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Nota di contenuto	<p>""1. Why a Reappraisal Is Necessary """"2. The Relevance of the Classical Framework ""; ""3. On the Two Kinds of Incompatibility ""; ""4. Wholeness and the Proper Logic for Complementarity ""; ""5. The Reduction of Duality ""; ""References ""; ""COMPLEMENTARITY OUT OF CONTEXT: ESSAY ON THE RATIONALITY OF BOHRa€S THOUGHT""; ""Abstract ""; ""1. Complementarity Contextualized ""; ""2. Complementarity: A Stumbling Block on the Way to Context ""; ""3. The Duality Route to Context ""; ""4. Incommensurability: Last Resorta€?and Last Exit ""; ""5. The Concept of Action Quantization ""</p> <p>""6. Tying Loose Ends """"Appendix ""; ""Notes ""; ""References ""; ""MOLECULAR INTEGRALS OVER SLATER-TYPE ORBITALS. FROM PIONEERS TO RECENT DEVELOPMENTS""; ""Abstract""; ""1.Introduction""; ""2.Early History of the Slater Orbitals""; ""3.History of the STO Computer Programs""; ""4.Slater Orbitals & Gaussian Orbitals""; ""5. Types of Exponentially Decaying Orbital, Based on Eigen-functions for One-Electron Atoms""; ""6.Types of Integral over Slater Orbitals""; ""6.1. One-Electron Integrals""; ""6.2.Two-Electron Integrals""; ""6.3.Three- and Four-Electron Integrals""</p> <p>""7.Methods in the Literature""""7.1.Single-Center Expansion""; ""7.2. Gaussian Expansion""; ""7.3.Gaussian Transform Method""; ""7.4. Fourier-Transform Method""; ""7.5.Use of Sturmians""; ""7.6.Elliptic Coordinate Method""; ""8.General Two-electron Exponential Type Orbital Integrals in Poly-Atomics without Orbital Translations""; ""8.1.</p>

Introduction"; ""8.2.Basis Sets""; ""8.3.Programming Strategy""; ""8.4. Avoiding ETO Translations for Two-Electron Integrals over Three and Four Centers""; ""8.5.Numerical Results of Coulomb Resolutions: Efficiency""
 ""8.6.Selected Exchange Integrals for the CH₃F Molecule (Evaluated Using the Coulomb Resolution)""""8.7.Conclusions""; ""9.Explicitly Correlated Methods for Molecules""; ""10.Highly Accurate Calculations Using STOs""; ""11.Closing Remarks""; ""Acknowledgements""; ""References""; ""TUNNELING DYNAMICS AND ITS SIGNATURES IN COUPLED SYSTEMS""; ""Abstract""; ""1.Introduction""; ""2.Historical Development""; ""A.Tunneling in Physics""; ""B.Tunneling in Chemistry""; ""C.Tunneling in Coupled Systems""; ""3.The Method""; ""A.Dynamics of the Coupled System in the Absence of Driving""
 ""B.Dynamics of the Coupled System in the Presence of External Driving""

Sommario/riassunto

This volume gives larger and deeper coverage of the electronic matters through the physical, chemical and biological ordered systems. With their increasing complexity, the matter structure from the physical to chemical to biological manifestations in an inter-disciplinary cross-fertilisation manner is gradually introduced. The book presents and reviews the avant-garde contributions for the XXI century with equilibrated contents provided by important scientists world-wide demonstrating a valuable impact on quantum fundamentals and applications. In fact, the present volume attempts to serve the unification of the physical-chemical-biological manifestation of atoms in molecules and in nanostructures by means of expanding the quantum frontiers by conjunction, either with relativity, topological information or graph theories as well.
