Non-local Correlations Effects in Transition Metal Compounds

Alexander Lichtenstein

University of Hamburg

Keywords: non-local correlation effects

We present a quantum theory of the non-local metal-insulator transition (MIT) in transition metal compounds. Strong competition between the local Coulomb interaction and chemical bonding in a Metal-Metal pair results in a small insulating gap. The standard LDA calculations show that the bonding-antibonding splitting is not enough to open a gap and correlation effects are important. A conventional single site DMFT cannot reproduce an insulating phase for any reasonable values of the Coulomb interaction since it leads to the reduction of the bonding-antibonding splitting. A cluster LDA+DMFT scheme is applied to describe the non-local correlation effects in these compounds. We investigate the MIT in different transition metal compounds and show that the many body non-local Coulomb interactio ns are essential for a simultaneous description of the low-temperature insulating and high-temperature metallic states.