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 computational tasks:

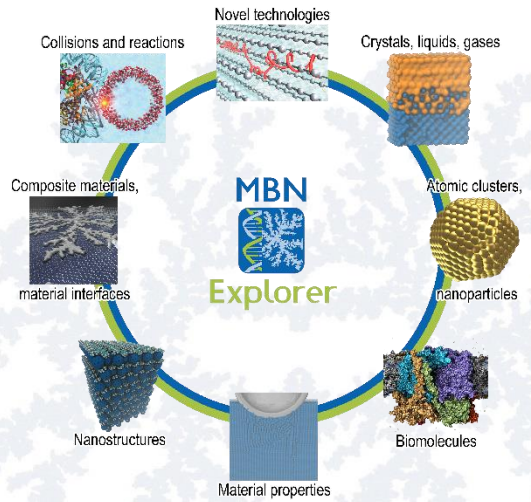
- Energy calculation
- Structure optimisation
- Molecular dynamics
- Euler rigid body dynamics
- Relativistic dynamics
- Kinetic Monte Carlo simulations
- Irradiation driven molecular dynamics

MBN Explorer features:

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

MBN Explorer includes 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 practical work with the software.

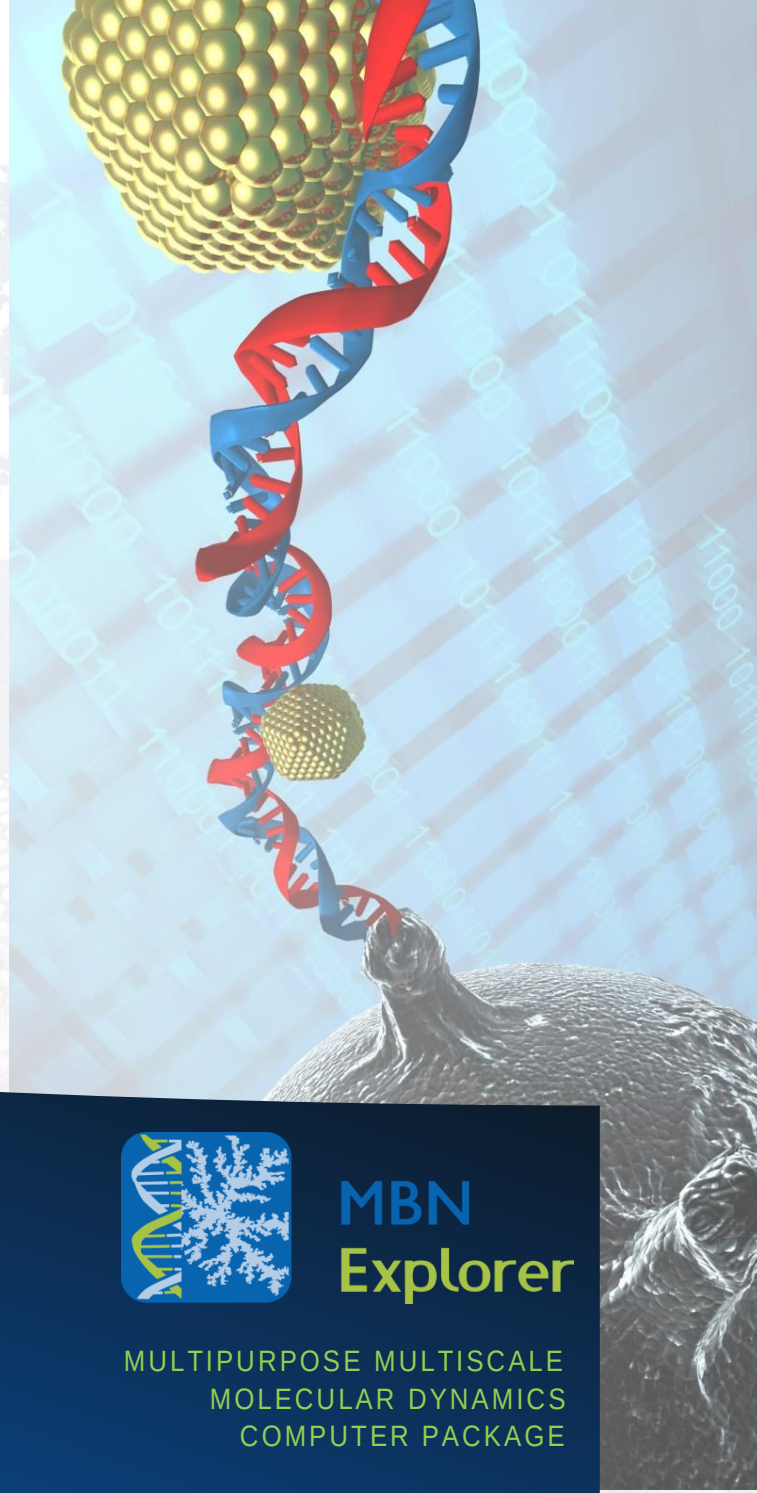
Read more on: www.mbnresearch.com



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, Materials Science, and Industry. A broad variety of algorithms and interatomic potentials implemented in the program allows simulations of structure and dynamics of a broad range of systems with the sizes from the atomic up to the mesoscopic scales.

MBN Explorer is being developed and distributed by MBN Research Center, which organises hands-on tutorials for the software, 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 book *"Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer"* published by Springer in 2017, ISBN 978-3-319-56085-4.

MBN Research Center

Contact:

Prof. Dr. Andrey V. Solov'yov
Altenhöferallee 3
60438 Frankfurt am Main, Germany
Tel.: +49-(0)69-348-75-600
Fax: +49-(0)69-348-75-628
E-mail: solovyov@mbnresearch.com

www.mbnresearch.com

MBN Explorer

MULTIPURPOSE MULTISCALE MOLECULAR DYNAMICS COMPUTER PACKAGE

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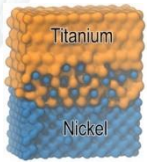
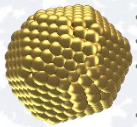


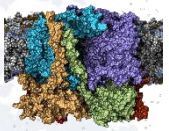
CRYSTALS, LIQUIDS, GASES

