Theoret. Chim. Acta (Berl.) 57, 265 (1980)

THEORETICA CHIMICA ACTA © by Springer-Verlag 1980

Book Review

C. A. Nicolaides and D. R. Beck (Eds.):

Excited States in Quantum Chemistry. Proceedings of the NATO Advanced Study Institute held at Kos, Greece, 1978. Dordrecht, Holland: D. Reidel Publishing Company 1979. IX + 572 pp. Cloth Dfl. 115.-/US-\$59.00

This volume is devoted to advanced quantum chemical methods applicable to the molecular excited state. As the Editors pointed out, the recent successes of experimental spectroscopy and photochemistry constitute a definite challenge to quantum chemists: "There is a need to create and/or apply general and useful approaches to the many-electron problem of the excited state which go beyond the independent particle model" capable of reproducing accurate experimental results and, if possible, provide guidance to experimentalists. The book is a quite successful attempt to describe the theoretical methods that hold promise to achieve this goal. These are based on configuration interaction, Green's functions, polarization propagator techniques, coherent potential and random phase approximations, many-body perturbation theory, cluster expansions, among others. The greatest contributors to this volume are Buenker and Peyerimhoff (BP) and Nicolaides and Beck (NB) with four chapters each. BP discuss the applications of their highly successful MRD-CI method to excitation energies and oscillator strengths for Rydberg and valence-shell states, vibrational energies and wavefunctions and molecular dissociation processes. NB deal with many body theory of photoabsorption in atoms and molecules including correlation, relativistic and radiation effects and the theory of non-stationary states within the coordinate rotation method. Other theoretical chapters are contributed by Linderberg (the polarization propagator), Von Niessen's group (Green's functions methods), Robb's group (many body perturbation methods), Öhrn (electron binding energies), Economou (disordered systems), Altick (atomic photoionization cross sections), Kunz (transition metal oxides), Collins (excitons in solids), Ladik (excited states of polymers) and Koutecky (surface states and chemisorption). In addition the book contains some important experimental chapters on lifetime measurements (Martinson), Auger electron spectra (Siegbahn) and the role of excited states in organic photochemistry (Michl).

The book is a valuable summary of the state of the art of many-body approaches to the treatment of the excited states of atoms, molecules and solids. It can be highly recommended to quantum chemists, spectroscopists, photochemists and to all other scientists interested in electronic excited states.

C. Sandorfy, Montréal

Received July 3, 1980