1. Record Nr. UNISALENTO991003876789707536

Autore	Thurber, James
Titolo	Further Fables for Our Time/ James Thurber
Pubbl/distr/stampa	Harmondsworth : Penguin Books, 1960
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia

2. Record Nr. UNINA9911035051403321

Autore	Martín-Fernández Carlos
Titolo	Computational Methods for the Analysis of Non-Covalent Interactions / / edited by Carlos Martín-Fernández, Stuart A. Macgregor
Pubbl/distr/stampa	Cham : , : Springer Nature Switzerland : , : Imprint : Springer, , 2025
ISBN	9783032015433
Edizione	[1st ed. 2025.]
Descrizione fisica	1 online resource (446 pages)
Collana	Structure and Bonding, , 1616-8550 ; ; 190
Altri autori (Persone)	MacgregorStuart A
Disciplina	542.85
Soggetti	Chemistry - Data processing Quantum chemistry Coordination compounds Organometallic chemistry Chemistry, Inorganic Bioinorganic chemistry Computational Chemistry Quantum Chemistry Coordination Chemistry Organometallic Chemistry Main-Group Chemistry Bioinorganic Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia

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.