1. Record Nr. UNINA9910830133103321

Titolo	Chemical reactivity in confined systems : theory, modelling and applications / / edited by Pratim K. Chattaraj, Debdutta Chakraborty
Pubbl/distr/stampa	2021 Hoboken, New Jersey : , : John Wiley & Sons, Inc., , [2021]
ISBN	1-119-68338-6 1-119-68335-1 1-119-68323-8
Descrizione fisica	1 online resource (451 pages)
Disciplina	541.39
Soggetti	Reactivity (Chemistry)
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Cover -- Title Page -- Copyright -- Contents -- Preface -- List of Contributors -- Chapter 1 Effect of Confinement on the Translation Rotation Motion of Molecules: The Inelastic Neutron Scattering Selection Rule -- 1.1 Introduction -- 1.2 Diatomics in C60: Entanglement, TR Coupling, Symmetry, Basis Representation, and Energy Level Structure -- 1.2.1 Entanglement Induced Selection Rules -- 1.2.2 H@C60 -- 1.2.3 H2@C60 -- 1.2.3.1 Symmetry -- 1.2.3.2 Spherical Basis and Eigenstates -- 1.2.3.3 Energy Level Ordering with Respect to -- 1.2.4 HX@C60 -- 1.3 INS Selection Rule for Spherical (Kh) Symmetry -- 1.3.1 Inelastic Neutron Scattering -- 1.3.2 Group Theory Derivation of the INS Selection Rule -- 1.3.2.1 GroupTheory Based INS Selection Rule for Cylindrical (Cv) Environments -- 1.3.2.2 GroupTheoryBased INS Selection Rule for Spherical (Kh) Environments -- 1.3.3 Specific Systems, Quantum Numbers, and Basis Sets -- 1.3.3.1 H@sphere -- 1.3.3.2 H2@sphere -- 1.3.3.3 HX@sphere -- 1.3.4 Beyond Diatomic Molecules -- 1.3.4.1 H2O@sphere -- 1.3.4.2 CH4@sphere -- 1.3.4.3 Any Guest Molecule in any Spherical (Kh) Environment -- 1.4 INS Selection Rules for NonSpherical Structures -- 1.5 Summary and Conclusions -- Acknowledgments -- References -- Chapter 2 PressureInduced Phase Transitions -- 2.1 Pressure, A Property of All Flavours, and Its Importance for the Universe and Life --

