Paul and Tatiana Ehrenfest book *Conceptual Foundations of the Statistical Approach in Mechanics* (Dover, 1990) involving "hypothetical functions as constants of the motion." He stops short of saying that such functions are nonmeasurable, a mathematical notion denoting the impossibility of writing tables of values. ("Nonmeasurable" is equivalent to a physicist's "nonexistent.") Since considering such hypothetical functions as observables had a pernicious influence, and because of the prestige of the Ehrenfests' treatment, this section could have been a good place for a few more critical details.

A concise analysis of the classical kinetic theory follows. The theory derives and illustrates the Boltzmann equation from a critical perspective. To students, it will be inspiring to find here topics that must otherwise be pursued through the literature, (such as Mark Kac's ring model or Paul Ehrenfest's urn model). Dorfman continues with a physical discussion of the meaning of recurrence, ergodicity, or mixing, concepts that are not yet in the cultural heritage of most physicists (chapters 3–6). The Green–Kubo formulae are discussed in chapter 7, in which the van Kampen objections are exposed carefully and in some detail.

Then Dorfman attempts to link the "classical" and the more recent views on chaos. His choice of the baker's maps to illustrate chaotic motion properties is motivated by their mathematical simplicity. However, "simplicity" is very subjective, and it is not entirely clear that he has made the best choice. The possibility of "computing everything" may induce some readers to lose sight of conceptual difficulties and understandings and to think that everything boils down to technicalities, despite Dorfman's repeated warnings.

Symbolic dynamics, Lyapunov exponents, and Kolmogorov–Sinai (KS) entropy are introduced mostly from the viewpoint of the corresponding properties of the baker's map. The SRB (Sinai–Ruelle–Bowen) distributions, the nonequilibrium extension of the Boltzmann–Gibbs distribution, are the central theme of the second half of the book, and Dorfman makes an effort to clarify their meaning via relatively simple calculations. He briefly discusses the "escape rate formalism" that played an important part in showing that something as concrete as a transport coefficient could come out of the "new" ideas and be useful at interpreting simulations. He makes the basic ideas of the "thermodynamic formalism" accessible, stressing clearly its surprising relationship to one-dimensional lattice gas statistical mechanics; the "triviality" of the latter renders feasible the apparently intractable analysis of certain chaotic motions.

Dorfman's pace is fast, at places a bit too fast; it leads to, as he says, "combining almost everything discussed" into the exposition of the Lorentz–Boltzmann equation for Lyapunov exponents and KS entropy of the Lorentz gas—a remarkable novelty in kinetic theory, in which everyone hoped, but hardly expected, to see something new.

It is far from clear that the approach displayed in this book will maintain the rate of development shown so far, as Dorfman implies throughout. In any event, this will remain a first and needed step toward a systematic simple presentation of a developing methodology.

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Introduction to Quantum Mechanics in Chemistry

Mark A. Ratner and George C. Schatz
Prentice Hall, Upper Saddle River, N.J., 2001. $86.00 (305 pp.). ISBN 0-13-895491-7

The 1998 Nobel Prize in Chemistry, awarded to Walter Kohn and John A. Pople, demonstrated the influence that computational quantum chemistry has had on the entire field of chemistry. This influence is likely to grow and spill into other active research areas in the near future. An introductory text bridging the gap between the basics of quantum mechanics and the application of ab initio and semi-empirical quantum chemistry theories to problems of chemical interest is thus highly desirable. The textbook, *Introduction to Quantum Mechanics in Chemistry* by Mark A. Ratner and George C. Schatz, which is aimed at nontheoretical chemists and undergraduate students, effectively provides this link. It is a concise, easily readable, and understandable introduction to quantum chemistry and the methods currently used in chemical applications.

After a brief review of the laws of classical mechanics and wave theory, the reader is introduced to the quantum mechanical treatment of the par-

ticle in a box, the rigid rotor, the harmonic oscillator, and the hydrogen atom. The variational method, electron spin, Slater determinants, and Hartree–Fock theory are presented along with the treatment of helium and other many-electron atoms. This review leads to the discussion of ab initio, density-functional, and semiempirical quantum chemistry methods and their performance in typical applications. The suggested readings at the end of each chapter cite the classics in the field, to which interested students may go for more in-depth discussions of the topics.

