MULTISCALE MODELLING OF MESO-BIO-NANO (MBN) SYSTEMS WITH MBN EXPLORER AND MBN STUDIO

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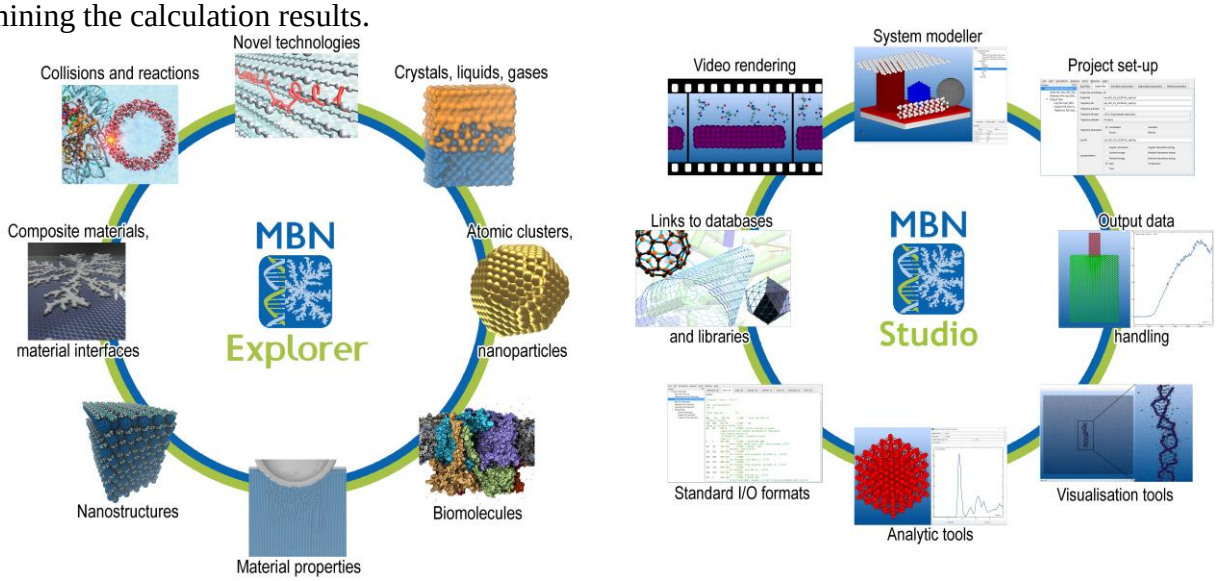
MBN Explorer is a multi-purpose software package developed by the MBN Research Center team for advanced multiscale simulations of complex molecular structure and dynamics [1]. A broad variety of interatomic potentials implemented in the MBN Explorer allows to study the structure and dynamics of very different molecular systems, such as clusters and nanoparticles, biomolecules (including proteins and DNA) and biomolecular systems, nanomaterials, liquids and crystals, composite bio-nano systems and material interfaces, see [2] and references therein. MBN Explorer has many unique features and a wide range of applications in Physics, Chemistry, Biology, Material Science, and related industries. A distinct feature of the package, which makes it significantly different from other codes, is in its universality and implemented multiscale features that make it applicable to the description of many very different Meso-Bio-Nano (MBN) systems with sizes ranging from atomic to mesoscopic [2]. MBN Explorer is combined with MBN Studio [3] a special multi-task software toolkit with graphical user interface. MBN Studio helps to set up calculations with MBN Explorer, monitoring their progress and examining the calculation results.



The talk will give an overview of the main features of the packages and will highlight a number of recent case studies of composite materials and material interfaces investigated by means of MBN Explorer and MBN Studio. Particular attention will be devoted to the modelling of thermo-mechanical properties of composites, material interfaces, phase and morphological transitions, mechanically, chemically and irradiation driven nanofabrication [2] studied by means of atomistic Molecular Dynamics (MD) simulations [2,4], and multiscale simulation techniques bases on the combined use of MD and MC (Monte Carlo) approaches [2,5]. The selected case studies are in the core of currently running European Research Projects supported within the HORIZON 2020, COST, Marie Skłodowska-Curie and Alexander von Humboldt Stiftung Programmes.

References

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