2.2 Pressure: Isotropic and Anisotropic, Positive and Negative -- 2.3 Changes of the State of Matter -- 2.4 Compression of Solids -- 2.4.1 Isotropic or Anisotropic Compressibility -- 2.4.2 Negative Linear Compressibility -- 2.4.3 Negative Area Compressibility -- 2.4.4 Anomalous Compressibility Changes at High Pressure -- 2.5 Structural SolidSolid Transitions -- 2.5.1 Structural Phase Transitions Accompanied by Volume Collapse -- 2.5.2 Effects of Volume Collapse on Free Energy.
2.5.3 StructureInfluencing Factors at Compression -- 2.5.4 Changes in the Nature of Chemical Bonding upon Compression and upon Phase Transitions -- 2.6 Selected Classes of Magnetic and Electronic Transitions -- 2.6.1 High Spin-Low Spin Transitions -- 2.6.2 Electronic Com vs Disproportionation -- 2.6.3 MetaltoMetal Charge Transfer -- 2.6.4 NeutraltoIonic Transitions -- 2.6.5 Metallization of Insulators (and Resisting It) -- 2.6.6 Turning Metals into Insulators -- 2.6.7 Superconductivity of Elements and Compounds -- 2.6.8 Topological Phase Transitions -- 2.7 Modelling and Predicting HP Phase Transitions -- Acknowledgements -- References -- Chapter 3 Conceptual DFT and Confinement -- 3.1 Introduction and Reading Guide -- 3.2 Conceptual DFT -- 3.3 Confinement and Conceptual DFT -- 3.3.1 Atoms: Global Descriptors -- 3.3.2 Molecules: Global and Local Descriptors -- 3.3.2.1 Electron Affinities -- 3.3.2.2 Hardness and Electronic Fukui Function -- 3.3.3 Inclusion of Pressure in the E &amp -- equals -- E [N,v] Functional -- 3.4 Conclusions -- Acknowledgements -- References -- Chapter 4 Electronic Structure of Systems Confined by Several Spatial Restrictions -- 4.1 Introduction -- 4.2 Confinement Imposed by Impenetrable Walls -- 4.3 Confinement Imposed by Soft Walls -- 4.4 Beyond Confinement Models -- 4.5 Conclusions -- References -- Chapter 5 Unveiling the Mysterious Mechanisms of Chemical Reactions -- 5.1 Introduction -- 5.1.1 Context -- 5.1.2 Ideas and Methods -- 5.1.3 Application -- 5.2 Energy and Reaction Force -- 5.2.1 The Reaction Force Analysis (RFA) -- 5.2.2 RFABased Energy Decomposition -- 5.2.3 Marcus Potential Energy Function -- 5.2.4 Marcus RFA -- 5.3 Electronic Activity Along a Reaction Coordinate -- 5.3.1 Chemical Potential, Hardness, and Electrophilicity Index -- 5.3.2 The Reaction Electronic Flux (REF).
5.3.2.1 Physical Decomposition of REF -- 5.3.2.2 Chemical Decomposition of REF -- 5.4 An Application: the Formation of Aminoacetonitrile -- 5.4.1 Energetic Analysis -- 5.4.2 Reaction Mechanisms -- 5.5 Conclusions -- Acknowledgments -- References -- Chapter 6 A Perspective on the SoCalled Dual Descriptor -- 6.1 Introduction: Conceptual DFT -- 6.2 The Dual Descriptor: Fundamental Aspects -- 6.2.1 Initial Formulation -- 6.2.2 Alternative Formulations -- 6.2.2.1 Derivative Formulations -- 6.2.2.2 Link with Frontier Molecular Orbital Theory -- 6.2.2.3 StateSpecific Development -- 6.2.2.4 MO Degeneracy -- 6.2.2.5 Quasi Degeneracy -- 6.2.2.6 Spin Polarization -- 6.2.2.7 Grand Canonical Ensemble Derivation -- 6.2.3 RealSpace Partitioning -- 6.2.4 Dual Descriptor and Chemical Principles -- 6.2.4.1 Principle of Maximum Hardness -- 6.2.4.2 Local Hardness Descriptors -- 6.2.4.3 Local Electrophilicity and Nucleophilicity -- 6.2.4.4 Local Chemical Potential and Excited States Reactivity -- 6.3 Illustrations -- 6.3.1 Woodward Hoffmann Rules in DielsAlder Reactions -- 6.3.2 Perturbational MO Theory and Dual Descriptor -- 6.3.3 Markovnikov Rule -- 6.4 Conclusions -- References -- Chapter 7 Molecular Electrostatic Potentials: Significance and Applications -- 7.1 A Quick Review of Some Classical Physics -- 7.2 Molecular Electrostatic Potentials -- 7.3 The Electronic Density and the Electrostatic Potential -- 7.4 Characterization of Molecular Electrostatic

Inducing Chemical Bond Between Two Ngs -- 14.5 XNgY Insertion Molecule: Confinement in One Direction -- 14.6 Conclusions -- Acknowledgements -- References -- Chapter 15 Effect of Both Structural and Electronic Confinements on Interaction, Chemical Reactivity and Properties -- 15.1 Introduction.
15.2 Geometrical Changes in Small Molecules Under Spherical and Cylindrical Confinement.

Sommario/riassunto

"This book provides a theoretical basis for the molecular phenomena observed in confined spaces. State-of the-art theoretical and computational approaches are described, with a focus on obtaining physically relevant understanding, enabling the reader to build a good appreciation of the underlying chemical principles. aI²²EReal life' examples of confined systems are presented, highlighting how the reactivity of atoms and molecules changes upon encapsulation. Recent developments related to the following host-guest systems are discussed. *AI² Cucurbit[n]uril *AI² ExBox 4 *AI² Clathrate hydrates *AI² Octa acid cavitand *AI² Metal organic frameworks (MOFs) *AI² Covalent organic frameworks (COFs) *AI² Zeolites *AI² Fullerenes *AI² Carbon nanotubes."--

