Glenn's legacy to science is contained in that sentence. He was a great scientist, administrator, and public figure, whose remarkable success was largely attributable to hard work.

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Molecular Electronic-Structure Theory

Trygve Helgaker, Poul Jørgensen, and Jeppe Olsen
Wiley, New York, 2000. $300.00 (908 pp.). ISBN 0-471-96755-6

The molecular electronic-structure problem lies at the heart of chemistry and of molecular physics. The full electronic Hamiltonian in the Born–Oppenheimer approximation can be solved exactly only for the hydrogen atom, but the development of powerful approximate methods over the past 70 years has invalidated P. A. M. Dirac's famous statement that "the underlying physical laws for understanding . . . all of chemistry are thus completely known, . . . it is only that application of these laws leads to equations much too complicated to be soluble."

A number of commercially available programs now exist that use different methods and approaches to solve for the ground-state electronic structure of small- to medium-sized molecules in the nonrelativistic limit. Some of these programs also extend to excitation properties, relativistic corrections, and semiempirical and density functional schemes. While many discussions are also available in the textbook, review, and journal literature concerning electronic-structure theory, in the authors' view, no "comprehensive, up-to-date, technical monograph" on the subject has been written.

Molecular Electronic-Structure Theory, by Trygve Helgaker, Poul Jørgensen, and Jeppe Olsen is, as is pointed out in its preface, precisely such a comprehensive monograph. Up to now, no single source has provided, in a unified form and with a unified, convenient notation, a comprehensive description of the actual methods for carrying out ab-initio electronic structure. This book will be useful to those workers who wish to use such calculations with more than "black-box" knowledge. In its 900 pages, it gives detailed, clear, numerically illustrated, and extensively discussed presentations of "all the important aspects of modern ab-initio non-relativistic wavefunction-based molecular electronic structure theory."

This text is focused and, within its focus, quite complete. In the first 15 chapters, it covers second quantization, exact and approximate wavefunctions, standard models, atomic basis functions, Gaussian basis sets, molecular integral evaluation, Hartree–Fock theory, configuration interaction theory, multiconfigurational self-consistent field theory, coupled cluster theory, and perturbation theory. The sixteenth chapter, roughly 100 pages long, many times the length of any of the others, is devoted to calibration of electronic structure models. In this chapter, a set of sample atoms and molecules is examined for various strengths and weaknesses. It also contains sections on errors in quantum mechanical calculations, equilibrium distances, equilibrium structures, dipole moments, atomic and molecular energies, atomization energies, reaction enthalpies, and conformational barriers.

The formal presentations and derivations are quite complete. Referencing is adequate. A particular strength of the text is the presence in each chapter of a set of comprehensive exercises accompanied by the solutions to those exercises. Most of these exercises are formal and manipulative, rather than numerical.

Although a number of electronic structure codes were used in the writing of this book, there is very little reference within the text to specific codes. Rather, the authors discuss the principles involved in electronic structure theory at the ab-initio level, and how those principles can be utilized in the derivation and optimization of algorithms for such calculations. Indeed, the authors suggest in their preface, "you will be able to write a computer program without too much difficulty." This is a strong statement, but both the detail and the precision of the text make it a correct statement. The book also has a useful list of acronyms and a very well-constructed index.

Because of the tight focus on ab-initio methodology and analysis of molecular ground state properties, the text misses some subjects that might have been expected. For example, both density functional theory and relativistic corrections are largely absent. (Density functional theory is discussed briefly in the last few pages, and some examples of relativistic corrections are given in the last chapter.) Because this is largely a book on formal derivations and methodology, several of the interpretative aspects that one might have expected are absent: There is no population analysis, no Bader analysis of bonding properties, no discussion of the Morokuma energy partitioning, no physical discussion of bonding properties. While the standard textbook analysis of Koopmans' theorem is extended to include electron affinities as well as ionization energies, the authors do not point out that the electron affinities are almost always substantially worse numerically than the ionization energies. Nor do they explain why this is true.

Other aspects that do not appear include semiempirical theories and energy derivative methods. Despite the extremely important work that these authors have done in the development and application of response theories for the calculation of excited state properties and molecular response properties, no extended discussion of the response properties appears in the text.

The specific problem of molecular electronic-structure theory and models requires analysis at many levels. On balance, this text provides what I believe to be a comprehensive, careful, meticulous, and clear development of the formalism of wavefunction-based ab-initio electronic-structure theory for molecules. It is the most complete and satisfying presentation of the actual armament involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basis of contemporary molecular electronic structure methods.

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100 Years of Planck's Quantum

Ian Duck and E. C. G. Sudarshan
World Scientific, River Edge, N.J., 2000. $86.00 (545 pp.)
ISBN 981-02-4309-X

Ian Duck and E. C. G. Sudarshan's *100 Years of Planck's Quantum* is an unusual hybrid of a reprint volume and a running commentary on the papers being reprinted. The authors, who are "interpreters" as much as editors, believe that one should have as a basis the actual words of the scientists as they went through their creative processes. At the same time, they are aware that history has selected the important from the unimportant, changing the emphasis from what the creators might have thought was important to what seems important in light of subsequent events. In some cases of course, the originators had it exactly right!

Duck and Sudarshan believe that their selection requires a continuing commentary to place the papers within a modern historical context. Their aim is clearly not to provide the reader with a historical document as such.