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Quantum mechanics can describe the detailed structure and behavior of matter, from electrons, atoms, and molecules, to the whole universe. It is one of the fields of knowledge that yield extraordinary precessions, limited only by the computational resources available. Among these methods is density functional theory (DFT), which permits one to solve the equations of quantum mechanics more efficiently than with any related method.

The present volume represents the most comprehensive summary currently available in density functional theory and its applications in chemistry from atomic physics to molecular dynamics. DFT is currently being used by more than fifty percent of computational chemists.

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