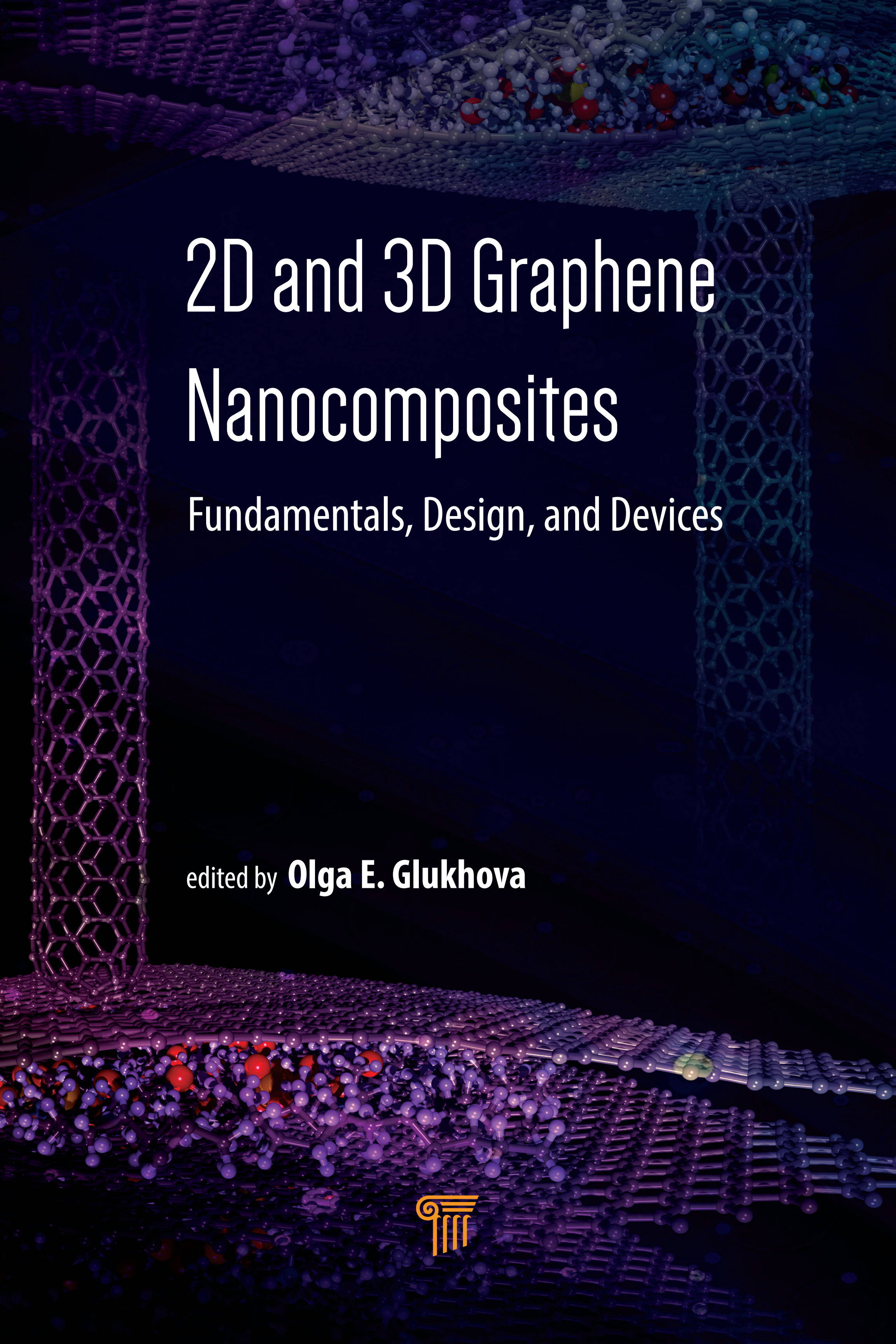

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edited by **Olga E. Glukhova**

