



# Polymer- & Soft-Matter-Seminar

## Prof. Viktor Ivanov

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**“To what extent can mesoscale computer simulation be used to predict properties of (macro)molecular systems?”**

**Tuesday,  
26<sup>th</sup> June 2018**

**at: 5.15pm**

**VDP4 1.27,  
Von-Danckelmann-Platz 4,  
06120 Halle**

In this talk, I will give an overview about recent work in my group on the mesoscale computer simulation of conformational and dynamic properties of several (macro)molecular systems. In our studies, we have used the dissipative particle dynamics (DPD) method [1,2]. Following the multiscale computer simulation approach, we have developed coarse-grained (CG) models for polymer nanocomposites [3], organic and water solutions of lecithin and bile-salts [4,5], polyimides [6], precursors of polyacrylonitrile fibers, polyurethanes. I will use some of these examples to demonstrate how to keep in a CG model the most important information about the chemical structure of (macro)molecules which is crucial for correct representation of macroscopic properties of these systems. I will discuss the arising problems in detail, including methodological aspects of DPD method with special attention to the issue of whether the conditions of excluded volume and non-phantomness of polymer chains can be satisfied in the course of simulations with «soft» potentials.

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- [2] P. Español, P.B. Warren, Perspective: Dissipative particle dynamics, *J. Chem. Phys.*, v.146, p.150901 (2017).
- [3] Komarov P., Markina A., Ivanov V., Influence of surface modification of halloysite nanotubes on their dispersion in epoxy matrix: Mesoscopic DPD simulation, *Chemical Physics Letters*, v.653, p.24 (2016).
- [4] Markina A., Ivanov V., Komarov P., Khokhlov A., Tung S.H., Self-assembly of micelles in organic solutions of lecithin and bile salt: Mesoscale computer simulation, *Chemical Physics Letters*, v.664, p.16 (2016).
- [5] A. Markina, V. Ivanov, P. Komarov, A. Khokhlov, and S. H. Tung, Self-Assembly of Lecithin and Bile Salt in the Presence of Inorganic Salt in Water: Mesoscale Computer Simulation, *J. Phys. Chem. B*, v.121, p.7878 (2017).
- [6] A. Markina, V. Ivanov, P. Komarov, S. Larin, J. Kenny, S. Lyulin, Effect of polymer chain stiffness on initial stages of crystallization of polyetherimides: coarse-grained computer simulation, *Journal of Polymer Science, Part B: Polymer Physics*, v.55, p.1254 (2017).