1. Record Nr. UNINA9910855368403321

Autore	Matta Cherif F
Titolo	Electron Localization-Delocalization Matrices / / by Chérif F. Matta, Paul W. Ayers, Ronald Cook
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2024
ISBN	9783031514340 3031514343
Edizione	[1st ed. 2024.]
Descrizione fisica	1 online resource (235 pages)
Collana	Lecture Notes in Chemistry, , 2192-6603 ; ; 112
Altri autori (Persone)	AyersPaul W CookRonald
Disciplina	541.22
Soggetti	Chemistry, Physical and theoretical Mathematical physics Chemistry - Data processing Chemometrics Mathematics Statistics Theoretical Chemistry Theoretical, Mathematical and Computational Physics Computational Chemistry Mathematical Applications in Chemistry Applications of Mathematics Statistics in Engineering, Physics, Computer Science, Chemistry and Earth Sciences
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	An Introduction to Electron Localization-Delocalization Matrices -- The Physics of Electron Localization and Delocalization -- The Quantum Theory of Atoms in Molecules and Electron Localization and Delocalization -- Localization-Delocalization Matrix Representation of Molecules -- Molecular Fingerprinting using Localization-Delocalization Matrices: Computational Aspects -- Principal Component Analysis of Localization-Delocalization Matrices --

Localization-Delocalization Matrices Analysis for Corrosion Inhibition -- Localization-Delocalization Matrices Analysis in Predicting Mosquito Repellency -- Modeling Enzyme-Substrate Interaction with Localization-Delocalization Matrices -- Localization-Delocalization Matrices of Large Systems -- Closing remarks.

Sommario/riassunto

This book builds bridges between two yet separated branches of theoretical and mathematical chemistry: Chemical Graph Theory and Electronic Structure Calculations. Although either of the fields have developed their own techniques, problems, methods, and favorite benchmark cases independent from each other, the authors have managed to bring them together by using the localization-delocalization matrix (LDM). The LDM is a novel molecular descriptor that fingerprints a molecule by condensing the complicated electronic information in one, mathematically manageable, object. In this book, the authors introduce the readers to modeling techniques based on LDMs. Their technique offers a high accuracy as well as robust predictive power, often dramatically surpassing the potential of either of the constituting methods on their own. In addition to the comprehensive and accessible introduction to this new field of theoretical chemistry, the authors offer their self-developed software free to download, so that readers can try running their own simulations. The described methods are very general and can easily be implemented for calculating various properties and parameters such as mosquito repelling activity, ionic liquid properties, local aromaticity of ring molecules, log P's, pKa's, LD50, corrosion inhibition activities, and Lewis acidities and basicities – to only name a few. The free downloadable software helps readers automate the analysis of the matrices described in this book and hence facilitates application of the described methodology. .