d Theory in Electronic Structure Calculations: \\ Applications to so

Table of Contents

Dynamical Mean Field Theory in Electronic Structure Calculations: Applications to solids with f and d electrons

Gabriel Kotliar

Department of Physics and Astronomy, Serin Physics Laboratory, Rutgers University, Piscataway N.J. (USA)

Existent electronic structure methods deal successfully with electrons which are extended or core like. A recent breaktrhu in many body technique allows to treat strongly correlated electronic systems which are neither fully itinerant or well localized. We have developed and implemented these ideas within an LMTO band structure method to construct an ab−intio framework for performing electronic structure calculations. The method gives the total energy the interacting local spectral function and can be used to compute transport coefficients. We will outline the physical and the formal content of the method. We will then illustrate its usefulness with two concrete applications to two strongly correlated electron systems containing f and d electrons: fcc Pu and the perovskite $La_{1-x}Sr_xTi\ O_3$. We will conclude with directions for future developments.
