Molecular Crystals and Liquid Crystals

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

A Review of: "Molecular Modelling for Beginners"

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Version of record first published: 31 Aug 2006

To cite this article: Joel F. Liebman & Susan K. Gregurick (2005): A Review of: "Molecular Modelling for Beginners", Molecular Crystals and Liquid Crystals, 442:1, 203-205

To link to this article: http://dx.doi.org/10.1080/154214090964762

Mol. Cryst. Liq. Cryst., Vol. 442, pp. 203–205, 2005

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/154214090964762

Taylor & Francis
Taylor & Francis Group

Book Review

Molecular Modelling for Beginners, by Alan Hinchliffe, John Wiley & Sons, 2003; xviii + 410, pp., $117.00, cloth; $46.00, paper.

This book is Hinchliffe's most recent contribution to the pedagogical literature of molecular modeling. Hinchliffe states, "The focus is on Molecular Mechanics, Monte Carlo and Molecular Dynamics." For example, the reader is selectively introduced to MM1 and MM2 (but not MM3 or MM4), and AMBER (but not CHARM). In fact, the book also has a thorough introduction to classical physics and an extensive treatment of molecular quantum mechanics ranging from the semiempirical to the Hartree–Fock (both restricted and unrestricted) level to numerous contemporary post–Hartree–Fock methods such as the G1, G2, and G3 hierarchy. This thoroughness makes this book a powerful addition to the library of any user of molecular modeling methods, because few individuals are knowledgeable of the majority of them. There are few examples given and no problems or exercises accompany the text. The reader of this book (student and professor) must be self-motivated: this is a reasonable although not always fulfilled aspiration for a volume at the level of this book. The reader, however, is given numerous citations to the literature (118 in total), many of which are the pioneering studies themselves but too few are current studies.

There are two related features of this book about which the reviewers admit their ambivalence. The first is that although an informal first-person point of view is used for many topics, many methods are described using the original authors' own words, most often taken from the abstract of "keynote papers." However, good science and good pedagogy do not always correspond any more than good researchers and good teachers, and beginning students might not be ready to learn from the primary literature whose authorship rarely aims for them. The second is the paucity of chemical examples used to illustrate the more mathematics- and physics-oriented text. This allows the reader to discuss species of direct interest and experience. However, the one molecule that appears with any enthusiasm or frequency, phenylalanine, is consistently misspelled in the text and the index as

"phenylanine." Errors in writing are unavoidable, but this continuing occurrence can fuel the erroneous conclusion that physical and theoretical chemistry is orthogonal to organic, medicinal, and biochemistry, the areas in which molecular modeling has made the majority of its applications and resultant successes.

Let us now turn to some specific aspects of molecular modeling in our review.

Pp. 123–142, molecular dynamics: The chapter on molecular dynamics is well illustrated with examples and a good basis of theory. However, some fundamental potential-energy equations are not given and should be included. These include the hard spheres, square well, and Lennard–Jones equations.

Pp. 143–150, Monte Carlo: The chapter on Monte Carlo simulations is reasonably well stated and gives a good overview of the simulation techniques. There are, however, no illustrated examples, as in the molecular dynamics case, of these types of simulations as applied to real systems. Moreover, the program provided is not documented well.

Pp. 151–169, introduction to quantum modeling: This chapter is well written and easy to understand but is in every contemporary physical-chemistry text. As such, this chapter does not relate well to molecular modeling.

Pp. 170–195, quantum gases: This is an excellent chapter and one of the nicest explanations of a Drude model of metals ever given.We commend the author: it is very difficult to find such a clear discussion of statistical mechanics in an undergraduate (or first-year graduate) text.

Pp. 245–260, simple molecules: This chapter is both too complete and incomplete. Although it discusses H_2^+ and H_2 at great length, most of the methods are specialized to just these species or just to diatomics. Because it does not appear elsewhere in the text, we may wonder why a discussion of other diatomic molecules wasn't made and thereby a mention (a brief reminder?) of σ and π orbitals, bonding and antibonding, and bond order included.

Pp. 346–359, density functional theory: The equations given for the DFT theory are hard to follow for a beginner. Because most of the intended readers are novices, this chapter will be a challenge. However, the history of DFT is quite interesting. We could not understand why numerical integration is given in this chapter and again the application is the "phenylanine" molecule.

Overall: The book is a good secondary reference but not a good text for a course. The book is too far reaching and covers every topic; thus, only the surface is scratched for most issues, save a few. However, the book is fun to read and is a very nice reference.

We thus feel that Hinchliffe's book is a recommended read, both rewarding and rough, but unfortunately only with exceptional effort for the beginning audience explicitly targeted.

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