



Topological Modelling of Nanostructures and Extended Systems (Carbon Materials: Chemistry and Physics)

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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.

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