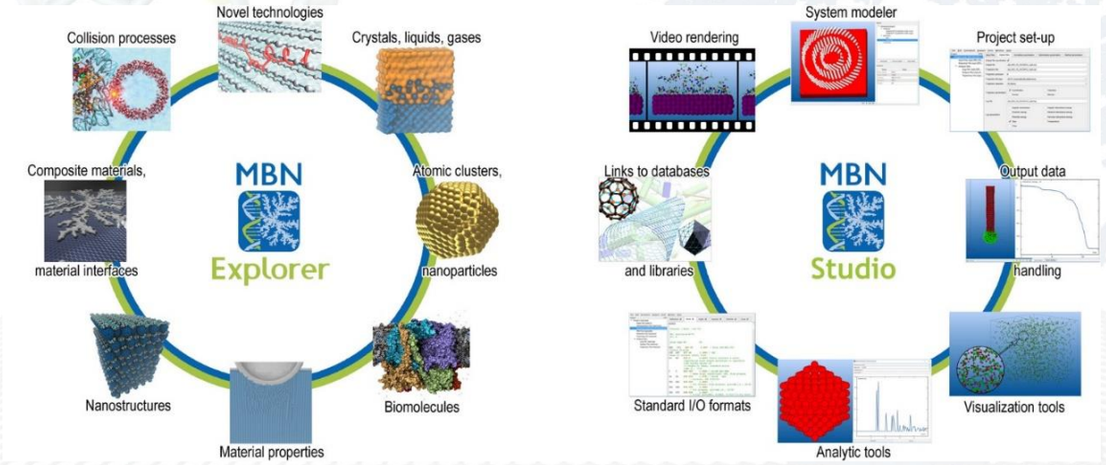
Training course on **Multiscale Computational Methods for Complex Molecular Systems**

October 26-27, 2017 / Polo Scientifico Tecnologico - Università degli Studi di Ferrara, via Saragat 1

The course aims at exploring physical models and computational approaches used for the simulations of Meso-Bio-Nano (MBN) systems and the investigation of their structure and dynamics at the atomic level of detail. The course is based on practical exercises with the advanced computational software **MBN Explorer** and **MBN Studio**.



The hands-on tutorial will cover the case studies of atomic clusters and nanoparticles; biomolecular systems; nanomaterials; composite materials and material interfaces; crystalline, liquid and gaseous systems; thermo-mechanical properties of materials; dynamical, collision- and irradiation-driven multiscale phenomena. Relevant physical concepts, mathematical techniques and computational methods will be introduced, including force fields and algorithms used in molecular dynamics and Monte Carlo simulations on parallel computers. Special attention will be devoted to modeling crystalline structures, propagation of relativistic projectiles in crystals, quantitative analysis of the channeling and related phenomena.

The tutorial is designed for graduate students, postdoctoral researchers and staff in computational bio-/nanophysics and chemistry, materials science, radiochemistry and radiobiology, who seek to extend their research skills to include computational and theoretical expertise, as well as for all other researchers interested in theoretical & computational physics and chemistry.

The training course is organized by MBN Research Center (Frankfurt am Main, Germany) together with Università degli Studi di Ferrara.

The detailed information about the training course and the registration for it can be found on www.mbnresearch.com/tutorial-7-scope

Deadline for registration: October 1, 2017

October 26:

10:00 - 10:15	**Training course opening**
10:15 - 11:00	**Basics of MBN Explorer and MBN Studio:** Short description of main features of MBN Explorer and MBN Studio: universality, tuneable force fields, multiscale approach, computational efficiency, etc.; areas of application of MBN Explorer and MBN Studio
11:00 - 11:20	Coffee break
11:20 - 11:50	**Setting up the calculation:** Specification of input files and formats, and instructions on how to run MBN Explorer
11:50 - 12:50	**MBN Studio:** An introduction to MBN Studio - a multipurpose toolkit for MBN Explorer - and an overview of its main features; overview of the MBN Explorer examples library, which contains the trial case studies demonstrating capacities of the program
12:50 - 14:00	Lunch
14:00 - 15:00	**Gases, liquids, crystals:** Description of setting up simulations of crystalline, liquid and gaseous media with MBN Explorer; different types of boundary conditions; energy and temperature control
15:00 - 16:00	**Atomic clusters and nanoparticles:** Description of setting up calculations involving atomic clusters and nanoparticles; construction of clusters and nanoparticles with MBN Studio
16:00 - 16:30	Coffee break
16:30 - 17:30	**Biomolecular systems:** Exploration of dynamical processes with biomolecular systems; use of the molecular mechanics potential for setting up calculations of biomolecular systems; simulation of bond breakage processes in biomolecular systems using MBN Explorer
17:30 - 18:30	**Collision- and irradiation-induced processes:** MD simulation of collision and irradiation-induced processes in organic and inorganic molecular systems and materials

October 27:

9:30 - 10:30	**Multiscale modelling of composite materials and material interfaces:** Application of the kinetic Monte Carlo method for simulations of fractal structures growth and their post-growth relaxation
10:30 - 11:30	**Nanostructured materials:** Application of classical MD for simulations of carbon-based nanomaterials
11:30 - 12:00	Coffee break
12:00 - 13:00	**Thermo-mechanical properties of materials:** Investigation of thermo-mechanical properties of crystalline, nanostructured and amorphous materials by means of MD simulations of the nanoindentation process
13:00 - 14:00	Lunch
14:00 - 16:00	**Propagation of particles through medium:** MD simulations of particles propagation through media (heterocrystalline structures, bent crystals, amorphous materials, solids, nanotubes, biological environment, etc.); modelling of particles' propagation in crystalline media by means of Geant4
16:00 - 16:30	Coffee break
16:30 - 17:30	**Irradiation-induced transformations of biomolecular systems:** Exploration of dynamical processes related to the irradiation induced thermo-mechanical damage of molecular and biomolecular systems
17:30 - 18:30	**Modelling of focused electron beam-induced deposition:** Introduction to the concept of irradiation-driven molecular dynamics; MD simulations of the focused electron-beam induced deposition process
18:30 - 18:45	**Tutorial closing and concluding remarks**