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Structure visualization for microgel polymer systems adsorbed on a solid substrate

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Nanostructures and nanoparticles are on the top of technique and biomedical application. A special class of such systems is the polymers adsorbed on a substrate. Confinement at the surface changes their physical and chemical properties with respect to a bulk system that open a new possibility for the usage in long-time biomedical applications also at body temperature. Formation of stimuli responsive surface structures using microgel particles as colloidal building blocks is an active field of research.

A variety of experimental methods such as static and dynamic light scattering, neutron scattering, nuclear magnetic resonance, etc.[1-3] were used for the characterization of the microgel bulk phase morphology, the internal network structure and the dynamics. The more complicated task is the investigation of systems adsorbed on a surface. Methods such as atomic force microscopy, grazing incidence small-angle neutron/X-ray scattering (GISANS/GISAXS) can reveal characteristic parameters of the studied systems. But the data analysis in this case is not a trivial task. Use of modern computer methods opens a new opportunity for visualization of the samples and their structures.

In our research we use the BornAgain[4] software package (actively developing at JCNS) to simulate and decode structure of poly(ethylene glycol)(PEG)-based microgel particles adsorbed on a Si substrate. The characteristic parameters of the system obtained from GISANS data are used for system simulation in BornAgain and at the same time the simulation results provide better understanding of the experimental results. This closed circle of simultaneous analysis of the real and virtual data makes it possible to obtain a model of the system and visualize the structure of the microgel particles.

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