Quantum simulations of materials and biological systems

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This book features contributions from leading world experts in the fields of density functional theory (DFT) and its applications to material and biological systems.
The recent developments of correlation functionals, implementations of Time-dependent algorithm into DFTB+ method are presented. The applications of DFT method to large materials and biological systems such as understanding of optical and electronic properties of nanoparticles, X-ray structure refinement of proteins, the catalytic process of enzymes and photochemistry of phytochromes are detailed. In addition, the book reviews the recent developments of methods for protein design and engineering, as well as ligand-based drug design. Some insightful information about the 2011 International Symposium on Computational Sciences is also provided.