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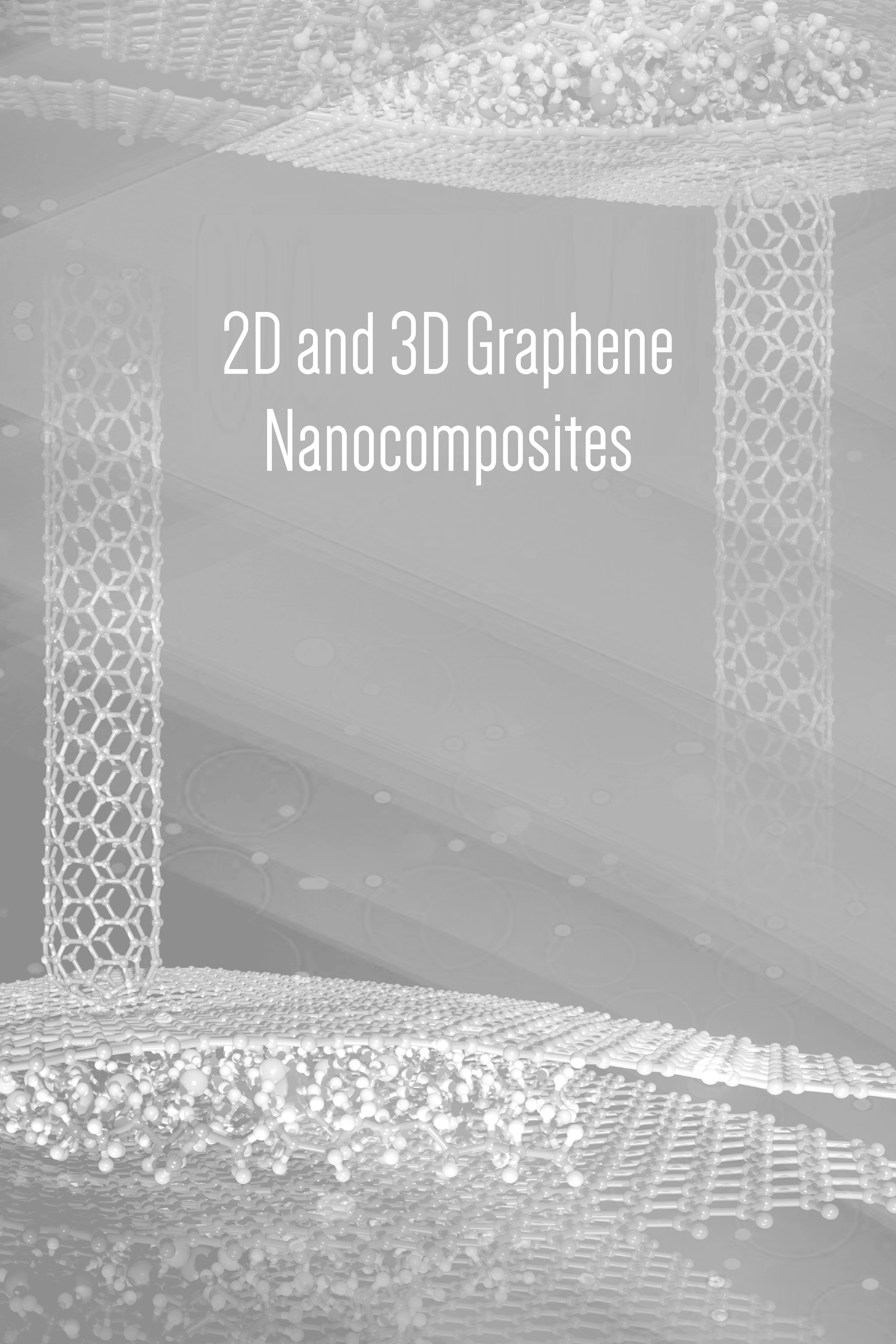

