



Density Functional Theory in Quantum Chemistry

Takao Tsuneda

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In this book, density functional theory (DFT) is introduced within the overall context of quantum chemistry. DFT has become the most frequently used theory in quantum chemistry calculations. However, thus far, there has been no book on the fundamentals of DFT that uses the terminology and methodology of quantum chemistry, which is familiar to many chemists, including experimentalists. This book first reviews the basic concepts and historical background of quantum chemistry and then explains those of DFT, showing how the latter fits into the bigger picture. Recent interesting topics of DFT in chemistry are also targeted. In particular, the physical meanings of state-of-the-art exchange-correlation functionals and their corrections are described in detail. Owing to its unconventionality, this book is certain to be of great interest not only to chemists but also to solid state physicists.

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