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Armchair Graphene Nanoribbons; 4.2.3 Graphene Nanoribbons with Finite Length; 4.2.4 Surface Chemical Adsorption; 4.3 Mechanical and Electromechanical Properties of GNRs; 4.4 Summary; Acknowledgements; References; 5 Cutting Graphitic Materials: A Promising Way to Prepare Graphene Nanoribbons; 5.1 Introduction; 5.2 Oxidative Cutting of Graphene Sheets; 5.2.1 Cutting Mechanisms 5.2.2 Controllable Cutting 5.3 Unzipping Carbon Nanotubes; 5.3.1 Unzipping Mechanisms Based on Atomic Oxygen; 5.3.2 Unzipping Mechanisms Based on Oxygen Pairs; 5.4 Beyond Oxidative Cutting; 5.4.1 Metal Nanoparticle Catalyzed Cutting; 5.4.2 Cutting by Fluorination; 5.5 Summary; References; 6 Properties of Nanographenes; 6.1 Introduction; 6.2 Synthesis; 6.3 Computation; 6.4 Geometry of Zigzag-Edged Hexangulenes; 6.5 Geometry of Armchair-Edged Hexangulenes; 6.6 Geometry of Zigzag-Edged Triangulenes; 6.7 Magnetism of Zigzag-Edged Hexangulenes; 6.8 Magnetism of Zigzag-Edged Triangulenes
6.9 Chimeric Magnetism 6.10 Magnetism of Oligocenes, Bisanthene-Homologs, Squares and Rectangles; 6.10.1 Oligocene Series: C4m+2H2m+4 (na = 1; m = 2, 3, 4 . . .); 6.10.2 Bisanthene Series: C8m+4H2m+8 (na = 3; m = 2, 3, 4 . . .); 6.10.3 Square and Rectangular Nano-Graphenes: C8m+4H2m+8 (m = 2, 3, 4 . . .); 6.11 Concluding Remarks; Acknowledgment; References; 7 Porous Graphene and Nanomeshes; 7.1 Introduction; 7.1.1 Graphene-Based Nanomeshes; 7.1.2 Graphene-Like Polymers; 7.1.3 Other Relevant Subjects; 7.1.3.1 Isotope Separation; 7.1.3.2 Van der Waals Correction for Density Functional Theory
7.1.3.3 Potential Energy Surfaces for Hindered Molecular Motions Within the Narrow Pores

Sommario/riassunto

"The aim of this book is to deliver a comprehensive view of graphene chemistry from various perspectives out of theoretical and computational investigations"--