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Preface

The discovery of graphene by A. K. Geim and K. S. Novoselov in 2004 divided the modern history of materials science into *before* and *after*. The research boom that began after the release of the first publication on graphene has affected many strategically important high-tech industries: energy conversion and energy storage, environmentally friendly technologies, medicine, electronics, and space applications. One of the new stages in the development of graphene materials science is associated with the study of composite materials based on graphene and other carbon nanostructures, including carbon nanotubes and fullerenes. A large number of scientific papers are devoted to theoretical and experimental studies of composite materials based on 2D graphene and 1D carbon nanotubes. There are several topological types of graphene–carbon nanotube composites that vary in the method of joining nanotubes and graphene as well as their mutual orientation. 3D pillared vertically aligned carbon nanotube–graphene composites and graphene–carbon nanotube composite films with horizontally aligned nanotubes are of most interest to researchers. The reason for such increased attention to graphene–carbon nanotubes composite materials is the improvement of their properties compared with conventional carbon materials due to the synergistic effect of nanotubes and graphene. The first results of research of new carbon composite structures showed their superiority over individual nanotubes and graphene in electrical, optical, and electrochemical properties, which opens up new ways to develop promising practical applications based on these materials.

Hybrid carbon nanosystems consisting of C_{60} fullerene films deposited on a monolayer graphene have broad prospects. Reports about this material began to appear in scientific papers only a few years ago, however, it is already predicted that electronic nanodevices, including photovoltaic devices, will be developed on the basis of graphene/C_{60} hybrid systems. It is predicted that a new promising direction in electronics will be the development of sensitive graphene-based sensors of single biomolecules, in particular, the DNA molecule. An important task in this area is to study the electronic energy and electrically conductive properties of graphene/DNA nucleotide molecular complexes from the standpoint of identifying the greatest sensitivity of graphene for the efficient operation of a DNA sensor.

An interesting and promising kind of graphene material is glass-like carbon, which is called an intermediate carbon material between layered graphene and fullerenes. This material has an irregular highly porous structure and a highly developed surface. There are two topological types of glass-like carbon: graphitized type—a material from multi-layered graphene flakes forming layers, and non-graphitized type—a material consisting of randomly distributed curved layers of graphene flakes and fragments of layered fullerenes, which form numerous nanopores. The presence of a porous structure makes this material suitable for filling with atoms of various chemical elements in order to control its characteristics in a wide range of values.

Numerous 2D graphene-like materials have already been distinguished into a separate class of materials, in the structure of which either carbon atoms in the lattice sites are replaced by atoms of a different chemical type or various adsorbed atoms are present. One of the main purposes of such modifications is the opening of the band gap in graphene, the value of which can be controlled, for example, by varying the concentration of adsorbed atoms. In particular, the functionalization with hydrogen and fluorine atoms leads to the appearance of a band gap in graphene. The new graphene modifications obtained in this way—hydrogenated graphene (graphane) and fluorinated graphene (fluorographene)—are intensively investigated by many scientific groups.

The progress achieved in the research of graphene and graphene-based composite materials to date would not be possible without computer simulation methods that significantly complement the results of full-scale experiments and in some cases can replace them due to the special complexity or impossibility of performance. With the emergence of new structural varieties of graphene, the physical and mathematical apparatus is also being developed for their study.

This book covers the fundamental properties of new 2D/3D composite materials based on graphene and its modifications and discusses their potential application areas. It provides an interpretation of interesting physical effects discovered for the first time for graphene materials under consideration. It contains a description of the experimental methods for obtaining and characterizing samples of chemically modified graphene and the conceptual foundations of popular methods for computer modeling of graphene nanostructures as well as original computational techniques developed by the authors of the book chapters. The book is a result of the joint work of many highly qualified specialists in the field of experimental and theoretical research of graphene and its derivatives. The book will be useful for a wide audience, including students, graduate students, and researchers in academic institutions and also specialists in industrial engineering.

Olga E. Glukhova
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