**MBN Explorer: a universal tool for advanced multiscale modelling 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, 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 suitable for:**
- Energy calculation
- Structure optimisation
- Molecular dynamics
- Euler rigid body dynamics
- Relativistic dynamics
- Kinetic Monte Carlo simulations
- Irradiation driven molecular dynamics

**Program features:**
- Universality
- 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 **MBN Research Center**: [http://www.mbnresearch.com](http://www.mbnresearch.com)

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**Fields of Application**

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

**Novel and emerging 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