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



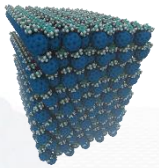
ATOMIC CLUSTERS AND NANOPARTICLES

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



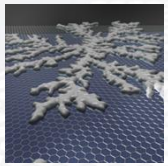
BIOMOLECULAR SYSTEMS

- 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 biomolecular nanomaterials
- Crystalline superlattices of nanoparticles
- Nanofilms
- Self-assembly and growth
- Nanoscale phase and structural transitions

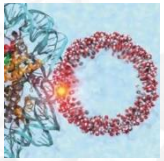


COMPOSITE MATERIALS AND MATERIAL INTERFACES

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

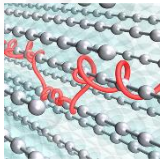
THERMO-MECHANICAL PROPERTIES OF MATERIALS

- Thermo-mechanical properties
- Tribological properties
- Nanoindentation, scratching
- Elastic and plastic deformations
- Dynamics of dislocations
- Nanoscale phase and structural transitions



COLLISIONS AND REACTIONS

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



NOVEL TECHNOLOGIES

- Biomedical applications driven by irradiation, nanoprocesses and technologies
- Surface deposition processes
- 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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ENTERPRISE LICENSING

Accessible individual and multi-users license agreements are offered for commercial exploitation of MBN Explorer.

Purchased license rights provide access to

- MBN Explorer software and its updates
- MBN Explorer documentation package
- MBN Explorer user's workshops

Special packages including education, dedicated hands-on training and helpdesk are also available. Contact us or visit our website www.mbnresearch.com for more details.