1. Record Nr.   UNINA9910437796903321

Titolo   Topological modelling of nanostructures and extended systems / / Ali Reza Ashrafi ... [et al.], editors

Pubbl/distr/stampa   New York, : Springer, 2013

ISBN   94-007-6413-8

Edizione   [1st ed. 2013.]

Descrizione fisica   1 online resource (xv, 575 pages) : illustrations (some color)

Collana   Carbon materials : chemistry and physics, , 1875-0745

Altri autori (Persone) AshrafiAli Reza

Disciplina   541

Soggetti   Nanostructures - Design and construction
                        Nanoscience

Lingua di pubblicazione Inglese

Formato   Materiale a stampa

Livello bibliografico   Monografia

Note generali   "ISSN: 1875-0745."

Nota di bibliografia   Includes bibliographical references and index.

Nota di contenuto   Helical Wrapping of Graphene sheets and their Self-assemble into Core-Shelled Composite Nanostructures with metallic particles -- First-Principles Study of the Electronic and Magnetic Properties of Defects in Carbon Nanostructures -- Structural defects on the Electronic Transport Properties of Carbon-based Nanostructures -- Topological versus Physical and Chemical Properties of Negatively Curved Carbon Surfaces -- Topochemistry of spatially extended sp2 nanocarbons: fullerenes, nanotubes, and grapheme -- A Pariser-Parr-Pople Model Hamiltonian based approach to the electronic structure and optical properties of graphene nanostructures -- Topological invariants of Möbius-like graphenic nanostructures -- Spanning Fullerenes as Units in Crystal Networks -- Introducing „Colored" Molecular Topology by Reactivity Indices of Electronegativity and Chemical Hardness -- Nanostructures and Eigenvectors of Matrices -- Theoretical analysis of the reactivity of carbon nanotubes: local versus topological effects -- Computation of the Szeged index of some nanotubes and dendrimers -- The Edge-Wiener index and its computation for some nanostructures -- Study of Fullerenes by Some New Topological Index -- Topological Study of (3,6)- and (4,6)-Fullerenes -- Enumeration of Hetero – Molecules by Using Pólya Theorem.

Sommario/riassunto	Topological Modelling of Nanostructures and Extended Systems completes and expands upon the previously published title within this series: The Mathematics and Topology of Fullerenes (Vol. 4, 2011) by gathering the latest research and advances in materials science at nanoscale. It introduces a new speculative area and novel concepts like topochemical reactions and colored reactive topological indices and provides a better understanding of the physical-chemical behaviors of extended systems. Moreover, a charming new family of space-filling fullerenic crystals is here analyzed for the first time. Particular attention is given to the fundamental influences exercised by long-range connectivity topological mechanisms on the chemical and physical properties of carbon nanostructures. Systems consisting in graphenic layers with structural and topological defects are investigated in their electronic and magnetic behaviors also in presence of metallic particles. More specifically, the book focuses on: · Electronic Properties of low dimensional nanostructures including negatively-curved carbon surfaces;- Pariser-Parr-Pople model hamiltonian approach to graphene studies; ·Topochemistry and Toporeactivity of extended sp2-nanocarbons: PAH, fullerenes, nanoribbons, Moebius-like nanoribbons, nanotubes and grapheme; ·Novel class of crystal networks arising from spanning fullerenes; ·Nanostructures and eigenvectors of matrices and an extended treatise of topological invariants; ·Enumeration hetero-fullerenes by Polya theory. Topological Modelling of Nanostructures and Extended Systems represents a valuable resource to advances graduates and researchers working in mathematics, chemistry, physics and material science.