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Dynamical Mean-Field Theory for Strongly Correlated Materials

This is the first book that provides a detailed summary of one of the most successful new condensed matter theories - dynamical mean-field theory (DMFT) - in both static and dynamical cases of systems of different sizes. DMFT is one of the most successful approaches to describe the physical properties of systems with strong electron-electron correlations such as bulk materials, multi-layers, surfaces, 2D materials and nanostructures in both metallic and insulating phases. Strongly correlated materials usually include partially-filled localized d- or f-orbitals, and DMFT takes into account crucial for these systems time-resolved interaction between electrons when they "meet" on one atom and occupy one of these orbitals. The First Part of the book covers the general formalism of DMFT as a many-body theory, followed by generalizations of the approach on the cases of finite systems and out-of-equilibrium regime. In the last Chapter of the First Part we discuss generalizations of the approach on the case when the non-local interactions are taken into account. The Second Part of the book covers methodologies of merging DMFT with ab initio static Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) approaches. Such combined DFT+DMFT and DMFT+TDDFT computational techniques allow one to include the effects of strong electron-electron correlations at the accurate ab initio level. These tools can be applied to complex multi-atom multi-orbital systems currently not accessible to DMFT. The book helps broad audiences of students and researchers from the theoretical and computational communities of condensed matter physics, material science, and chemistry to become familiar with this state-of-art approach and to use it for reaching a deeper understanding of the properties of strongly correlated systems and for synthesis of new technologically-important materials.

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