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BOOK REVIEW

Roman F. Nalewajski: "**Fundamentals and methods of quantum chemistry. Lectures**" (in Polish).
Polish Edition: ,,**Podstawy i metody chemii kwantowej. Wykłady**", PWN Warszawa 2001.
ISBN 83-01-13536-0.

Teaching quantum chemistry is not an easy task: on the one hand its basics are largely abstract and require mathematical and physical backgrounds beyond the average level of an undergraduate chemistry student, unless he really desires to specialize in this field. On the other hand, over the years, the field accumulated advanced computational technology, which is at present widely and successfully used throughout most chemistry and physics, enough to mention the Nobel prize for Pople and Kuhn of 1999. Taking advantage of these developments requires a great deal of understanding of both the fundamental principles, their applications, and the involved numerical technology. Nalewajski's book aims at providing such knowledge, at the contemporary level of theory, for students whose major is chemistry (or physics).

The reviewed book, published in Polish, is an extended and amended version of a quantum chemistry lecture notes prepared by the Author for undergraduate and graduate students of chemistry at Jagiellonian University. The Author, a renowned theoretician, specializes in density functional theory and the theory of chemical bond, and has been teaching quantum chemistry course over many years.

Unfortunately, the result falls somewhat short of expectations since, in my opinion, this book will be too difficult for most students. The contents has a form of extensive, but often too loosely bound lecture notes (in the spirit of the "Lecture Notes in Chemistry" of Springer). Quite unfortunately for an undergraduate course, it is also written in a recondite and esoteric language. The Author focuses on formal derivations, paying less attention to elucidation of concepts, to providing examples, exercises, and applications. The best academic books are not written in this way, *cf*. Feynman lectures in physics or Kolos's and Golebiewski's quantum chemistry books, which strove to keep high standard in this respect. One may evoke the statement of Rabi: "The power of physics is in words". Concepts, intuitive ideas, imaginative pictures and applications are equally important. Last not least, a successful book should make a good and involving reading.

The book is structured into 4 Sections, and Sections are dissected into individual Lectures.

The first two Sections lay out the fundamental concepts of quantum mechanics, and discuss the most important simple models: a one-dimensional free particle, a particle constrained by some potential, the rigid rotor and the harmonic oscillator – the essentials covered by many other well established textbooks.

Section 3 derives basic approximate methods of solving Schroedinger equation: the perturbation theory and variation method, and presents fundamental physical models behind the contemporary theory of electronic structure: the Born-Oppenheimer and one-electron approximations, and ends with atomic and diatomic terms. To merge all these subjects under one title of "approximate methods" is somewhat conceptually unusual, but individual fragments are consistently and well presented.

Section 4 is crucial from the point of view of contemporary applications of computational quantum chemistry. It is about methods of calculations of electronic structure of molecules, primarily from first principles. The presentation starts with the Hartree-Fock theory, describes contemporary theories of chemical bond, explores the idea of potential energy surfaces, introduces the post-Hartree-Fock theories within the framework of the configuration interaction formalism and valence bond theory. Finally, the essentials of density functional theory are presented, and its representation within the Kohn-Sham orbital approximation. Particular fragments are meticulously written, and many arguments and derivations I have found useful for didactic purposes.

Of the Lectures in Sec. 4 the chemical bond part belongs to the best, interesting and competently written with the feeling characteristic for somebody who has been actively involved in the relevant research himself. It includes the classic Mullikan charges, discusses the topological analysis of Bader, and finally describes ingenious Hirschfeld's "stockholder atoms". It winds up with the outlook toward the recent developments by the Author himself, which derive from the information theory: "The measure of the number of bonds in a molecule might then be provided by information distances between the molecule and the related pro-molecule that determine the specific molecular information noise" (translated from Polish by the Reviewer). Discouraging as this may sound – the Holy Grail of all chemists, the chemical bond, is reduced to the information noise – it is undoubtedly exciting.

Other two Lectures in Sec. 4, which are worth recommendation, are those about the density functional theory, and the Kohn-Sham method. They represent a small monograph of the subject, which is still relatively new, and so far have not been adequately covered by any textbook. It is thoroughly and competently described, to the best of my knowledge for the first time in a student course. The drawback is that applications are practically missing: both in the form of simple examples and exercises, as well as more complex, but realistic applications. This is a general problem with this book, which is heavily biased towards presentations of formalisms. And while formalisms may appear to be very elegant, the true beauty of a theory is only revealed in how it handles particular cases. In addition, in the case of the density functional theory, there is an extra problem of control of its reliability in a variety of applications.

I would recommend this book for undergraduate and graduate students, who specialize in theoretical chemical physics and physical chemistry, and for researchers, who seek a better understanding of intricate formalisms of contemporary quantum chemistry. They should be warned, however, that the book makes a hard reading.

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