

1. Record Nr.	UNINA9910855368403321
Autore	Matta Chérif F
Titolo	Electron Localization-Delocalization Matrices
Pubbl/distr/stampa	Cham : , : Springer International Publishing AG, , 2024 ©2024
ISBN	3-031-51434-3
Edizione	[1st ed.]
Descrizione fisica	1 online resource (235 pages)
Collana	Lecture Notes in Chemistry Series ; ; v.112
Altri autori (Persone)	AyersPaul W CookRonald
Disciplina	541.22
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Intro -- Foreword -- Preface -- Acknowledgments -- Contents -- About the Authors -- 1 An Introduction to Electron Localization-Delocalization Matrices -- References -- 2 The Physics of Electron Localization and Delocalization -- 2.1 What do we mean by Electron (De)Localization? -- 2.2 Pauli's Exclusion Principle and the Formation of Localized Electron Pairs -- 2.3 Conclusions -- References -- 3 The Quantum Theory of Atoms in Molecules and Electron Localization and Delocalization -- 3.1 The Electron Density: Introductory Concepts -- 3.2 From the Topography of the Electron Density to the Topology of a Bonded Structure -- 3.3 The Zero-Flux Surface as a Condition for a Well-Defined Quantum Subsystem -- 3.4 Examples of Properties of Atoms in Molecules -- 3.4.1 Examples of Bond Properties -- 3.4.2 Examples of Atomic Properties -- 3.5 Localization of Electrons within and their Delocalization between Atoms in a Molecule -- 3.6 The Delocalization Indices and Chemical Bonding by Example -- 3.6.1 Bonding to Titanium -- 3.6.2 Delocalization Indices and NMR Spin-Spin Coupling Constants -- 3.7 The Electron Localization-Delocalization Matrix (LDM) -- 3.8 The Interacting Quantum Atoms (IQA) Matrix (IQAM) -- 3.9 Closing Remarks -- References -- 4 Localization-Delocalization Matrix Representation of Molecules -- 4.1 Networks, Graphs, and Matrices: General Considerations -- 4.2 The Molecule as an Incomplete Network of Bond Paths -- 4.3 The Molecule

as Complete Network of Exchange Channels -- 4.4 Dissimilarity of Two Molecules as the Distance between their LDMs -- 4.5 Problems and Solutions of the LDM Representation of a Molecule -- 4.5.1 The Non-Uniqueness of an LDM in Specifying a Chemical Structure -- 4.5.2 Unequally-Sized Molecules or Molecules not Sharing a "Recognizable Common" Skeleton -- 4.5.3 Insensitivity to Optical Isomerism. 4.5.4 Conformational Flexibility -- 4.6 Closing Remarks -- References -- 5 Molecular Fingerprinting using Localization-Delocalization Matrices: Computational Aspects -- 5.1 Computational Implementation of LDM Analysis -- 5.2 The Triangle Inequality -- 5.2.1 Test Case 1: The First Four Saturated Aliphatic Hydrocarbons -- 5.2.2 Test Case 2: The Iso-Electronic Series with $N = 50$ Electrons -- 5.2.3 Test Case 3: Halogenated Benzoic Acids -- 5.3 Basis Set Effects -- 5.4 Closing Remarks -- References -- 6 Principal Component Analysis of Localization-Delocalization Matrices -- 6.1 The Localization-Delocalization Matrix as Tabulated Data -- 6.2 The Statistical Concepts of Covariance and Correlation -- 6.3 Some Basics of Principal Component Analysis (PCA) -- 6.3.1 A Numerical Example: H_2O -- 6.3.2 A More Elaborate Numerical Example: Imidazole -- 6.4 Factor Analysis (FA) Contrasted with Principal Component Analysis (PCA) -- 6.5 General Protocol for Applying PCA and FA to LDMs -- 6.6 Closing Remarks -- Appendix -- Proof that the Eigenvectors of a Symmetric Matrix Corresponding to Different Eigenvalues are Orthogonal -- Proof that the Eigenvalues of a Real and Symmetric Matrix are Real -- References -- 7 Localization-Delocalization Matrices Analysis for Corrosion Inhibition -- 7.1 Corrosion Inhibition Efficiency -- 7.2 The Exorbitant Economic Costs of Corrosion -- 7.3 First Case Study: Quantum Chemical Prediction of Corrosion Inhibitors' Efficiency -- 7.3.1 LDM Prediction of Corrosion Inhibitors' Efficiency Outperforms a Traditional Approach -- 7.3.2 Methodology of the LDMs Modeling of Corrosion Inhibitors' Efficiency -- 7.3.3 LDMs' Prediction of Corrosion Inhibitors' Efficiency -- 7.4 Second Case Study: Predicting Stress Corrosion Cracking Inhibitors' Efficiency -- 7.4.1 Stress Corrosion Cracking (SCC) Costs Lives and Treasury. 7.4.2 Structure-Activity Relationship of Stress Corrosion Cracking Inhibitors -- 7.4.3 Methodology of the LDMs Modeling of Stress Corrosion Cracking Inhibitors' Efficiency -- 7.4.4 QSAR and Mechanistic Insight into the Active Molecular Species of SCC Inhibitors -- 7.5 Third Case Study: PCs of the LDMs for the Modeling of General Corrosion Inhibition -- 7.5.1 Introductory Remarks -- 7.5.2 Heterocyclic Diazoles Corrosion Inhibitors for Iron in a Strong Acidic Medium -- 7.5.3 Heterocyclic Diazoles Corrosion Inhibitors for Aluminum Alloys in a Strong Acidic Medium -- 7.5.4 Classifying Corrosion Inhibitors by a Latent Class Analysis of the PCs of the LDMs -- 7.6 Closing Remarks -- References -- 8 Localization-Delocalization Matrices Analysis in Predicting Mosquito Repellency -- 8.1 Insect Olfaction and the Mitigation of Mosquito-Transmitted Diseases -- 8.2 Steps for an LDMs Predictive Modeling of Mosquito Repellency -- 8.3 Modeling of Semiochemical Toxicants for Mosquitoes -- 8.4 Modeling of Semiochemical Toxicity Against *Aedes Aegypti* -- 8.5 Modeling of Odorant Binding by Odorant Binding Proteins (OBPs) -- 8.6 Modeling Mosquito Repellent Response of the Odorant Receptor of *Culex quinquefasciatus* -- 8.7 Closing Remarks -- Appendix -- References -- 9 Modeling Enzyme-Substrate Interaction with Localization-Delocalization Matrices -- 9.1 Enzyme Catalysis: Some Generalities -- 9.2 Method -- 9.3 Modeling Carbamates Inhibitors of Acetylcholinesterase as Alzheimer Disease Slowing Agents -- 9.4 Organophosphorus Hydrolysis by Phosphotriesterase -- 9.5 Closing

Remarks -- References -- 10 Localization-Delocalization Matrices
of Large Systems -- 10.1 The Scaling Problem of Quantum Chemical
Calculations -- 10.2 The Kernel Energy Method (KEM) -- 10.3
Fragmentation Without Capping -- 10.4 Closing Remarks -- References
-- 11 Closing Remarks -- Index.
