

1. Record Nr.	UNISA996211955203316
Titolo	Clusters and colloids [[electronic resource]] : from theory to applications // edited by Gunter Schmid
Pubbl/distr/stampa	Weinheim ; ; New York, : VCH, c1994
ISBN	1-281-75885-X 9786611758851 3-527-61607-1 3-527-61606-3
Descrizione fisica	1 online resource (573 p.)
Altri autori (Persone)	SchmidGunter <1937->
Disciplina	541.3
Soggetti	Microclusters Colloids Molecular theory
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Includes bibliographical references and index.
Nota di contenuto	Clusters and Colloids; Contents; 1 General Introduction; 2 Electronic Structure of Metal Clusters and Cluster Compounds; 2.1 Introduction; 2.2 The Description of the Clusters Electronic Structure; 2.2.1 Wave Function Based Methods; 2.2.2 Density Functional Methods; 2.2.3 Simplified Methods; 2.3 Structure and Properties of Naked Clusters; 2.3.1 The Theoretical Description of Metal Clusters; 2.3.2 Structure, Bonding, and Stability; 2.3.2.1 Geometrical Structures; 2.3.2.2 The Jellium Model; 2.3.2.3 Fluxionality; 2.3.2.4 Stability and Fragmentation; 2.3.2.5 Bond Lengths 2.3.2.6 Electron Delocalization in Clusters 2.3.3 Ionization Potentials and Electron Affinities; 2.3.4 Electronic States, "Band Structure", and Band Gap; 2.3.5 Optical Responses; 2.3.6 Clusters in External Fields; 2.3.6.1 Magnetic Behavior; 2.3.6.2 Electric Polarizability; 2.4 Structure and Properties of Ligated Clusters; 2.4.1 The Metal - Ligand Interactions; 2.4.2 Structures and Bond Lengths; 2.4.2.1 Geometrical Structures; 2.4.2.2 Metal - Metal Bond Lengths; 2.4.2.3 The Ligand Polyhedron; 2.4.3 Topological Relationships and Simplified Bonding Models

2.4.3.1 The Effective Atomic Number (EAN) Rule; 2.4.3.2 The Polyhedral Skeletal Electron Pair (PSEP) Model; 2.4.3.3 Topological Electron Counting (TEC); 2.4.3.4 Electron Counting Based on the Extended Huckel Approach; 2.4.3.5 Clusters Stabilized by s-s Interactions: A Unified View; 2.4.4 Quantum Chemistry of Organometallic Clusters: A Deeper Look into the Bonding; 2.4.4.1 Semiempirical Calculations; 2.4.4.2 Limitations of Simplified Approaches; 2.4.4.3 Bare Versus Ligated Clusters: The Effect of the Ligands; 2.4.4.4 Ligand-Field Effects in Clusters; 2.4.4.5 The Strength of the Metal-Metal Bonds; 2.4.4.6 Clusters with Interstitial Atoms; 2.4.5 Physical Measurements and Chemical Bonding; 2.4.5.1 Photoelectron Spectroscopy; 2.4.5.2 Optical Spectroscopy; 2.4.5.3 Magnetic Susceptibility Measurements; 2.4.5.4 ESR Spectra; 2.4.5.5 NMR Spectra; 2.4.5.6 Specific Heat; 2.4.5.7 Redox Properties; 2.5 Conclusions; 2.5.1 The Role of Theory in Clusters Research; 2.5.2 On the Analogy between Metal Clusters and Surfaces; References; 3 Clusters in Ligand Shells; 3.1 Introduction; 3.2 Low-valent Organometallic Clusters; 3.2.1 Interplay Between Electronic and Steric Factors in the Growth of Transition Metal Molecular Clusters in Ligand Shells; 3.2.2 Bonding and Spectroscopic Behavior of Carbon Monoxide; 3.2.3 Stereochemical Non-rigidity of Clusters in Ligand Shells; 3.2.4 Homo- and Heterometallic Transition Metal Clusters; 3.2.4.1 Synthesis of High Nuclearity Clusters by Ligand Elimination; 3.2.4.2 Synthesis of Higher Nuclearity Clusters by Elimination of Metal Fragments; 3.2.4.3 Synthesis of Higher Nuclearity Clusters by Redox Processes; 3.2.4.4 Structural Features of Homo- and Heterometallic Clusters; 3.2.5 Transition Metal Clusters Containing Main Group Elements

Sommario/riassunto

This book offers a comprehensive overview of the rapidly developing field of cluster science. In an interdisciplinary approach, basic concepts as well as recent developments in research and practical applications are authoritatively discussed by leading authors. Topics covered include 'naked' metal clusters, clusters stabilized by ligands, clusters in solids, and colloids. The reader will find answers to questions like: * How many metal atoms must a particle have to exhibit metallic properties? * How can the large specific surface of clusters and colloids be employed in catalysts?
