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Altri autori (Persone)	MacgregorStuart A
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Nota di contenuto	Interpreting Non Covalent Bonds with the Block Localized Wave Function (BLW) Method -- Local Energy Decomposition of Coupled Cluster Energies Principles and Applications -- Electron Density based Energy Decomposition Analysis from QM to QM/MM calculations -- GKS EDA method for intermolecular interactions in complex systems -- SAPT and many body dispersion: Intermolecular interactions at cubic scaling cost -- Survey of contemporary applications of Quantum Chemical Topology -- The Interpenetration Index and its applications in chemistry -- Exhibiting noncovalent interactions in dynamic environments using aIGM method.
Sommario/riassunto	This volume showcases state-of-the-art computational methodologies

for the description and analysis of non-covalent interactions. Each chapter focusses on a specific approach, outlining a theoretical framework for the method in hand that is then illustrated by cutting-edge applications. A range of energy decomposition analyses and real-space topological and geometrical schemes are covered, providing a menu of approaches from which to draw insight into non-covalent interactions. The book serves as a comprehensive resource for computational chemists, as well as experimental chemists seeking to understand how computational techniques can be applied in their research.
