Joint Theory Seminar
European XFEL, CFEL & University of Hamburg

Thursday, 16 March 2023, 16:00 *XHQ/E1.173, in hybrid mode*

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Multiscale modelling of irradiation driven processes

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Most of the irradiation driven processes in condensed matter systems are essentially multiscale and occur on different spatial and temporal scales. Examples of such processes include most of the radiobiological case studies, irradiation driven technologies for nanofabrication, astrochemistry and many more. Computational modelling of such complex processes and phenomena became possible only recently through the development of the multiscale theories and related powerful computational techniques enabling to interconnect outcomes of theoretical analysis at different temporal and spatial scales. The talk will give an overview of the recent developments of the multiscale techniques and their realisation in the advanced software packages MBN Explorer and MBN Studio.

MBN Explorer is a multi-purpose software package for advanced multiscale simulations of complex molecular structure and dynamics developed by the team of the MBN Research Center [1]. A broad variety of algorithms implemented in the MBN Explorer allows studying 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, gases and plasmas, composite bio-nano systems and material interfaces, see [2,3] and references therein. MBN Explorer has many unique features and a wide range of applications in Physics, Chemistry, Biology, Material Science, and related industries. MBN Explorer is supplemented with MBN Studio [4] a special multi- task software toolkit with graphical user interface. MBN Studio helps to set up calculations with MBN Explorer, monitor their progress, analyse results of simulations.

The talk will give an overview of the main features of the packages and will highlight a number of recent multiscale case studies investigated by means of MBN Explorer and MBN Studio. Particular attention will be devoted to the modelling of irradiated MesoBioNano (MBN) systems studied by means of reactive and irradiation driven Molecular Dynamics (RMD and IDMD) and multiscale simulation techniques based on the combined use of quantum methods (many body theory, collisions theory, DFT, TDFT), molecular dynamics (MD) and MC (Monte Carlo) approaches, as well as by means of stochastic dynamics [2-4].

Particular attention will be devoted to the discussion of advances in the field relevant to a number of modern technologies achieved by means of RMD and IDMD [5,6], stochastic dynamics [7] and multiscale modelling [2,3,8]. The selected case studies are in the core of currently running European Research Projects supported within the HORIZON 2020 (N-Light and RADON), Horizon Europe (TECHNO-CLS) and Deutsche Forschungsgemeinschaft (DFG) frameworks as well as the COST Action MultIChem, see www.cost.eu/actions/CA20129/

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