

# Preface

The number of observed or guessed atomic architectures formed by elemental carbon has unexpectedly increased in the last decades. In addition to graphite and diamond, a multiplicity of other structures – such as well ordered fullerenes and nanotubes, or less ordered structures like nanoporous and amorphous carbon – have been synthesized and studied. Similarly to what happens for diamond with respect to graphite, the new metastable phases (although basically  $sp^2$ -bonded) are definitely other than graphite (still to consider as the most stable phase) as for their physical and chemical features in a wide range of temperatures and pressures. Interestingly, the mechanical, structural, and electronic properties of these new forms of carbon are extremely different, ranging from soft to hard, from compact to open, from insulating to metallic.

Theory and simulations have largely contributed to understand and characterize the new carbon-based systems and led to the prediction of new ones. The multiplicity of possible arrangements, the diversity of behaviors, and the complex interplay between structures and properties poses a formidable challenge to theoretical and computational physicists. A number of different methods are therefore needed, ranging from model-potential molecular dynamics, to tight-binding calculations, to first-principles simulations. As a general feeling, it is also becoming evident that their combination into a unique theoretical and computational tool is actually needed to make new progress in this field.

This volume presents a unique survey of the theoretical modeling of all phases of carbon – other than single fullerene molecules or nanotubes – from natural crystalline forms found on earth and in meteorites to artificial (hypothetical) nanofoams. In addition, the present volume deals with the computational techniques used to understand and predict the structure and properties of such carbon systems, as well as reports about the present state of the art, including controversial aspects like the occurrence of magnetism, and presents open questions for the future. Although the main focus is on carbon-based systems, the computational challenges posed by their diverse structural, bonding, mechanical and electronic properties are relevant for all materials and make the present volume valuable for the whole community of computational condensed matter physics.

Each chapter is a self-contained authoritative exposition by scientists with an international reputation, sharing their knowledge and tricks of the trade. As a whole, the book provides a basis towards a unified theoretical description of carbon, the most fascinating element in Nature.

The first part of the volume is mostly devoted to the structural properties of several novel carbon structures.

Chapter 1 by Ghiringhelli and Meijer opens with a description of the phase diagram of carbon that includes its traditional phases, diamond, graphite and liquid carbon. Graphite and diamond melt into a liquid with a network-like microscopic structure at extremely high values of pressure and temperature. The phase diagram of carbon is experimentally poorly known and recent simulations give access to its determination.

The diamond structure can also become extremely stable at the nanoscale, as extensively discussed in Chapter 2 by Galli, where nanoparticles with diamond-like structures, formed in a wide variety of natural environments (around stars or in CVD phases) or under very high pressure and temperature conditions, are investigated.

Since the discovery of fullerenes and nanotubes, that are not treated in detail here, several other new forms of nanostructured carbon mostly based on the graphitic  $sp^2$  bond configuration have been identified. Chapter 3 by Seifert, Kuc and Heine introduces the carbon nanofoams, hypothetical ordered graphitic structures that display interesting analogies with carbon nanotubes. Although not yet firmly established, these structures might have been possibly experimentally realized.

The second part of the volume is more focused on the physico-chemical properties of several exotic carbon architectures.

Chapter 4 by Carlsson introduces a more general type of structure based on  $sp^2$  bonding called nanoporous carbon, a class of materials that have been obtained by a number of experimental methods. Nanoporous carbon and nanofoams promise to have specific catalytic action and great potential for chemical applications.

Chapter 5 by Marks examines amorphous carbon, currently among the most interesting materials for applications. Computer simulations have largely contributed to the complex characterization of this disordered type of structure. The contribution provides a critical exam of the criteria for theory to be accurate enough to discern between different structural models.

Chapter 6 by Blase, Benedek and Bernasconi examines the exceptional mechanical properties of clathrate structures. The criteria for designing hard materials are examined, also in connection with electronic properties and possible occurrence of superconductivity.

Finally in Chapter 7 by Ganchenkova, Vehviläinen and Nieminen, the intriguing, but still controversial observation of ferromagnetism in nanostructured carbon, such as polymerised fullerenes and ion-irradiated graphitic materials is examined and the conditions for ferromagnetic ordering defect-related magnetism are explored.

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