



Time-Dependent Density-Functional Theory: Concepts and Applications (Oxford Graduate Texts)

Carsten A. Ullrich

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Time-dependent density-functional theory (TDDFT) describes the quantum dynamics of interacting electronic many-body systems formally exactly and in a practical and efficient manner. TDDFT has become the leading method for calculating excitation energies and optical properties of large molecules, with accuracies that rival traditional wave-function based methods, but at a fraction of the computational cost.

This book is the first graduate-level text on the concepts and applications of TDDFT, including many examples and exercises, and extensive coverage of the literature.

The book begins with a self-contained review of ground-state DFT, followed by a detailed and pedagogical treatment of the formal framework of TDDFT. It is explained how excitation energies can be calculated from linear-response TDDFT. Among the more advanced topics are time-dependent current-density-functional theory, orbital functionals, and many-body theory. Many applications are discussed, including molecular excitations, ultrafast and strong-field phenomena, excitons in solids, van der Waals interactions, nanoscale transport, and molecular dynamics.

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