MesoBioNano (MBN) Explorer is a multi-purpose software package for advanced multiscale simulations of complex molecular structure and dynamics. It is suitable for the following tasks:

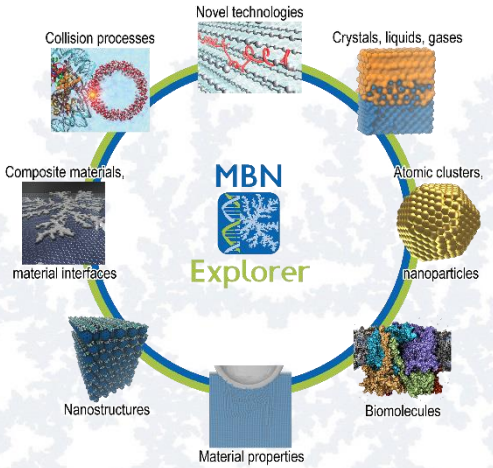
- Energy calculation
- Structure optimisation
- Molecular dynamics
- Euler rigid body dynamics
- Relativistic dynamics
- Kinetic Monte Carlo simulations

MBN Explorer features:

- Universality and applicability to a broad range of problems and molecular systems
- MPI and OpenMP parallelisation
- Extendibility
- Convenient interface
- Compatibility with standard visualisation software

MBN Explorer includes User's guide and a comprehensive database with examples of simulated molecular systems of various degree of complexity. They illustrate the implemented algorithms and serve as a convenient starting point for the basic acquaintance with the program.

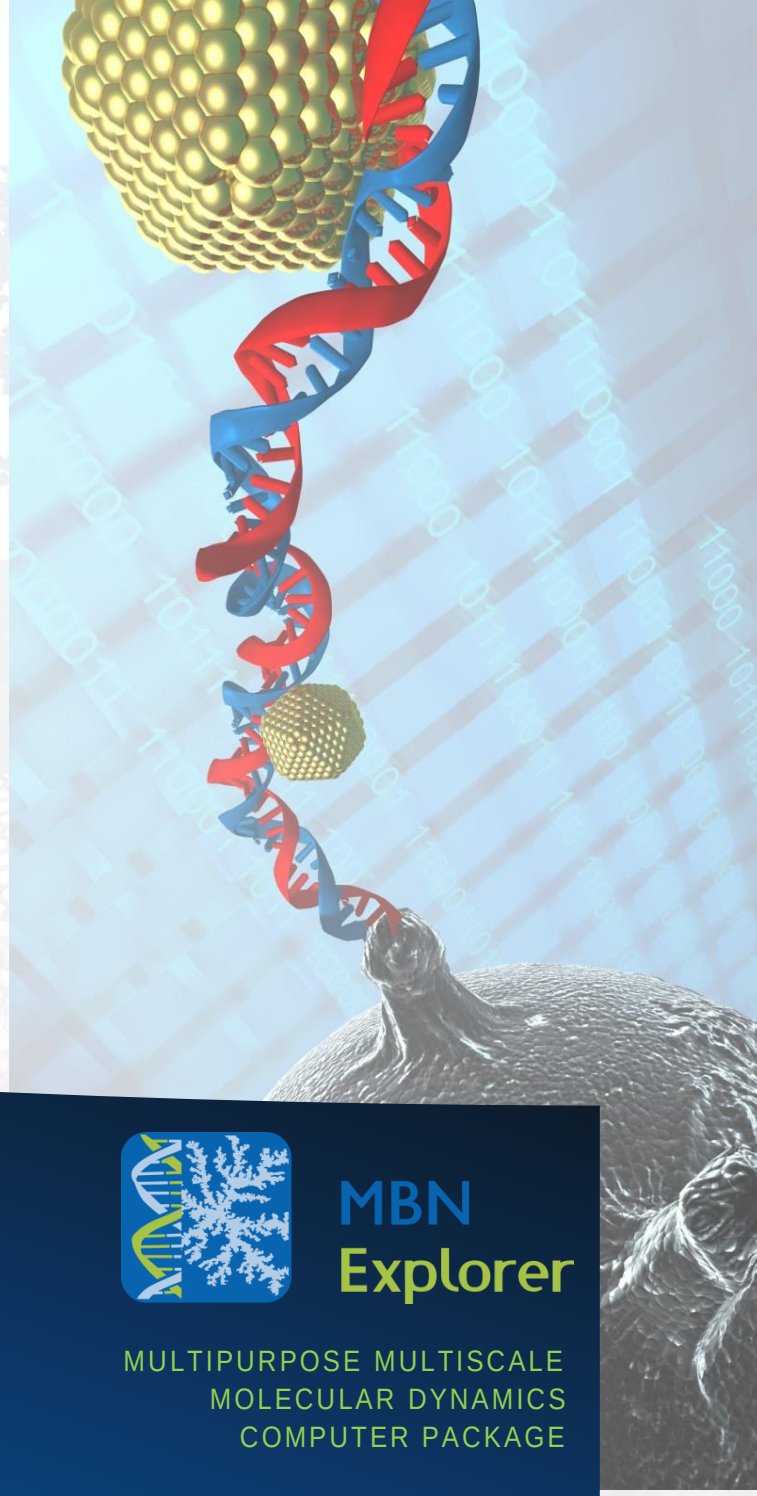
Read more on: www.mbnexplorer.com
www.mbnresearch.com



