realistic many-body investigation of complex materials

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Novel materials based on the combination of different known bulk features provide the possibility for a new era in condensed matter physics. For instance, emerging electronic phases within the interface region between e.g. bulk compounds of band- or Mott-insulating character pose a formidable problem beyond the scope of either conventional density functional theory (DFT) or minimal model-Hamiltonian approaches. By means of the charge self-consistent combination of DFT with many-body schemes such as dynamical mean-field theory (DMFT) an advanced realistic methodology is available that may tackle such challenges. In this talk the theoretical framework will be presented and the application to intricate materials systems discussed.

I thereby mainly focus on two concrete problems. First, the delta-doping of distorted-perovskite Mott-insulating titanates with a single SrO layer along the [001] direction gives rise to a rich correlated electronic structure. From a realistic superlattice study, layer- and temperature-dependent multi-orbital metal-insulator transitions are revealed. Furthermore, breaking the spin symmetry in delta-doped GdTiO$_3$ results in blocks of ferromagnetic itinerant and ferromagnetic Mott-insulating layers which are coupled antiferromagnetically. Second, a report on recent studies of doped Ruddlesden-Popper iridates will be given. There the interplay between spin-orbit coupling and local Coulomb interactions gives rise to demanding bulk physics. In these compounds, nonlocal self-energies are likely relevant to differentiate between the electron- and hole-doped regime.