**MBN Explorer: a universal tool for modeling and visualisation of complex molecular structure and dynamics**

*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 simulations of structure and dynamics of very different molecular systems with sizes ranging from atomic to mesoscopic, and their visualisation.

**MBN Explorer is suitable for the following tasks:**
- Energy calculation
- Structure optimisation
- Molecular dynamics
- Euler rigid body dynamics
- Relativistic dynamics
- Kinetic Monte Carlo simulations

**Program 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

The program is being developed and distributed by the **MBN Research Center**: [http://www.mbnresearch.com](http://www.mbnresearch.com)

### Fields of Application

**Crystals, liquids, gases**
- Crystalline structures
- Liquids and soft matter
- Amorphous structures and glasses
- 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
- Multiscale modeling

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

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

**Composite materials and material interfaces**
- Nanocomposites and composites
- Material interfaces
- Functional nanoparticles and surface coatings
- Nanofractals
- Deposition, diffusion and surface pattern formation, morphological transitions
- Multiscale modeling

**Thermo-mechanical properties of materials**
- Thermo-mechanical properties
- Tribological properties
- Elastic and plastic deformations
- Nanindentation
- Dislocations
- Nanoscale phase and structural transitions
- Multiscale modeling

**Collisional processes**
- Collisional processes involving clusters, nanoparticles and biomolecules
- Molecular association and dissociation
- Collision induced fragmentation
- Laser, thermal, collision induced desorption
- Particles propagation through a medium
- Collision induced thermo-mechanical medium effects

**Emerging technologies**
- Biomedical applications driven by nanophases and technologies, e.g. advanced radiotherapies
- Deposition technologies: sputtering, CVD, PVD, FEBID, etc.
- Crystalline undulator-based novel light sources
- Virtual design of materials
- Computational nano- and microscope

**MBN Research Center**
Altenhöferallee 3
60438 Frankfurt am Main, Germany
E-mail: solovyov@mbnresearch.com
Web: [www.mbnresearch.com](http://www.mbnresearch.com)

© Copyright MBN Research Center 2015