Contribution ID: **84** Type: **Invited Talk**

Multiscale modelling of complex dynamical processes in solids with MBN Explorer and MBN Studio

Thursday, 12 September 2019 09:50 (20 minutes)

The multiscale modeling of complex molecular systems is a hot topic of the modern theoretical and computational research. To fully understand the dynamics of molecular systems and exploit it in different technological applications, such as hadron therapy, surface deposition and nanofabrication technologies, construction of novel light sources and others, one needs to consult many disciplines ranging from physics and chemistry to materials and life sciences, software engineering and high performance computing.
The MBN Explorer software package [1] is powerful and universal instrument of computational research that allows to build up, with the help of implemented algorithms operating at different space-and-time scales, multiscale models for the description of various molecular systems and processes therein for numerous biomedical and nanotechnology applications [2]. MBN Studio [3] is a graphical user interface for MBN Explorer that has been developed to facilitate setting up and starting MBN Explorer calculations, monitoring their progress and examining the calculation results.
There are several research areas in which multiscale simulations performed with the use of MBN Explorer and MBN Studio play an important role, e.g.in constructing of novel light sources based on charged particles propagation in crystalline undulators [4]. The talk will present novel theoretical and computational approaches and methodologies implemented in MBN Explorer and MBN Studio as well as related case studies.

Summary

Topic

1. Crystal Channeling and related mathematical, physical and chemical issues

Primary authors: KOROL, A. V. (MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany); SOLOV'YOV, A. V. (MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany)

Presenter: KOROL, A. V. (MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany)

Session Classification: Invited Talk