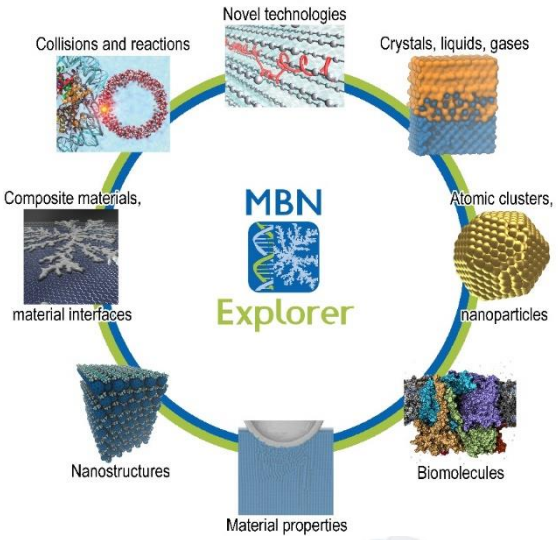
MBN Explorer: a universal tool for advanced multiscale modelling of complex molecular structure and dynamics

MBN Research Center



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:

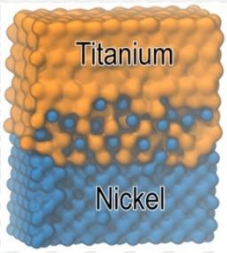
- Energy calculation
- Structure optimisation
- Molecular dynamics
- Euler rigid body dynamics
- Relativistic dynamics
- Kinetic Monte Carlo simulations
- Irradiation driven molecular dynamics

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

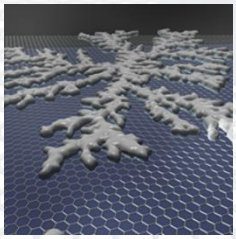
The program is being developed and distributed by **MBN Research Center**: http://www.mbnresearch.com

Fields of Application



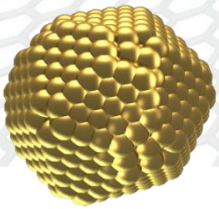
Crystals, liquids, gases

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



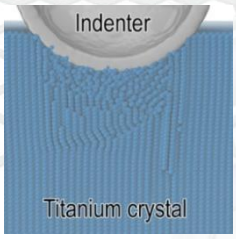
Composite materials and material interfaces

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



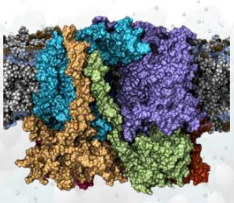
Atomic clusters and nanoparticles

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



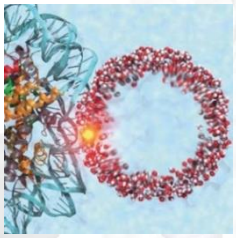
Thermo-mechanical properties of materials

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



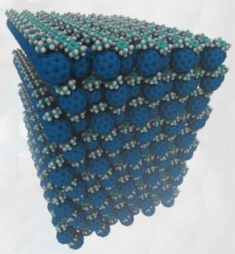
Biomolecular systems

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



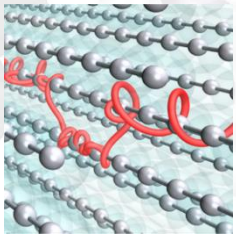
Collisions and reactions

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



Nanostructured materials

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



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

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