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Titolo	Human behavior analysis for library and information science / / Mu-Yen Chen [and three others], editors
Pubbl/distr/stampa	[Place of publication not identified] : , : Emerald Publishing Limited, , 2017
ISBN	1-78754-009-X
Descrizione fisica	1 online resource (225 pages)
Disciplina	150.721
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Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia

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Titolo	Applications of Topological Methods in Molecular Chemistry / / edited by Remi Chauvin, Christine Lepetit, Bernard Silvi, Esmail Alikhani
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ISBN	3-319-29022-3
Edizione	[1st ed. 2016.]
Descrizione fisica	1 online resource (582 p.)
Collana	Challenges and Advances in Computational Chemistry and Physics, , 2542-4491 ; ; 22
Disciplina	540
Soggetti	Chemistry, Physical and theoretical Topology Theoretical and Computational Chemistry
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Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Part I. Topological Methods : Definition, State of the Art and Prospects

-- 1. On quantum chemical topology -- 2. Localization-Delocalization and Electron Density-Weighted Connectivity Matrices: A Bridge Between the Quantum Theory of Atoms in Molecules and Chemical Graph Theory -- 3. Extending the Topological Analysis and Seeking the Real-Space Subsystems: The Case of Non-Coulombic Systems with Homogenous Potential Energy Functions -- 4. Exploring Chemistry Through the Source Function for the Electron and Spin Densities -- 5. Emergent Scalar and Vector Fields in Quantum Chemical Topology -- 6. Topology of Quantum Mechanical Current Density Vector Fields Induced in a Molecule by Static Magnetic Perturbations -- 7. Topological Analysis of the Fukui Function -- 8. Topological Tools for the Study of Families of Reaction Mechanisms: the Fundamental Groups of Potential Surfaces in the Universal Molecule Context -- 9. Quantum Chemical Topology Approach for Dissecting Chemical Structure and Reactivity -- Part II. Topological Methods for the Characterization of -Electron Delocalization and Aromaticity -- 10. Paradise Lost - -Electron Conjugation in Homologs and Derivatives of Perylene -- 11. Rules of Aromaticity -- 12. Localized Structures at the Hückel Level, a Hückel-Derived Valence Bond Method -- 13. Magnetic Properties of Conjugated Hydrocarbons from Topological Hamiltonians -- Part III. Topological Methods for the Characterization of Weak Bonding Interactions -- 14. What Can be Learnt from a Location of Bond Paths and from Electron Density Distribution? -- 15. Following Halogen Bonds Formation with Bader's Atoms-in-Molecules Theory -- 16. Charge Transfer in Beryllium Bonds and Cooperativity of Beryllium and Halogen Bonds -- 17. A Complete NCI Perspective: From New Bonds to Reactivity -- 18. Diversity of the Nature of the Nitrogen-Oxygen Bond in Inorganic and Organic Nitrites in the Light of Topological Analysis of Electron Localisation Function (ELF) -- 19. Quantum Chemical Topology in the Field of Quasirelativistic Quantum Calculations. .

Sommario/riassunto

This is the first edited volume that features two important frameworks, Hückel and quantum chemical topological analyses. The contributors, which include an array of academics of international distinction, describe recent applications of such topological methods to various fields and topics that provide the reader with the current state-of-the-art and give a flavour of the wide range of their potentialities.