Molecular Crystals and Liquid Crystals

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Book Review

Joel F. Liebman [a]

[a] Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, 1000 Hilltop Circle, Baltimore, MD 21250

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Book Review

Density Functional Theory: A Practical Introduction, by David S. Sholl and Janice A. Steckel, John Wiley & Sons, 2009; xii +238 pages; $90.00; ISBN 978-0-470-37317-0.

Quoting from its back cover, the book states "Density functional theory (DFT) is one of the most frequently used computational tools for studying and predicting the properties of isolated molecules, bulk solids and materials interfaces [...] [this book offers] [...] a concise [...] introduction to the key concepts and practical applications of DFT." For the research practitioner who is the reader of the journal in which this review appears, all of this suggests this is a good read to gain knowledge of a powerful contemporary technique in computational chemistry. The reader is told there are problem sets in each chapter that give readers the opportunity [...] to perform [...] their own calculations," "worked examples that [...] solve real-world problems," and "[f]urther readings [...] enabling readers to investigate specific topics in greater depth." This suggests that the educator who is the reader of the journal in which this book review appears should find much to include in a graduate classroom environment. I concur with these assertions for the materials scientist or physical chemist who is educated in sophisticated mathematics and physics. However, I do not share the authors' optimism for the organic chemically inclined investigator or even the molecularly oriented physical chemist. I disagree with the claim that "anyone in math, science, and engineering can master DFT calculations" from what is found in this book.

Elemental crystals are discussed at length in the book, but these are atomic, not molecular, in composition and structure. Oxides are also discussed, but these return us to species of simple stoichiometry. Where are polyatomics? Few molecules "decorate" the pages of the book (despite the cover), and most of these have no more than two atoms. The Perdue–Wang functional (PW91) dominates the discussion in this book, and however powerful it is, it is not the B3LYP functional that is the workhorse of the molecular chemist who uses DFT. Likewise, plane waves dominate Gaussian basis functions. I suspect these omissions may chase away, or at least disappoint, many readers

despite a highly useful first chapter entitled "What is Density Functional Theory?" The authors themselves acknowledge this divide "[a]lthough many of the foundations [. . .] (a)re also relevant to complementary approaches used in the chemical community for isolated molecules, there are enough differences in the applications of these two groups of methods that including both methods would only have been possible by significantly expanding the scope of the book. Moreover, several resources already exist that give a practical 'hands-on' introduction to computational chemistry calculations for molecules." By their statement, acknowledging what they believe the book covers, the authors take the risk of assuming that what they have included in the book meets the needs of readers whom this author believes may not fully understand or use what the authors present.

This schism is regretted because the basic principles of DFT are independent of this choice of species and functional. It is unfortunate that this last disclaimer is in small print as opposed to being positioned more prominently on the book jacket. After all, to give a culinary and even ethnic metaphor, despite how many stars for the restaurant, all of this seems like a belated look at a menu after finding a restaurant, discovering that one must order burritos at a beer garden, or bratwurst at a cantina. Or, admitting wry humor, that there must be mayonnaise accompanying sauerkraut at a delicatessen to accompany the food tastes of all and hence few, customers.

Joel F. Liebman
Department of Chemistry and Biochemistry,
University of Maryland, *Baltimore County*,
1000 Hilltop Circle,
Baltimore, *MD 21250*