Quantum Chemistry (5th Edition)

Ira N. Levine
Synopsis

Integrating many new computer-oriented examples and problems throughout, this modern introduction to quantum chemistry covers quantum mechanics, atomic structure, and molecular electronics, and clearly demonstrates the usefulness and limitations of current quantum-mechanical methods for the calculation of molecular properties. Covers such areas as the Schrödinger Equation, harmonic oscillator, angular momentum, hydrogen atom, theorems of quantum mechanics, electron spin and the Pauli Principle, the Virial Theorem and the Hellmann-Feynman Theorem, and more. Contains solid presentations of the mathematics needed for quantum chemistry, clearly explaining difficult or subtle points in detail. Offers full, step-by-step examinations of derivations that are easy to follow and understand. Offers comprehensive coverage of recent, revolutionary advances in modern quantum-chemistry methods for calculating molecular electronic structure, including the ab initio and semiempirical methods for molecular calculations. Now integrates over 500 problems throughout, with a substantial increase in the amount of computer applications, and fully updated discussions of molecular electronic structure calculations. For professionals in all branches of chemistry.

Book Information

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Customer Reviews

I’m a grad physics student, rather than a chemist. But I’m using this book in a Physical Chemistry class because my school doesn’t have an Atomic & Molecular class. Now, maybe I’m saying this
because I already have a background in Quantum Mechanics ... but this book is awesome. My instructor assigns all or nearly all of the end-of-chapter problems each week. And I’m able to flip to the back of the book and check to see if my numbers agree. It may be be Quantum Chemistry, rather than Quantum Mechanics, but aside from the chemical modeling which isn’t as applicable for physicists, Levine just does a better job of conveying quantum mechanics than most Q.M. books I’ve seen. He’s able to keep things simple, and not clog up the logic process with mathematical proofs. If you need a math proof, he gives you the reference. But the important stuff is proven, and he gives a lot of examples to help the process. As a bonus to physicists, a lot of the problems require some number crunching. And in this age of physical symbolism, it is easy to get rusty at dealing with real numbers, real units and real dimensions. I’ll even go so far as to say that before I read Levine, I never really had a complete grasp of Q.M.. And I’ve used decent books before this; Merzbacher, Saxon, a little Cohen-Tenoudji, Ter Har, Lim and Griffiths. This one is my favorite, and imagine, it’s not even officially a physics book!

This is the best introductory book for learning Quantum Chemistry. Especially for those who are not particularly mathematically inclined, or even for those who are, this book is simply great. It starts with an introduction to the Schrodinger’s equation. The most important fact is that, after this introduction, the author leads us through a range of wide topics in which the mathematical preliminaries are first explained. Whether it is differential equations or power series solutions, the author carefully guides you through everything. That makes the book self contained. Further on, there’s a wonderful chapter on Angular Momentum. In later chapters, we get a very good introduction to most of the important approximation methods and other computational methods used in modern Quantum Chemistry. This includes the variational method, perturbation theory, Hartree-Fock methods, and an enlightening chapter on the Feynman-Hellman theorem. The book ends with a look at computational methods like GAUSSIAN programs which are used routinely today in electronic structure calculations. I would very strongly recommend the book to anyone who is interested in learning what molecular structure is about.

Quantum chemistry a special field of the quantum-mechanical theory has always been a very tricky course for all the chemistry students around the world, because of the demanding mathematical background they have to possess in order to comprehend the extremely difficult concepts and applications of the best - up to now - theory we have to understand phenomena at the atomic and molecular level. This textbook is the best I know in the field because Pf. Ira Levine provides the
necessary Maths in a really instructive way which chemists will appreciate with a great relief! All the mathematics they will need is contained in this book so they won’t have to study it from a different source, wasting time and getting disappointed! On the other hand, the order of the chapters is excellent and the problems at the end of each chapter solidify your understanding of what you have already read during the chapter. There are also answers to selected problems at the end of the book! Highly recommend this textbook to all the chemists who would love to really understand Quantum Chemistry!

I had written a review of the 4th edition, published in International Journal of Quantum Chemistry, vol. 43, 439-441 (1992). This 5th edition is about 100 pages longer than the 4th one. All the new material it contains is clearly listed in the preface. I still highly recommend this book. I regret however that no paperback edition seems to be available.

I read the fourth edition of this book as an undergraduate student in chemistry. Now that I am a grad student involved in research problems in quantum chemistry, I find myself reaching for this book everytime I need to refresh this concept or that. The best part about this book is the level of detail at which a lot of basic quantum chemistry topics have been treated. I highly recommend this book for any serious student of quantum chemistry and those from other fields who need to learn some quantum chemistry on their own for their work.

I am amazed at the sheer depth of detail that Levine succeeds in conveying while somehow keeping the subject highly organized and extremely readable. Like a good teacher, he has a knack for anticipating your questions and problems and addresses them. He also seems to know exactly which points deserve attention and emphasis, and which don’t. His constant referencing of previous equations even when not absolutely necessary minimizes the student’s chance of getting lost or forgetting previous material and not remember where to find it again. Very mathematical, but all required mathematics are expertly reviewed before being introduced. My only complaints are a few critical typos in the angular momentum section, and the fact that that section and the section on symmetry could have been more clearly presented (especially the section on symmetry!). But overall, nobody’s perfect, and this is as close as you get. Definitely a class about Lowe’s textbook.

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