

# Preface

MesoBioNano (MBN) Explorer is a multi-purpose software package for advanced multiscale simulations of complex molecular structure and dynamics. It has many unique features and a wide range of applications in physics, chemistry, biology, materials science, and related industries. A variety of algorithms and interatomic potentials implemented in the program allow for the simulation of the structure and dynamics of a broad range of systems with the sizes from the atomic up to the mesoscopic scales. This provides the necessary molecular level quantitative details for the construction of the multiscale approaches in many areas of modern research. MBN EXPLORER is equipped with a special multi-task toolkit—the MBN STUDIO, which enables construction of input files, simple start of simulations, as well as visualization and analysis of the results obtained. The systematic description of the capabilities of these universal and powerful software packages and their applications in numerous areas of research are discussed in the book chapters.

This book attempts to present the state-of-the-art understanding of the mechanisms of clustering, self-organization, growth and structure formation in complex MBN systems on the basis of modern theoretical and computational physics approaches. Due to the large diversity of the systems and processes, the book does not even consider touching many of them. Instead, it is focused on the description of the key research methodologies that proved to be successful and led to the better understanding of some of the above-mentioned problems. These methodologies often rely on novel computational approaches, algorithms and high-performance computing, which are introduced and discussed via the exemplar case studies of clustering, self-organization and structure formation in various MBN systems.

The material is arranged as follows. In the introductory chapter we describe the field of MBN science, introduce main concepts and computation approaches related to the field, explain the basic features of MBN EXPLORER and MBN STUDIO. Chapter 2 presents a summary of main theoretical methods on which MBN EXPLORER is based, elaborates the key algorithms implemented in the package, outlines the basic ideas towards the multiscale description of MBN systems by means of kinetic Monte Carlo approach and the irradiation driven molecular dynamics. Chapter 3 introduces general aspects of the computational approach based on MBN EXPLORER,

the type of computational problems that can be addressed with the use of this software as well as of the multi-functional toolkit MBN STUDIO.

In Chaps. 4–10 we present case studies of various MBN systems which can be investigated by means of MBN EXPLORER. The results of computer simulations as well as of theoretical studies of structure and dynamics of atomic and molecular clusters of different materials are discussed in Chap. 4. Case studies of transformations of biomolecular systems at different thermal and biologically relevant conditions as well as at various external stresses are presented in Chap. 5. In Chap. 6 we provide examples of nanostructured materials that can be studied with MBN EXPLORER, in particular, with the tools based on the kinetic Monte Carlo algorithm which allows simulation of multiscale phenomena in complex MBN systems. Chapter 7 provides an introduction to the fascinating field of research related to simulation of novel composite complex molecular systems, materials consisting of components of different nature, ordered or disordered, materials interfaces. Examples of the simulations of mechanical properties and thermal effects of a broad variety of the materials are discussed in Chap. 8. MBN EXPLORER-based molecular dynamics simulations of the nano- and microscale conformational, morphological and phase transitions, proteins folding, nanoparticle and molecular diffusion, particle propagation through medium, collision and fragmentation processes, laser induced acoustic desorption are elaborated in Chap. 9. Chapter 10 shows that MBN EXPLORER is a very useful and powerful tool for the exploration of the challenging interdisciplinary research problems arisen in connection with the development of new technologies. The last Chap. 11 of the book gives an outlook for future perspectives of MBN EXPLORER and MBN STUDIO, presents the main ideas and the key directions for further development of the software, describes the ways for obtaining the software together with a bunch of supplementary material.

The current release of MBN EXPLORER, which is the heritage of a long-standing development, has been thoroughly tested, benchmarked and proven to be reliable in calculations. We express our deep gratitude to Andrey Koshelev, Pavel Nikolaev, Mikhail Panshenskov, Andrey Shutovich, Ilia Volkovets and Gennady B. Sushko who contributed a lot to the development, construction and maintenance of the code at different stages of its evolution. We acknowledge collaborative work with Victor Bezchastnov, Catherine Bréchnignac, Jean-Patrik Connerade, Veronika Dick, Leonid G. Gerchikov, Kaspar Haume, Elsa Henriques, Adilah Hussien, Vadim K. Ivanov, Chris Kexel, Andrey G. Lyalin, Nigel J. Mason, Oleg I. Obolensky, Mikhail Panshenskov, Roman G. Polozkov, Stefan Schramm, [Klaus Schulten], Gennady B. Sushko, Eugene Surdutovich, Pablo de Vera, Alexey V. Verkhovtsev, Sergiy N. Volkov, Alexander Yakubovich together with whom many of the theoretical and numerical results presented in the book were obtained. We express our gratitude to Alexey Verkhovtsev for his help in preparation of the textual and graphical material presented in Sect. 9.2.

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