

*Books Received*

**Quantum Systems in Chemistry and Physics. Volume 1: Basic Problems and Model Systems, Volume 2: Advanced Problems and Complex Systems, Granada, Spain (1997).** Edited by Alfonso Hernández-Laguna (Estación Experimental del Zaidein, C.S.I.C., Granada, Spain), Jean Maruani (CNRS, Paris, France), Roy McWeeny (Università di Pisa, Italy) and Stephen Wilson (Rutherford Appleton Laboratory, Oxfordshire, UK). Kluwer (<http://www.wkap.nl>): Dordrecht. March 2000, 432 pp. NLG 345.00 / USD 182.00 / GBP 114.00. Hardbound Vol. 1, ISBN 0-7923-5969-0. 416 pp. NLG 335.00 / USD 178.00 / GBP 110.00. Hardbound Set of 2 volumes, ISBN 0-7923-5971-2

**Shu-Kun Lin**

Molecular Diversity Preservation International (MDPI), Saengergasse 25, CH-4054 Basel, Switzerland  
Tel.: +41 79 322 3379, Fax: +41 61 302 8918, E-mail: [lin@mdpi.org](mailto:lin@mdpi.org), <http://www.mdpi.org/lin/>

*Received: 7 September 2000 / Published: 30 September 2000*

These two volumes [1] are volumes 2 and 3 of the series *Progress in Theoretical Chemistry and Physics* [2,3]. They comprise forty papers coming from the most outstanding contributions to the Third European Quantum Systems in Chemistry and Physics Workshop held in Granada, Spain (1997). These books cover a very broad spectrum of scientific research work from quantum-mechanical many-body methods to important applications and computational developments, and from atoms and molecules to condensed matter.

The first volume is subtitled *Basic Problems and Model Systems*, and includes the following topics: density matrices and density functionals, electron correlation effects, relativistic formulations, valence theory, and nuclear motions.

The second volume is subtitled *Advanced Problems and Complex Systems* and covers the following topics: response theory, condensed matter, reactive collisions and chemical reactions, and computational chemistry and physics.

Contents: Preface. **1.** Density Matrices and Density Functionals. 3-Body Correlation Effects in Third Order Reduced Density Matrices; *C.Valdemoro, et al.* **2.** Electron Correlation Effects. Ab Initio Summation Over States/CI Singles for Static and Dynamic First Hyperpolarizabilities of Small

Molecules; *M. Spassova, et al.* Comparing (SC)<sup>2</sup>CAS-SDCI and Externally Corrected CCSD Methods; *G. Peris, J.P. Malrieu.* The Size-Consistent Self-Consistent SDCI Method for Excited States and Ionization Potentials; *J. Pitarch-Ruiz, et al.* Influence of Electron Correlation on the Electronic Structure of Superconducting Y-Ceramics; *I.G. Kaplan, et al.* **3.** Relativistic Formulations. Perspectives in Relativistic Thomas-Fermi Calculations for Atomic Systems; *I.Porrás, A. Moya.* Expectation Values for Ground State Atoms from a Modified Thomas-Fermi-Diract Approach; *A. Moya, I. Porrás.* Relativistic oscillator strengths for excited-state transitions in halogen atoms. Regularities; *C. Lavin, et al.* Extension of the Relativistic Quantum Defect Orbital Method to the Treatment of Many-valence Electron Atoms. Atomic Transition in Ar II; *I. Martíin, et al.* **4.** Valence Theory. **5.** Nuclear Motions. The Effect of the Pseudopotential on the Torsional Energy Levels of Hydrogen Peroxide and Deuterium Peroxide; *M.L. Senent, Y.G. Smeyers.* **6.** Response Theory. Duality in Two-ways Interferometers: The Symmetric Quanton-Detecton System; *J. Martínez-Linares, D.A. Harmin.* Atomic Resonances in External Field; *R. González-Ferez, W. Schweizer.* **7.** Condensed Matter. Diffusion Monte Carlo Calculations of Quasibound States of Rare Gas-halogen Clusters: a Diabatic Approach; *G.García-Rizo, et al.* **8.** Reactive Collisions and Chemical reactions. Electro-nuclear Quantum Mechanics Beyond the Born-Oppenheimer Approximation. Towards a Quantum Electronic Theory of Chemical Reaction Mechanisms. **9.** Computational Chemistry and Physics. N-O and P-O Bond Nature in Hypervalent Compounds. Is Bader Analysis Basis Set and Geometry Independent? *J.A. Dobado, et al.* A Theoretical Study of the Radical Addition to the Xylenes; *V.-H.Uc, et al.* Theoretical Study of the Proton Affinities of Some Substituted Derivatives of Histamine and Homologous Compounds. Structure-Activity Relationships.

## References and Notes

1. <http://www.wkap.nl/book.htm/0-7923-5971-2>.
2. Website <http://www.wkap.nl/series.htm/PTCP>.
3. Please contact Customer Services ([services@wkap.nl](mailto:services@wkap.nl)) for set price information.