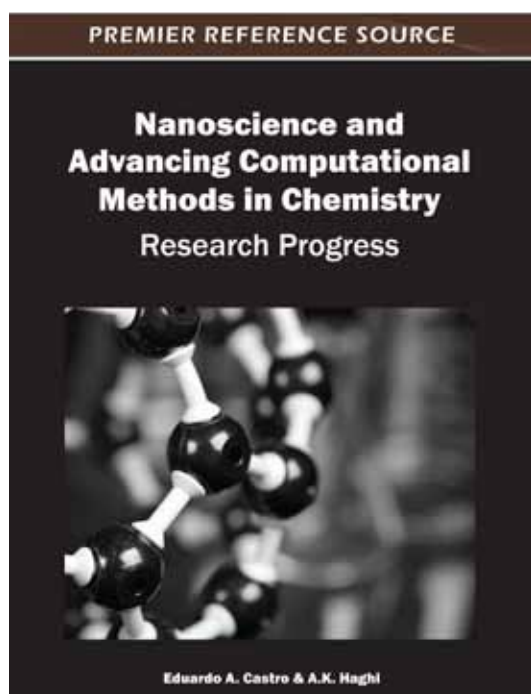


An Excellent Addition to Your Library!

Released: May 2012

Nanoscience and Advancing Computational Methods in Chemistry: Research Progress



Eduardo A. Castro (Research Institute of Theoretical and Applied Physical-Chemistry (INIFTA), Argentina)
& A.K. Haghi (University of Guilan, Iran)

The budding field of nanotechnology offers enormous potential for advances in medical science, engineering, transportation, computers, and many other industries. As this growing field solidifies, these technological advances may soon become a reality.

Nanoscience and Advancing Computational Methods in Chemistry: Research Progress provides innovative chapters covering the growth of educational, scientific, and industrial research activities among chemical engineers and provides a medium for mutual communication between international academia and the industry. This book publishes significant research reporting new methodologies and important applications in the fields of chemical informatics and discusses latest coverage of chemical databases and the development of new experimental methods.

Topics Covered:

- Basic principles on nanoscience
- Silver Nanoplates
- Nanostructure materials and Nanomodification Techniques
- Current Directions in Nanomachining
- Electronegativity and Hardness among Nanomaterials
- Nanoroots of Quantum Chemistry
- Low Dimensional Inorganic Nanomaterials
- Ionocovalency and Applications
- Biological Synthesis of Nanoparticles
- Donor–Acceptor Chemical Interactions

ISBN: 9781466616073; © 2012; 321 pp.

Print: US \$195.00 | Perpetual: US \$295.00 | Print + Perpetual: US \$390.00

Market: This premier publication is essential for all academic and research library reference collections. It is a crucial tool for academicians, researchers, and practitioners and is ideal for classroom use.

Eduardo A. Castro's career was launched by studying Physical Chemistry at the Faculty of Chemistry of the La Plata National University of La Plata, Buenos Aires, Argentina, during 1963-70. His diploma work to get his PhD Degree was on calculation of HMO and related semi empirical methods of beta-carotene for analyze chemical reactivity and electronic spectrum. Incidentally, his only available computational resource on that time was a diagonalization subroutine for symmetric matrices and his only disposable instruction book was Andrew Streitwieser's on Theoretical Organic Chemistry. From 1971-72 he performed his Ph.D. work at the Physics Department of the National La Plata University, working under supervision of Manuel Sorarrain. After that we find him as a research scientist at the Theoretical and Applied Research Institute located at La Plata National University where he founded the Group for Theoretical Chemistry in 1974. Then, he was appointed as a member of the Scientific Researcher Career in the Argentina National Research Council, and he continues up to the present time as a Superior Researcher.

Chapter 1

Cluster Origin of Solvent Features of Fullerenes, Single-Wall Carbon Nanotubes, Nanococones, and Nanoborns

Torrens Francisco (Institut Universitari de Ciència Molecular, Universitat de València, Spain)
Castellano Gloria (Cátedra Energésis de Tecnología Interdisciplinar, Universidad Católica de Valencia, Spain)

Chapter 2

Dipole Moment as a Possible Diagnostic Descriptor of the Conformational Isomerism of the Ammonia Molecule

Ghosh Dulal C. (University of Kalyani, India)
Rajak Sandip Kumar (University of Kalyani, India)

Chapter 3

Commonality in the Origin and the Manifestation in the Real World of Electronegativity and Hardness

Islam Nazmul (University of Kalyani, India & Techno Global-Balurghat, India)
Ghosh Dulal C. (University of Kalyani, India)

Chapter 4

Nanoroots of Quantum Chemistry: Atomic Radii, Periodic Behavior, and Bondons

Putz Mihai V. (Laboratory of Computational and Structural Physical Chemistry, West University of Timisoara, Romania)

Chapter 5

DFT Correlation of the Site Selectivity of Donor-Acceptor Chemical Interaction

Ghosh Dulal C. (University of Kalyani, India)
Bhattacharyya Soma (University of Kalyani, India)

Chapter 6

Biological Synthesis of Silver Nanoparticles and their Functional Properties

Prabhawathi Veluchamy (Indian Institute of Technology Madras, India)
Sivakumar Ponnurengam Malliappan (Indian Institute of Technology Madras, India)
Doble Mukesh (Indian Institute of Technology Madras, India)

Chapter 7

Nanostructured Metal Oxide Gas Sensor:

Mazloom Jamal (University of Guilan, Iran)
Ghodsi Farhad E. (University of Guilan, Iran)

Chapter 8

On the Modeling of Carbon Nanotubes as Drug Delivery Nanocapsules

Alisafaei F. (University of Wyoming, USA)
Ansari R. (University of Guilan, Iran)

Chapter 9

Probing the Reactive Center for Site Selective Protonation in a Molecule by the Local Density Functional Descriptors

Rajak Sandip K. (University of Kalyani, India)
Islam Nazmul (University of Kalyani, India)
Ghosh Dulal C. (University of Kalyani, India)

Chapter 10

On the Method of the Determination of the Global Hardness of Atoms and Molecules

Islam Nazmul (University of Kalyani & Techno Global-Balurghat, India)
Ghosh Dulal C. (Techno Global-Balurghat, India)

Order Your Copy Today!

Name: _____

Organization: _____

Address: _____

City, State, Zip: _____

Country: _____

Tel: _____

Fax: _____

E-mail: _____

Enclosed is check payable to IGI Global in
US Dollars, drawn on a US-based bank

Credit Card Mastercard Visa Am. Express

3 or 4 Digit Security Code: _____

Name on Card: _____

Account #: _____

Expiration Date: _____