**IN SUMMARY**

MesoBioNano (MBN) Studio is a special multi-task software toolkit with graphical user interface developed to facilitate the practical work with MBN Explorer. It simplifies modelling of MBN systems, setting up calculations, monitoring their progress, visualising and examining the calculation results. MBN Studio can be utilised for any type of calculations supported by MBN Explorer.

MBN Studio has a number of built-in analytic tools allowing the calculation of specific characteristics that are determined by the output of simulations. A special modelling plug-in of MBN Studio allows us to easily construct a large variety of molecular systems of different geometry built of arbitrary atomic and molecular constituents.

MBN Studio allows setting up application-specific projects which involve special algorithms. Such projects are designed for the particular tasks that are linked to the applications of significant impact and importance, such as novel and emerging technologies.

MBN Studio assists in utilising libraries and databases that provide coordinates and geometries for atomic clusters, nanoparticles, biomolecules, crystals and other MBN systems.

MBN Studio can be utilised for any type of calculations that are supported by MBN Explorer, such as single-point energy calculations, structure optimisation, molecular dynamics (non-relativistic, relativistic, Euler, irradiation driven) and kinetic Monte Carlo simulations. MBN Studio is being continuously developed by the joint participation of world class scientists and professional IT developers. Being tested by several research groups worldwide, the MBN Studio software toolkit is described in detail in the book of MBN Explorer and MBN Studio Tutorials, and also in the book “Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer” published by Springer in 2017, ISBN 978-3-319-56085-4.

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MesoBioNano systems
modelling with a single software

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Computational Physics at the Life Science interface: MesoBioNano Science
Computational Physics, Chemistry and Biology
Computational Material Science
High Performance Computing

OUTPUT DATA HANDLING
- Built-in drawing tool for plotting systems' characteristics
- Graphical representation of data
- Easy handling of output data and their representation

VISUALISATION TOOLS
- Visualisation of input and output data
- Visualisation of simulated atomic trajectories
- Modelling, virtual manipulation and design of MBN systems
- Different representation and colour schemes

ANALYTIC TOOLS
- Built-in tools for analysis of output data
- Calculation of diffusion coefficients of atoms and molecules, melting temperatures, heat capacities, radial distribution functions, etc.
- Applicable to any modelled system

STANDARD I/O FORMATS
- Working with the coordinate, trajectory, potential, topology, manipulation and chemical rules files
- Support of several popular file formats, including XYZ, DCD, PDB and PSF

LINKS TO DATABASES AND LIBRARIES
- Built-in library of illustrative examples
- Links to online resources containing coordinates and geometries of various molecular systems, as well as parameters of interaction force fields

VIDEO RENDERING
- Composing and editing of image frames
- Video rendering of results of MD and MC simulations
- Encoding of sets of frames as MPEG movies

SYSTEM MODELLER
- Creating of input files for MBN Explorer
- Construction of complex molecular systems of different geometry and composition
- Built-in tools for generating 1D, 2D and 3D objects of different shapes

COMPATIBLE WITH
- MICROSOFT WINDOWS
- LINUX
- MAC OS X

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