Theor Chem Acc (2003) 110: 358
DOI 10.1007/s00214-003-0481-z

Theoretical
Chemistry Accounts

Book review

Bernd A. Hess (ed): Relativistic Effects in Heavy-Element Chemistry and Physics

John Wiley & Sons, 2003. 307 pp (ISBN 0470841389) US $140

Uzi Kaldor

School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel

Published online: 4 November 2003

In the last few decades, quantum chemists began to realize that relativity has a profound effect on the chemical and physical behavior of atomic and molecular systems, particularly those including heavy elements. Much of the research effort in this field took place in Europe, and was greatly assisted by generous support of European granting bodies. The European Science Foundation established a REHE program which operated between 1993 and 1998, supporting many mutual visits as well as an impressive series of conferences and workshops. An even larger program (in financial terms) was sponsored by the German Science Foundation (DFG) between 1994 and 2000, funding some 30 research groups. This activity provided ample opportunity for establishing collaborations and fruitful exchange of ideas, and contributed significantly to the rapid development of the field. This book is the final report of the German REHE project.

The book is compact (300 pages in small format), and presents an intermediate between a monograph and a collection of articles. The seven chapters were written by seven groups of authors (although the table of contents and list of contributors do not tell who wrote which chapter; one has to go to the actual chapter to find that), but appear in uniform style and even have a joint bibliography. This attests to singular discipline on the part of the authors and/or very hard work on the part of the editor. Most major subjects in the field are covered, starting with quantum electrodynamics in strong fields, going through ab initio four-component methods, more approximate methods (two-component, pseudopotentials, relativistic density functional theory), and ending with two chapters where the methodology is applied to real "wet" chemistry.

Uniform appearance notwithstanding, not all subjects are covered at the same level. The first (and longest) chapter discusses quantum electrodynamics in strong fields in considerable detail. The second chapter, on the other hand, gives a rather brief description of four-component methods; this is compensated by a thorough compilation of applications, accompanied by an extensive bibliography, which the present reviewer found very useful. The third chapter, which combines the two rather disparate subjects of transformed Hamiltonians and effective core potentials, is also rather brief, but conveys the salient points of the two methods and is rich with pertinent examples. The theory and applications of relativistic density functional theory, a subfield showing rapid development in recent years, are described in detail in Chap. 4, followed by a separate chapter devoted to magnetic phenomena in solids, also studied by relativistic density functional theory. It is a nice touch to conclude the book with two chapters describing the strong interaction between theory and experiment, one discussing the generation and characterization of superheavy elements, and the other showing how relativistic effects influence the chemistry of heavy d and f elements. All chapters, regardless of their depth of coverage, give reliable account of their subjects.

This concise book cannot cover all aspects of the rapidly evolving field. It provides, however, a tantalizing taste of many important subjects, and, together with the comprehensive bibliography, can give the interested reader a valuable overview and starting point for further exploration.

e-mail: kaldor@jade.tau.ac.il