Many-Electron Bands in Transition Metal Compounds

A. Stoyanova and R. Broer
Theoretical Chemistry, Zernike Institute for Advanced Materials
Rijksuniversiteit Groningen
Nijenborgh 4, 9747 AG Groningen, The Netherlands

C. de Graaf
ICREA Researcher at the Department of Physical and Inorganic Chemistry
Universitat Rovira i Virgili
Marcel.l Domingo s/n, 43007 Tarragona, Spain

We present a new method for generating correlated many-electron bands for localized excited states, hole states and added-electron states in extended systems with strong electron correlation effects. The energy bands are obtained within an ab initio many-electron non-orthogonal tight-binding approach. The corresponding wave functions consist of optimized linear combinations of local many-electron basis functions. The local many-electron basis is obtained from multiconfiguration wave functions for large embedded clusters. Each local state is expressed in terms of its own optimized orbitals set. The method allows for a rigorous treatment of the local electronic relaxation and correlation that accompanies the excitation, electron-removal and electron-addition process. As a demonstration of the performance of the method we investigate the Bloch wave-vector dependence of the energies of the lowest added-electron states in the perovskite $CaMnO_3$. These states are important for understanding the interplay of conduction and magnetism in doped $CaMnO_3$.