

1. Record Nr.	UNINA9910457028503321
Titolo	Quantum frontiers of atoms and molecules [[electronic resource] /] / editor, Mihai V. Putz
Pubbl/distr/stampa	Hauppauge, N.Y., : Nova Science Publishers, c2011
ISBN	1-61324-867-9
Descrizione fisica	1 online resource (687 p.)
Collana	Chemistry research and applications
Altri autori (Persone)	PutzMihai V
Disciplina	541/.28
Soggetti	Chemical bonds - Mathematical models Dirac equation Quantum chemistry Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
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</p>

Coordinate Method""; ""8.General Two-electron Exponential Type Orbital Integrals in Poly-Atoms without Orbital Translations""; ""8.1. 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""

2. Record Nr.	UNISA996393291403316
Titolo	By the Lords-Justices and Council. A proclamation [[electronic resource]] : Charles Porter Tho: Coningesby. Whereas all due care has been taken for the keeping up and preserving the markets in all parts of this kingdom under their Majesties obedience, whereto all persons may resort with freedom and liberty of trade and commerce; .
Pubbl/distr/stampa	Dublin, : Printed by Andrew Crook assignee of Benjamin Tooke, printer to the King and Queen at thier Majesties printing-house on Ormonde-Key, [1691]
Descrizione fisica	2 sheets ([2] leaves)
Altri autori (Persone)	ConingsbyThomas Coningsby, Earl, <1656?-1729.>
Soggetti	Markets - Ireland Ireland History 17th century Early works to 1800 Ireland History War of 1689-1691 Early works to 1800
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Title from caption and opening words of text. Imprint from colophon.

"Given at the Council-Chamber in Dublin 25th. day of September,
1691."

For the encouragement of markets and agriculture.--Steele.

Steele notation: Arms 201. the said p.2) upon their.

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Sommario/riassunto

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