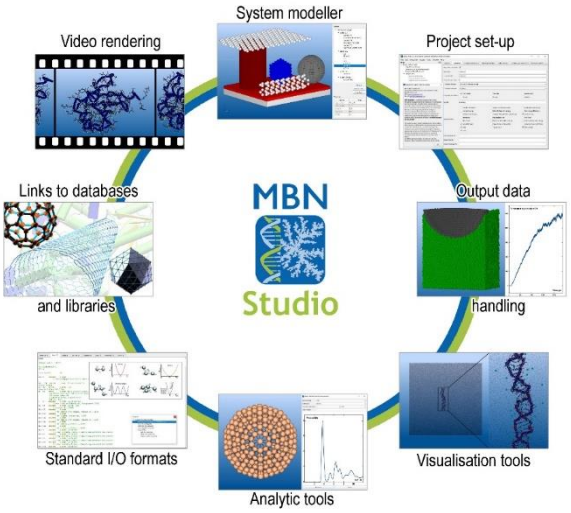
MBN Studio: a multi-task toolkit for MBN Explorer

MBN Research Center



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

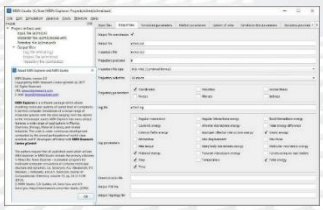
MBN Studio has a number of built-in analytic tools allowing the calculation of specific characteristics that are determined by the output of simulations. A special modelling plug-in of MBN Studio allows to easily construct a large variety of molecular systems of different geometry built of arbitrary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

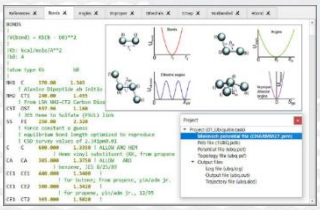
The program is being developed and distributed by **MBN Research Center**: http://www.mbnresearch.com

Main Features



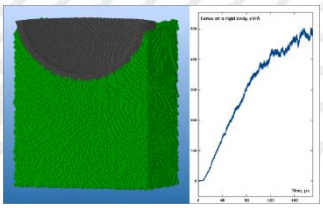
Project set-up

- User-friendly interface
- Support of all types of MBN Explorer calculations
- Setting-up standard and application specific projects
- Use of MBN Explorer examples library



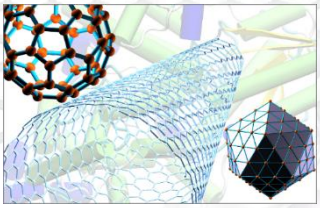
Standard input/output formats

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



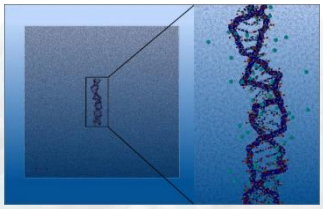
Output data handling

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



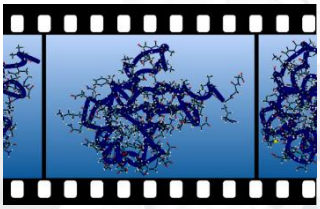
Links to databases and libraries

- 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 and potentials



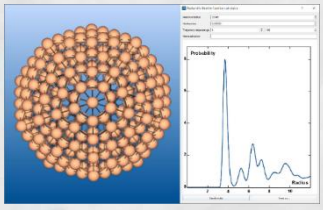
Visualisation tools

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



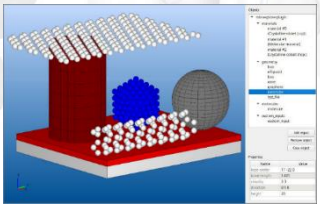
Video rendering

- Composing and editing of image frames
- Video rendering of results of MD (non-relativistic, relativistic, Euler, irradiation-driven) and MC simulations
- Encoding of sets of images as MPEG movies



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



System modeller

- Creating 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

MBN Research Center **Altenhöferallee 3, 60438 Frankfurt am Main, Germany** **E-mail: team@mbnexplorer.com** **Web: www.mbnresearch.com**