1. Record Nr. UNINA9910298597403321

Autore	Putz Mihai V
Titolo	Structural Chemistry : Principles, Methods, and Case Studies / / by Mihai V. Putz, Fanica Cimpoesu, Marilena Ferbinteanu
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2018
ISBN	3-319-55875-7
Edizione	[1st ed. 2018.]
Descrizione fisica	1 online resource (825 pages) : color illustrations
Disciplina	541.2
Soggetti	Chemistry, Physical and theoretical Building materials Theoretical and Computational Chemistry Structural Materials Physical Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Atomic Structure and Quantum Mechanics -- Wave Function Theories and Electron Structure Methods. Quantum Chemistry, from Atoms to Molecules -- Density Functional Theory: from conceptual level towards practical functionality -- Bond! Chemical Bond. Electron Structure Methods at Work -- New keys for Old Keywords. Hybridization and Aromaticity, Graphs and Topology -- The Coordination Bonding. Electronic Structure and Properties -- The Modelling in Molecular Magnetism -- Bonding in Rings and Clusters -- Add on. The Bondon-a new theory of electron effective coupling and density ensembles.
Sommario/riassunto	This book explains key concepts in theoretical chemistry and explores practical applications in structural chemistry. For experimentalists, it highlights concepts that explain the underlying mechanisms of observed phenomena, and at the same time provides theoreticians with explanations of the principles and techniques that are important in property design. Themes covered include conceptual and applied wave functions and density functional theory (DFT) methods, electronegativity and hard and soft (Lewis) acid and base (HSAB) concepts, hybridization and aromaticity, molecular magnetism, spin

transition and thermochromism. Offering insights into designing new properties in advanced functional materials, it is a valuable resource for undergraduates of physical chemistry, cluster chemistry and structure/reactivity courses as well as graduates and researchers in the fields of physical chemistry, chemical modeling and functional materials.