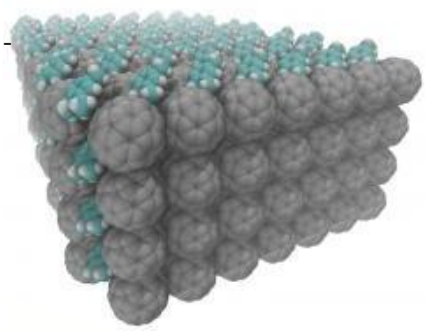


IN SUMMARY

MBN Explorer package allows to model molecular systems of varied level of complexity. Particularly suitable to compute system's energy, to optimize molecular structure, as well as to consider the molecular and random walk dynamics, MBN Explorer allows to use a broad variety of interatomic potentials, to model different molecular systems, such as atomic clusters, fullerenes, nanotubes, polypeptides, proteins, DNA, composite systems, nanofractals, etc. Despite its universality, the computational efficiency of MBN Explorer is comparable, and in some cases even higher, than the computational efficiency of other software packages.

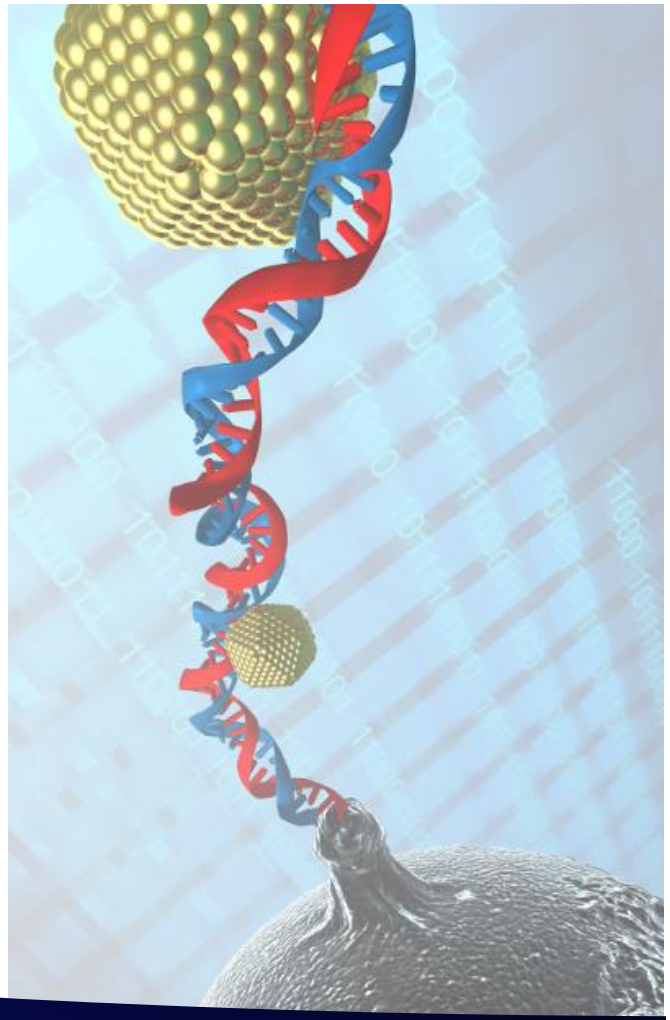
Read more on www.mbnexplorer.com

MBN Explorer can be used to study a broad range of MesoBioNano (MBN) systems ranging from individual atoms and/or molecules to complex bio-molecular complexes, featuring:

- Universal approach to MBN systems
- Rich library of interatomic potentials
- Possibility of particles gathering into rigid body
- High computation efficiency
- Force field compatibility
- Full compatibility with CHARMM force field
- VMD compatibility of output file

www.mbnexplorer.com

MBN Explorer includes a comprehensive database with examples on molecular systems of varied degrees of complexity, which are used to illustrate the implemented algorithms and can also be used as a starting point for the basic acquaintance with the program. Learn about our free tutorial courses and user's workshops from our website.



Early development of MBN Explorer started in 2000 with the compilation of a code to simulate structure and dynamics of many-body systems interacting via the Morse and the Lennard-Jones potentials. Molecular dynamics and single point energy calculations for biomacromolecules was introduced in 2005-2007 together with a growing variety of interatomic potentials and the possibility to freeze a group of atoms in rigid blocks. In parallel, efforts from professional developers have been spent to improve the code accessibility. The current release of MBN Explorer is indeed the heritage of more than a decade development. Tested by several research groups worldwide, the molecular dynamics simulation software is referenced in Journal of Computational Chemistry (2012).

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MBN Explorer

MULTIPURPOSE MULTISCALE MOLECULAR DYNAMICS COMPUTER PACKAGE

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Meso Bio Nano systems modeling with a single software

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Computational Physics at the Life Science interface: MesoBioNano Science
Computational Material Science
High Performance Computing

MBN Explorer is a multiscale molecular dynamics computer package that includes the possibility to perform, structure optimization, single point energy calculations, molecular dynamics simulations and random walk dynamics. It contains a broad variety of model potentials 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.

COMPATIBLE WITH

- WINDOW 7, XP, VISTA
- LINUX
- MAC OS X

A decade development now available for the community

ACADEMIC LICENSING

The use of MBN Explorer for non-commercial purpose is granted through a free of charge license. This licensing agreement is restricted to Universities and Research Centers aiming scientific publication of their results. Reference to MBN Explorer in reports, publications, or communication mentioning research results is requested in counterpart of academic license. All details about terms and conditions are available on www.mbnexplorer.com

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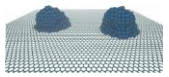
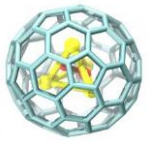


DEPOSITED NANOPARTICLES

Shown are silver nanoparticles (NP) deposited on graphite. Metal NPs on a surface experience deformation due to their interaction with the surface. MBN Explorer allows to simulate such interfaces and explore NPs diffusion.

NANOFRACTALS

Nanofractals arise when NPs are deposited on surfaces at certain conditions. MBN Explorer allows to simulate formation and evolution of nanofractals, as well as other nanostructured materials, using Monte Carlo dynamics approach.

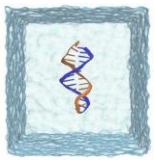


FULLERENES

Fullerenes, as well as all other allotropic forms of nanocarbon materials can be simulated with MBN Explorer. Unique thermo-mechanical properties of these materials, and the phase transitions between their different phases can be explored.

PROTEINS

Proteins are essential for functioning of living systems. MBN Explorer allows to simulate structure and dynamics of proteins in ubiquitous environments. Protein folding and many other process involving proteins can be studied.



BIOMOLECULES

MBN Explorer allows to simulated a large variety of biomolecules, biomolecular, hybrid bio-nano systems with various interfaces. Transformations of these systems at different thermal conditions and various external stresses can be explored.