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MBN Explorer: dynamics of biomolecular systems and self-organization

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Ilia A. Solov'yov, Gennady Sushko, Alexey Verkhovtsev, Andrei Korol and Andrey V. Solov'yov

MBN Explorer Tutorials Series: Volume II

URL: www.mbnresearch.com
E-mail: info@mbnexplorer.com

A hands-on guide how to use MBN Explorer – a universal computational suite for multiscale simulation of complex molecular structure and dynamics

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Referees:
V.K. Ivanov, doctor of physical-mathematical sciences, professor
Saint Petersburg State Polytechnic University, Russia

E. Surdutovich, Dr., professor,
Department of Physics, Oakland University, USA

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The book is a tutorial on the practical use of the software package MBN Explorer suitable for the multiscale modelling of structure and dynamics of complex molecular systems. The standard algorithms of molecular dynamics and optimisation are introduced in the book and explained in details invoking illustrative case studies. The original algorithms implemented in the code are described in a similar fashion. Many different problems arising in the studies of physical, chemical and biological systems and the processes occurring therein are analysed through numerical calculations of the system energy, optimisation of molecular structure accounting for dynamics of all the atoms in the system. The Monte Carlo approach is also introduced and applied to a number of case studies. Particular attention is paid to the problem of self-organisation in bio- and nanosystems and to the modelling of formation, growth and fragmentation of nanosystems, and in particular nanofractals and nanowires.

The book is aimed at scientists, post-graduate and graduate students specialising in the field of theoretical physics, computational physics, molecular, bio- and nanophysics, material science, as well as for teaching these disciplines in English.

Figures 44. Bibliography: 41 items

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