Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

A Review of "Time-Dependent Density-Functional Theory: Concepts and Applications"

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Version of record first published: 16 Nov 2012.

To cite this article: Joel F. Liebman (2012): A Review of "Time-Dependent Density-Functional Theory: Concepts and Applications", Molecular Crystals and Liquid Crystals, 569:1, 165-166

To link to this article: http://dx.doi.org/10.1080/15421406.2012.711647

Mol. Cryst. Liq. Cryst., Vol. 569: pp. 165–166, 2012

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421406.2012.711647

Taylor & Francis
Taylor & Francis Group

Book Review

Time-Dependent Density-Functional Theory: Concepts and Applications by Carsten A. Ullrich, Oxford University Press, Oxford, UK and New York, 2012, ISBN 978-0-18-956302-9, xiv + 526 pp, $82.99 (hardback).

This lengthy, largely photo-reproduced monograph is part of the series "Oxford Graduate Texts" and so is explicitly designed to educate both graduate students and the research practitioner who are interested in learning the theory and practice of a relatively unused approach of contemporary, calculational theoretical science, Time-Dependent Density Functional Theory (TDDFT). (The number of citations to this method is less than 10% of the "conventional" Density Functional Theory (DFT), the latter being an approach the volume's author does not discuss at any length after carefully distinguishing DFT from TDDFT.) Each chapter is accompanied by a collection of exercises that simultaneously educate the reader with new material as well as help calibrate the reader's level of understanding by providing an immediate appraisal of his/her knowledge. However worthy is that implicit goal, the reviewer wishes there was an accompanying answer book even if that would perhaps significantly increase the length and price of this new volume. There is an extensive bibliography to the primary literature (an impressive amount by the book's author), as well as to other reviews of the subject. The reader is also told about extant computer codes that allow the reader to make use of the current science and technology, rather than leaving the subject to be just a mathematical and abstract exercise in theorems and proofs about many-electron systems, these species being more commonly known as atoms, molecules, and very often polymers and solids. All of this is further amplified by introductory chapters and an extensive collection of appendices (15 in number) that provide some of the background (e.g., on atomic units, functionals, density matrices, Hartree–Fock calculations)—making the reviewer wonder if the reader in fact needs more than a casual reminder of these preliminary topics, then is s/he ready for the rest of the book?

What is missing in this book is a lengthier discussion of how TDDFT adds to our understanding of "classical chemistry"—the almost exclusive emphasis on spectroscopy and dynamics is not enough for this reviewer. (To be fair, the reviewer's concern about "classical chemistry" is more than that of many other theorists.) Let the reviewer now mention some species for which TDDFT has been recently applied, imidazolium hexafluorovanadium(III), dipyrazolo[3,4-b; 3′,4′-e]pyridine, "Nile red," N-ferrocenoyl-N′-ω-decenoyl-ethylenediamine, and the natural products, indotertine A and drimentine F. These studies document that TDDFT is a powerful theoretical approach with applications to a wide of variety of chemical phenomena, far more than the current book seems to suggest. The book is long on concepts and formalism, but short on applications: perhaps the author is planning another book.

Summarizing, the book is contemporary in content, mathematical in its approach, and encouragingly affordable but not as chemical as the reviewer would have hoped in order to enhance his own research.

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