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The physics of strongly correlated systems: A dynamical mean field theory approach

To this date, first-principles Density functional theory (DFT) has proven successful in the study of electronic structure of real materials. At the same time, we have plenty of program packages in which first-principles DFT has been implemented and are able to calculate material properties accurately and efficiently. However, the authors here in are concerned with the strongly correlated materials, where the electron-electron interaction heavily influences the electronic structure. It is a well known problem that first-principles DFT fails in describing these types of materials correctly. The reason for this failure is that first-principles DFT only includes electron-electron interactions in an average way. Many attempts have been proposed to solve this discrepancy. Among them is the inclusion of the Hubbard model in the electronic structure calculations. After working on many systems and more specifically ferroelectrics, we have faced some challenges posed by the Hubbard model in our day to day calculations. One, the calculation ceases being a first-principle to a semi-empirical like in the sense that you have an extrinsic energy in the system (DFT+U). Secondly, the application of the Hubbard model makes some systems loose their intrinsic properties like ferroelectrity. A good example is the loss of the O $2p$ and Ti $3d$ hybridization in $BaTiO_3$ when the Hubbard model is employed and thus rendering $BaTiO_3$ a paraelectric. In this work, the authors will highlight the recently developed dynamical mean field theory (DMFT). In principle, DMFT originates from the many-body approach in computational materials physics. DMFT has been combined with conventional DFT methods to help us conceptualize the physics of strongly correlated systems.

Keywords

DMFT, first-principles, Density functional theory

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