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| Nota di contenuto | Graphene Chemistry; Contents; List of Contributors; Preface; Acknowledgements; 1 Introduction; 2 Intrinsic Magnetism in Edge-Reconstructed Zigzag Graphene Nanoribbons; 2.1 Methodology; 2.1.1 Effective Valence Bond Model; 2.1.2 Density Matrix Renormalization Group Method; 2.1.3 Density Functional Theory Calculations; 2.2 Polyacene; 2.3 Polyazulene; 2.4 Edge-Reconstructed Graphene; 2.4.1 Energy Gap; 2.4.2 Frontier Molecular Orbitals; 2.4.3 Projected Density of States; 2.4.4 Spin Density in the Triplet State; 2.5 Conclusion; Acknowledgments; References 3 Understanding Aromaticity of Graphene and Graphene Nanoribbons by the Clar Sextet Rule 3.1 Introduction; 3.1.1 Aromaticity and Clar Theory; 3.1.2 Previous Studies of Carbon Nanotubes; 3.2 Armchair Graphene Nanoribbons; 3.2.1 The Clar Structure of Armchair Graphene Nanoribbons; 3.2.2 Aromaticity of Armchair Graphene Nanoribbons and Band Gap Periodicity; 3.3 Zigzag Graphene Nanoribbons; 3.3.1 Clar Formulas of Zigzag Graphene Nanoribbons; 3.3.2 Reactivity of Zigzag Graphene Nanoribbons; 3.4 Aromaticity of Graphene; 3.5 Perspectives; Acknowledgements; References 4 Physical Properties of Graphene Nanoribbons: Insights from First-Principles Studies 4.1 Introduction; 4.2 Electronic Properties of Graphene Nanoribbons; 4.2.1 Zigzag Graphene Nanoribbons; 4.2.2 |

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: $C_{4m+2}H_{2m+4}$ ($n_a = 1$; $m = 2, 3, 4 \dots$); 6.10.2 Bisanthene Series: $C_{8m+4}H_{2m+8}$ ($n_a = 3$; $m = 2, 3, 4 \dots$); 6.10.3 Square and Rectangular Nano-Graphenes: $C_{8m+4}H_{2m+8}$ ($m = 2, 3, 4 \dots$); 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"--