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MBN Explorer: simulations of nanomaterials structure and dynamics

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MBN Explorer Tutorials Series: Volume I

URL: www.mbnresearch.com
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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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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 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 studies of nanoscale systems and materials as well as the processes with their involvement are analysed through numerical calculations of the system energy, optimisation of molecular structure accounting for all the atoms in the system. Particular attention is paid to the studies of mechanical properties of nanostructured materials and propagation of particles in a medium by means of modern methods of molecular dynamics.

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

Figures 43. Bibliography: 46 items

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