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.

Rather, they want to provide the flavor of the original papers, most of which are excerpted rather than reprinted in full, and to help the reader interpret the papers within a context that was not apparent at the time the papers were written.

As a consequence, one gets a rather uncommon blending of original works colored strongly by a layer of interpretation, sometimes quite insightful and sometimes historical. It is rather like one of those music appreciation courses in which the pianist plays a passage of a famous piece and then dissects it; one ends up with less than a full picture of the whole, but generally with a much better idea of how the piece was put together and how its various parts interrelate.

Of course, within the framework of 100 years of the quantum, there is a lot of selecting to do. For this purpose, the authors make a conscious decision to limit themselves to nonrelativistic and non-field-theoretic aspects of the subject. They divide the book into four parts. The first deals with work that precedes modern quantum theory. Here they emphasize the work of Max Planck, Albert Einstein, Arthur Compton, and Niels Bohr. But they also include a prescient paper by Hendrik Kramers and Werner Heisenberg, and an explanatory paper on action variables by Karl Schwarzschild.

Part two is devoted to the classical development of the formalism of quantum theory, including Heisenberg's matrix formulation, the famous "dreimännerarbeit" of Max Born, Heisenberg, and Pascual Jordan, explaining Heisenberg's breakthrough in terms of orthodox matrix techniques and commutation relations, and P A. M. Dirac's independent reformulation of the theory, as well as Erwin Schrödinger's wave interpretation. They also discuss some of the early interpretational battles Heisenberg and Bohr had with Schroedinger. Part three is devoted to some classic interpretational questions, including Born's work on interpreting the magnitude of the wave function in terms of probability. It also includes Heisenberg's introduction of the uncertainty principle and Bohr's complementarity. Finally there is a discussion of the famous EPR (Einstein-Podolsky-Rosen) "paradox," and Bohr's answer. During the discussions, they manage to bring out the various personality conflicts involved.

The last part of the book includes modern developments such as John Bell's demonstration that one could distinguish experimentally between the EPR and Bohr points of view, the derivations of Bell's inequalities, and some of the now classic experiments such as Alain Aspect's, which tested these results and thus lent their weight to the conventional quantum interpretation. The authors also introduce the Feynman path integral as an especially important modern development.

The rest of the chapter is the only really debatable part of the book, so far as the authors' choice of material is concerned. It includes some modern attempts at alternative interpretations of the subject, and many readers would quibble at their selection. Included are papers by James Hartle, Hartle and Murray Gell-Mann, and Bryce DeWitt, on versions of decoherence and consistent-histories interpretations, because these offer a possibility of interpreting the concept of a wavefunction for the entire universe, necessary for a cosmological extension of quantum mechanics. This inclusion reflects the authors' own interest in particle physics, and although they are rather admirably constrained in their comments concerning an ultimate "theory of everything," they still seem to be somewhat infected by this particular bug, an occupational hazard for particle physicists. Other types of interpretations, such as Bohm's trajectories or many world interpretations, don't impress them as very relevant.

Finally, Duck and Sudarshan have very positive things to say about an informational interpretation of the wave function, and they discuss David Deutsch's introduction of quantum mechanical computers. However, whenever they discuss the "conventional" interpretation, they incorporate a density matrix approach and do not seem to believe that the wavefunction makes sense for an individual system. That would be the case for a frequency interpretation of probability. But one of the great strengths of an informational approach is that it gives meaning to the wavefunction for an individual system, because a single experiment can provide information about such a system. In contrast, a frequency interpretation only gives probabilities of occurrence within ensembles of systems. So their comments don't seem to me to take full advantage of the possibilities opened up by an informational approach.

At the end of the book, Duck and Sudarshan have some fun speculating about the future of quantum mechanics, although they are fully aware of the unreliability of such projections. They do have some interesting things to say about physicists themselves being partly responsible for the general lack of interest in the subject by nonphysicists.

When you have finished the book, you will have read parts of some papers that you probably would not have otherwise read, and you will have been given a guided tour through confusing territory by some wise and knowing guides. A different tour might have covered different landmarks, but you will have gotten your money's worth. Can't ask for more than that!

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Encyclopedia of Astronomy and Astrophysics

Edited by Paul Murdin
IOP (Nature Publishing Group), Philadelphia, 2001.
$650.00 set (3670 pp.).
ISBN 0-333-75088-8 (set)

This four-volume *Encyclopedia of Astronomy and Astrophysics* summarizes a great deal of what we knew in the astronomical sciences at the most recent millennium. An associated Web site http://www.ency-astro.com may keep much of it up-to-date for years to come. The contents are extensive indeed: The index alone consists of 76 pages, each with three columns of fine-type listings, and there are "nearly 700 main articles" in the words of Paul Murdin, editor-in-chief. Murdin was assisted by editorial and advisory boards comprising 33 persons, most of them prominent astrophysicists but including the celebrated amateur astronomer Patrick Moore.

The main articles are what make the new *Encyclopedia* worthwhile. They are generally by experts, who took much care in their preparation. Impressive examples are "Stellar Evolution" by Jørgen J. Christensen-Dalsgaard and "Venus: Interaction with Solar Wind," by Christopher T. Russell and Janet G. Luhmann. The degree to which the articles are illustrated and referenced, however, seems to depend on the inclination of the individual author. "Blue Stars at High Galactic Latitudes," by John S. Drilling, is less than four and one-half pages long, cites nine works published from 1965 through 1998, but is not illustrated. "Proper Motion: Optical/Infrared," by Arnold R. Klemola, runs seven pages, with two small geometric diagrams, six bibliographical citations, and a table of large astrometric catalogs with 20 footnoted references. On the other hand, articles on Saturn's rings and its satellites are heavily illustrated, but with just two or three citations in each.

The coverage of solar physics is especially thorough. There are numer-