IN SUMMARY

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, Material Science, and related industries. A broad variety of algorithms and interatomic potentials implemented in the program allows for the simulation of the structure and dynamics of a broad range of systems with the sizes from the atomic to the mesoscopic scales.

MBN Explorer is being developed and distributed by MBN Research Center, which organizes the hands-on tutorial courses, user's workshops and conferences.



MBN Explorer contains a large library of model force fields and allows for their flexible use. The current release of MBN Explorer has been thoughtfully tested, benchmarked and proved to be reliable in calculations. The code is under continuous development by the joined participation of world class scientists and professional IT developers. The current release of MBN Explorer is the heritage of a long standing development. Being tested by several research groups worldwide, the molecular dynamics simulation software is described in detail in the article *"MBN Explorer - a universal program for multiscale computer simulations of complex molecular structure and dynamics"* published in Journal of Computational Chemistry, **33** (2012) 2412, and in greater detail in the upcoming book *"Multiscale Computer Simulations of Complex Molecular Structure and Dynamics with MBN Explorer"* to be published by Springer in 2017.

MBN Research Center

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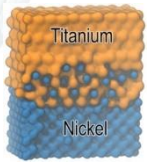
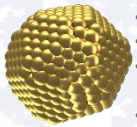


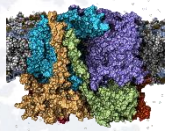
CRYSTALS, LIQUIDS, GASES

- Crystalline structures
- Liquids and soft matter
- Gaseous systems
- Physical and chemical phenomena with solids, liquids and gases
- Multiscale modeling



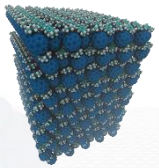
ATOMIC CLUSTERS AND NANOPARTICLES

- Atomic clusters
- Molecular clusters
- Finite nanosystems: fullerenes, nanotubes, graphene, etc.
- Deposited clusters and nanoparticles
- Dynamics of cluster and nanosystems



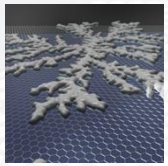
BIOMOLECULAR SYSTEMS

- Structure of biomolecules
- Biomolecular complexes
- Bio-nano systems
- Structural transitions, biomolecular processes
- Dynamics of DNA, RNA, and proteins
- Multiscale modelling



NANOSTRUCTURED MATERIALS

- Metallic, organic, inorganic and biological nanomaterials
- Crystalline superlattices of nanoparticles
- Nanofilms
- Self-assembly and growth
- Nanoscale phase and structural transitions

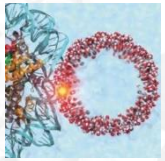


COMPOSITE MATERIALS AND MATERIAL INTERFACES

- Nanoalloys and composites
- Material interfaces
- Functional nanoparticles and surface coatings
- Nanofractals
- Deposition, diffusion and surface pattern formation, morphological transitions

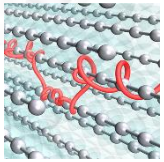
THERMO-MECHANICAL PROPERTIES OF MATERIALS

- Thermo-mechanical properties
- Tribological properties
- Elastic and plastic deformations
- Nanoindentation
- Dislocations
- Nanoscale phase and structural transitions



COLLISION PROCESSES

- Collision processes involving clusters, nanoparticles and biomolecules
- Molecular association and dissociation
- Particles propagation through a medium
- Collision induced thermo-mechanical medium effects



NOVEL TECHNOLOGIES

- Biomedical applications driven by nanoprocesses and technologies
- Deposition technologies
- Crystalline undulator based novel light sources
- Virtual design of materials
- Computational nano- and microscope

Longstanding development now available for the community

ACADEMIC LICENSING

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