



Integrative Research Institute for the Sciences

IRIS Colloquium

On Monday, July 04th, 2022, 15:15 – 16:30

Prof. Dr. Ilia Solov'yov

Department of Physics, Carl von Ossietzky Universität Oldenburg

*"Modelling of dynamical processes in molecular systems with
stochastic dynamics"*

Location: IRIS-Research Building, Conference Room 2'049
Zum Großen Windkanal 2, 12489 Berlin

Interested persons are warmly invited.

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Modelling of dynamical processes in molecular systems with stochastic dynamics

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Stochastic dynamics describes processes in complex systems having the probabilistic nature. They can involve very different dynamical systems and occur on very different temporal and spatial scale. This talk will discuss the concept of stochastic dynamics and its implementation in the popular program MBN Explorer [1-7]. MBN Explorer is a multi-purpose software package developed for advanced multiscale simulations of complex molecular structure and dynamics [1] by the MBN Research Center in Frankfurt (www.mbnresearch.com). It has many unique features and a wide range of applications in Physics, Chemistry, Biology, Material Science, and related industries.

Stochastic dynamics in MBN Explorer relies on the Monte Carlo approach and permits simulations of physical, chemical, and biological processes [7,8]. Stochastic dynamics can be used to describe many-body systems, where all their constituent elements can move stochastically and may experience transformations and reactions. These include different diffusion modes, dissociation and attachment (decay, fission and fusion), uptake and injections (creation and annihilation) processes, reactive transformations and particle type alteration. The system's constituent elements may have different nature, scale, properties, and a set of interactions with other components within the system that affect their stochastic dynamics. Establishing the fundamental principles and characteristics of stochastic dynamics of the system constituent elements might involve their hidden degrees of freedom and related interactions. Therefore, the developed approach in combination with molecular dynamics, quantum mechanics, collision and transport theories is instrumental in unravelling the multiscale nature of dynamical behaviour of numerous complex dynamical systems. The talk will present the basic theoretical concepts underlying stochastic dynamics implementation and provide several examples highlighting its applicability to different systems, such as diffusion and self-assembly of nano particles, irradiation driven transformations, studies of pattern formations. The chosen examples will be used to illustrate the diversity of applications that can be modeled by means of stochastic dynamics with MBN Explorer.

References

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