Exploration of irradiation/collision induced processes in Meso-Bio-Nano (MBN) systems by means of MBN Explorer and MBN Studio

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A new molecular dynamics (MD) approach for computer simulations and analysis of irradiation/collision driven chemical transformations of complex molecular systems, called irradiation driven molecular dynamics (IDMD), was recently suggested [1] and implemented in MBN Explorer [2]. The approach is based on the fact that irradiation induced quantum transformations can be treated as random, fast and local processes involving small molecules or molecular fragments. On this basis the quantum transformations, such as molecular bond breaks, creation and annihilation of dangling bonds, electronic charge redistributions, changes in molecular topologies, etc, can be incorporated into the molecular force fields, including the recently developed reactive CHARMM force field [3]. IDMD opens new possibilities to explore the irradiation/collision driven MD and chemistry in many complex MBN systems ranging from atomic clusters, nanoparticles and biomolecules to irradiated cells, surfaces, materials, as well as novel technologies such as radiotherapies, or focused electron/ion induced beam deposition (FEBID/IBID).

*MBN Explore*r is a multi-purpose software package for advanced multiscale simulations of complex molecular structure and dynamics [2]. It has many unique features and a wide range of applications in Physics, Chemistry, Biology, Materials Science, and Industry [4]. 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. A distinct feature of the package, which makes it significantly different from other codes, is in its universality and the implemented algorithms for multiscale modelling which make it very useful tool in to the exploration of many very different MBN systems beyond the limits of the classical MD schemes.

MBN Studio is a special multitask software toolkit with graphical user interface developed for MBN Explorer [5]. It helps setting up calculations with MBN Explorer, monitoring their progress and examining the calculation results. The graphical utility enables to visualise selected inputs and outputs. A number of built-in tools allows for the calculation and analysis of specific systems' characteristics. A special modelling plug-in allows constructing a large variety of molecular systems built of different atomic and molecular constituents.

The talk will give an overview of the main features of the software, its application areas and will highlight a number of recent case studies of irradiation/collision induced processes in MBN systems explored by means of MBN Explorer and MBN Studio. Particular attention will be devoted to simulations of the fusion and multifragmentation process in collisions involving metallic clusters, fullerenes and biomolecules [4,6] and the computational exploration of the FEBID processes [1,4]. It will be demonstrated that one can reproduce reasonably well experimental observations and make predictions about the morphology and molecular composition of nanostructures that emerge on the surface in the FEBID process.

References

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