2. Record Nr. UNINA9911019727103321

Autore	Imbriale W. A (William A.)
Titolo	Large antennas of the Deep Space Network / / William A. Imbriale
Pubbl/distr/stampa	Hoboken, N.J., : Wiley-Interscience, c2003
ISBN	9786610273416 9781280273414 1280273410 9780470321577 0470321571 9780471726197 0471726192 9780471728498 0471728497
Descrizione fisica	1 online resource (319 p.)
Collana	Deep-space communications and navigation series
Disciplina	621.382/54
Soggetti	Deep Space Network - Equipment and supplies Satellite dish antennas
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Large Antennas of the Deep Space Network; Table of Contents; Foreword; Preface; Acknowledgments; Chapter 1: Introduction; 1.1 Technology Drivers; 1.1.1 Frequency Bands Allocated to the Deep Space Network; 1.2 Analysis Techniques for Designing Reflector Antennas; 1.2.1 Radiation-Pattern Analysis; 1.2.2 Feed-Horn Analysis; 1.2.3 Spherical-Wave Analysis; 1.2.4 Dual Reflector Shaping; 1.2.5 Quasioptical Techniques; 1.2.6 Dichroic Analysis; 1.2.7 Antenna Noise-Temperature Determination; 1.3 Measurement Techniques; 1.3.1 Theodolite Measurements; 1.3.2 Microwave Holography 1.3.3 Aperture Gain and Efficiency Measurements1.3.4 Noise-Temperature Measurements; 1.4 Techniques for Designing Beam-Waveguide Systems; 1.4.1 Highpass Design; 1.4.2 Focal-Plane Matching; 1.4.3 Gaussian-Beam Design; 1.4.4 High-Power Design; 1.5 Summary; References; Chapter 2: Deep Space Station 11 : Pioneer-The

First Large Deep Space Network Cassegrain Antenna; 2.1 Introduction to the Cassegrain Concept; 2.2 Factors Influencing Cassegrain Geometry; 2.3 The DSS-11, 26-Meter Cassegrain System; References; Chapter 3: Deep Space Station 12: Echo; 3.1 The S-Band Cassegrain Monopulse Feed Horn
3.2 The 26-Meter S-/X-Band Conversion Project3.2.1 Performance Predictions; 3.2.2 Performance Measurements; 3.3 The Goldstone-Apple Valley Radio Telescope; References; Chapter 4: Deep Space Station 13: Venus; 4.1 The Dual-Mode Conical Feed Horn; 4.2 Gain Calibration; References; Chapter 5: Deep Space Station 14: Mars; 5.1 Antenna Structure; 5.2 S-Band, 1966; 5.3 Performance at X-Band; 5.3.1 Surface Tolerance; 5.3.2 Measured X-Band Performance; 5.4 Tricone Multiple Cassegrain Feed System; 5.4.1 Radio Frequency Performance; 5.4.2 New Wideband Feed Horns; 5.4.3 Dual-Hybrid-Mode Feed Horn
5.5 Reflex-Dichroic Feed System5.6 L-Band; 5.6.1 Design Approach; 5.6.2 Performance Predictions and Measurements; 5.6.3 L-Band System Modifications; 5.7 The Upgrade from 64 Meters to 70 Meters; 5.7.1 Design and Performance Predictions; 5.7.2 S- and X-Band Performance; 5.7.3 Ka-Band Performance; 5.7.4 Adding X-Band Uplink; 5.8 Distortion Compensation; 5.8.1 Deformable Flat Plate; 5.8.2 Array-Feed Compensation System; 5.8.3 The Array-Feed Compensation System-Deformable Flat-Plate Experiment; 5.8.4 Projected Ka-Band Performance; 5.9 Future Interests and Challenges; References
Chapter 6: Deep Space Station 15: Uranus-The First 34-Meter High-Efficiency Antenna6.1 The Common-Aperture Feed; 6.2 Dual-Reflector Shaping; 6.3 Computed versus Measured Performance; References; Chapter 7: The 34-Meter Research and Development Beam-Waveguide Antenna; 7.1 New Analytical Techniques; 7.2 Beam-Waveguide Test Facility; 7.3 The New Antenna; 7.3.1 Antenna Design Considerations; 7.3.2 Upper-Mirror Optics Design; 7.3.3 Pedestal Room Optics Design; 7.3.4 Bypass Beam-Waveguide Design; 7.3.5 Theoretical Performance; 7.3.6 Dual-Shaped Reflector Design
7.3.7 The Effect of Using the DSS-15 Main Reflector Panel Molds for Fabricating DSS-13 Panels

Sommario/riassunto

An important historical look at the space program's evolving telecommunications systemsLarge Antennas of the Deep Space Network traces the development of the antennas of NASA's Deep Space Network (DSN) from the network's inception in 1958 to the present. It details the evolution of the large parabolic dish antennas, from the initial 26-m operation at L-band (960 MHz) through the current Ka-band (32 GHz) systems. Primarily used for telecommunications, these antennas also support radar and radio astronomy observations in the exploration of the solar system and the universe. In addition,