Significant strengths of this book are the many exercises (and answers) that the authors disperse along the text and the wealth of problems given at the end of each chapter. These are extremely useful for working out derivations and deepening understanding of difficult parts. The "numerical" problems following the chapter "Applications of Electronic Structure Theory" involve the ab initio and density-functional computation of energies and structures of mostly small molecules and a comparison with the experimental and theoretical literature. Discussion of these problems allows the student to learn about the strengths and weaknesses of current computational methods. These problems are additionally well suited to an introductory, hands-on class in computational quantum chemistry. The last 30 pages of the book present solutions to the odd-numbered problems.

When writing a textbook that covers such a wide range of topics in only some 300 pages, the treatment of certain topics will surely require that compromises be made. Although one might argue that certain topics would deserve a more in-depth treatment, we feel that this textbook is well balanced overall. The book mentions, but does not discuss in detail, such advanced computational methods such as multiconfiguration, self-consistent field, or coupled-cluster theory. Nevertheless, it provides a basic understanding of the principles underlying quantum chemistry. The reader, armed with this knowledge, can then more easily study advanced books in quantum chemistry. The chapter, "Applications of Group Theory," however, might be difficult for undergraduates, because its coverage ranges from symmetry operations to constructing symmetry-adapted linear combinations—in a mere 20 pages. This chapter might well benefit from a more detailed discussion, or from a less ambitious coverage.

There is a conceptual similarity

between Ratner and Schatz's text and such other popular books in the subject as *Quantum Chemistry*, by Ira N. Levine (Prentice Hall, 1999). Levine's book offers a more detailed discussion (some 600 pages) on several topics, but it mostly addresses a different audience: graduate students. The attempt of Ratner and Schatz to offer a concise and easily understandable text to undergraduate students is highly commendable.

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Methods of X-Ray and Neutron Scattering in Polymer Science

Ryong-Joon Roe
Oxford U. Press, New York, 2000. $80.00 (331 pp.).
ISBN 0-19-511321-7

A great deal of similarity exists between x-ray and neutron scattering methods as applied to the study of the structure of matter. Historically, however, the two methods were developed at different times by different groups of scientists; as a result, very different terminologies often evolved to explain the same phenomena. By presenting the two methods together and emphasizing their similarities, Ryong-Joon Roe has written an introductory textbook that enables readers to become equally familiar with both techniques. For this reason, *Methods of X-Ray and Neutron Scattering in Polymer Science* meets a need that has not been adequately addressed by the many earlier textbooks and monographs, which have dealt principally with one method or the other.

Roe succeeds admirably in giving a balanced and unified presentation of the basic theory underlying both x-ray and neutron scattering. He uses a consistent set of symbols and nomenclature throughout the book and carefully explains and justifies any deviations from conventions used in specialized areas of the literature.

The book is aimed at readers with little prior exposure to scattering phenomena; it covers a range of topics at modest length without oversimplifying the subject matter or becoming bogged down in formalism. Expressions and relationships are developed clearly from first principles in most cases; in others, heuristic arguments are used effectively, or the reader is referred to one or more sources for a more rigorous treatment. Experimental results are used sparingly and only to illustrate how the theoretical concepts or the methods of analysis discussed are used in practice.

The first two chapters, covering the basic theory and experimental methods of x-ray and neutron scattering, are among the book's best and are not at all specific to polymer science. These chapters provide a firm foundation for understanding the applicability of the techniques to any type of material. Building on this basis, the subsequent chapters, on topics such as crystalline and amorphous polymers, blends, and copolymers, are presented as largely self-contained units that can be studied individually. Even among these more specialized chapters, there is much to recommend to a broad audience. For example, chapters 3 and 4, on scattering from crystalline and amorphous polymers, respectively, cover clearly and concisely the basics of crystal structure analysis, including methods of phase determination, diffraction-line broadening, crystal imperfections, short-range order, pair distribution functions, texture, and the like at a level that is both accessible and germane to students in any area of materials science.

Separate chapters address small-angle scattering and reflectivity, techniques that have probably had more impact on polymer science than any other area of materials science. In each case, Roe makes connections with the basic theory covered in the opening chapters to give the reader a unified view of diffraction. The chapter on small-angle scattering is particularly well organized and includes an excellent summary of the manifestations and analyses of lamellar structure so often encountered in polymer systems. The methods of deuterium labeling and contrast variation that give neutron scattering its unique role in characterizing structure in hydrogenous materials are also largely contained in a single chapter, which focuses on their application to polymer blends and block copolymers. The final chapter deals with inelastic neutron scattering and surveys succinctly the types of molecular motions that may be probed and the experimental techniques for doing so. The associated concepts and mathematical expressions are inherently more complex in this case, but here again Roe builds on and extends the foundation laid in the early chapters to present the material in a way that