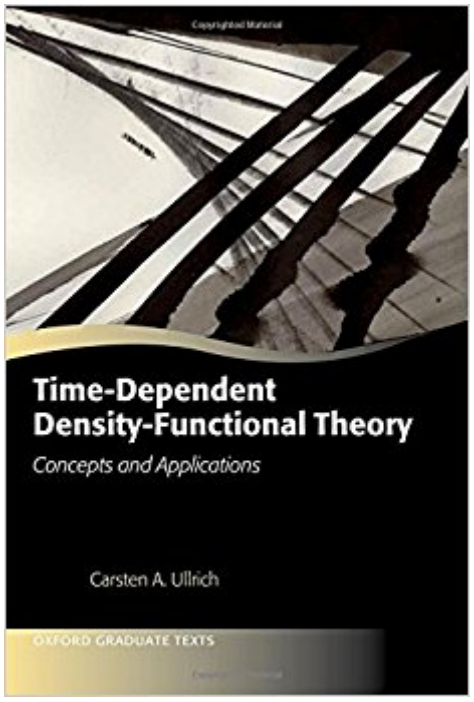
# Time-Dependent Density-Functional Theory: Concepts And Applications (Oxford Graduate Texts)



## Synopsis

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.

## Book Information

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## Customer Reviews

This is a very pedagogical introduction to the central ideas of time-dependent density-functional theory. The theory is described in depth and illustrated with many insightful examples and applications in atomic, molecular and condensed matter physics. This is a valuable book for both students and researchers. * Robert van Leeuwen, University of Jyvaskyla *

Carsten Ullrich is Associate Professor of Physics at the University of Missouri-Columbia.

It contains detail information about DFT and TD-DFT

I like this book for its review of many important developments within TDDFT in the last one or two decades. Quantum chemists should be careful as the viewpoint in this book is entirely given in the real-space representation (for densities, response functions, potentials, kernels). A plus is the use of common notation which makes the book readable even in case you do not directly originate from the TDDFT community.As it appears to me, some aspects are explained a bit in haste so that I just give 4 points. Others are explained quite lengthy though missing a clear highlighting of the underlying/basic principles/concepts. Some of the lengthy explanations may have been skipped (instead of giving a a sloppy summary) because they are indeed very well explained in other books, e.g., reading section 7.1 was much more enlightening using the Gross, Runge, Heinonen book on Many-Particle theory and basically most of the fundamental relations are ’borrowed’ from there, it seems.Coming back to the main track, so yes, it is a reliable and vast ressource of up-to-date TDDFT and as such highly recommended. As I have read the first edition from 2012, there is hope that the slight disorder/sloppiness in the text logic gets a clean up for the next edition? In this case, this book will get 5 points.

This is a very comprehensive book about time-dependent density functional theory (td-DFT), a theory that allows one to compute the excitation energies and, hence, the optical spectra of molecules and solids. The book is divided in four parts: Part 1 deals with the basic formalism of td-DFT, Part 2 covers linear-response theory and excitation energies, Part 3 discusses further developments of td-DFT such as td current-DFT and td-OEP (OEP = optimized effective potential), and Part 4 treats special topics (dispersion interactions, nanoscale transport, optimal control, etc.). At the end of the book there are more than fifty pages of Appendices (A through O), the last of which contains a list of both commercial and open-source td-dft computer codes that are available for research. Many references to the original literature are also provided by the author. The publication of this book is timely and it is highly likely that both students and computationally-oriented scientists will benefit from it.

In the preface the author has claimed that this book is both textbook and monograph. That’s exactly what it is so far for me. I find myself enlightened at the explanation of the RG theorem and TDKS

equation compared to the Lecture Notes in Physics books of the similar title but there is still a need to refer to other textbooks and review papers. So far it's the response theory section for me. Background reading has to be done before a student can thoroughly understand what's going on as recommended by the author himself.I would say Fundamentals in TDDFT or TDDFT (both Lecture Notes in Physics) and this book will couple well (other than the other references you would have to make).