
Molecular Crystals and Liquid Crystals

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# Book Review

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*Molecular Modelling for Beginner* (2nd ed.), Alan Hinchliffe, John Wiley & Sons, 2008, xix +411 pages; $170.00 (hardback), $70.00 (paperback). ISBN: 0470 51313 2 (hardback), 0 470 51314 9 (paperback).

This book is second edition of Hinchliffe's recent contribution to the pedagogical literature of molecular modeling: the field is advancing rapidly enough that this new work should be welcomed by the academic community though only five years have passed since first edition. In the name of brevity, the reader continues to be selectively introduced to molecular mechanics as realized in MM1 and MM2 (but not MM3 or MM4), AMBER (but not CHARM), QSAR "as routinely practiced in MM studies." The book also provides a thorough introduction to classical physics, and an extensive treatment of molecular quantum mechanics ranging from the all-but-forgotten semiempirical to the Hartree-Fock (both restricted and unrestricted) level to numerous contemporary post–Hartree Fock methods such as the Gl, G2, and G3 hierarchy. Quantum Mechanical/Molecular Mechanical hybrid ONIOM methods are also introduced. There is a new, highly appreciated, section "Sharing Out the Energy" which bridges key aspects of the microscopic and macroscopic understanding of molecular phenomena.

This book is written both for the student and the professional. Appendices provide much of the needed background in mathematics and physics as well as glossaries of symbols and abbreviations. Few examples are given, and problems and exercises are not found in the text. The reader is generally addressed to the primary literature for more information. This may be a rough entry to the discipline for some beginners, while others will be pleased to be invited to the research community. However, there is "a set of problems, together with solutions, is available on the associated Web site" to the book. As reviewer and educator, I am ambivalent about the use of this electronic supplement since Web sites seem more ephemeral than text to me. Yet, is this so different from an "instructor's manual" or "student's workbook" that often characterized textbooks from yesteryear?

I close by noting that the textbook is informally written and hence inviting. This is good, since it may appear mathematically and

computationally quite austere. There are few molecular structures that decorate the pages. I personally miss them, even though I can readily fill in the holes and ameliorate the omissions. Perhaps that was the author's intent. Maybe Hinchliffe is letting the reader choose those molecules of greatest personal interest—I note an encouragingly wide variety of species he has studied in his research. Let me thus be optimistic and so end this review as was done for the first edition: "Hinchliffe's book is a recommended read, both rewarding and rough."

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