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Hard matter–soft matter interface: Molecular dynamics

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Recent outcomes of nanotechnology allow for the development of multifunctional hierarchical nanoparticles and their application in numerous fields, including biomedicine. The use of hierarchicaly composed nanoparticles, possessing both the biological action and contrast physical properties, permits a combination of medical therapy and diagnostics into one procedure. Such an approach forms the basis for "theranostics" (therapy plus diagnostics), which is a rapidly growing direction in modern medicine, especially in oncology. As a rule, multifunctional nanoparticles with ahierarchical structure comprise an inorganic carrier and a soft bioactive part. The formation mechanism and the stability of such nanohybrids are determined by the effects within the soft matter–hard matter interface. Moreover, the interaction of nanoparticles with the cell membrane and the cellular uptake mechanism are the result of interaction effects within the hard matter–soft matter interface (HSI). Thus, the behavior of the subsystems at the HSI can determine the behavior of the whole system. Such heterogeneous interfaces are important and complex objects for study. The use of the so-called in silico approach provides a significant contribution to the comprehensive investigations of the soft matter systems and the phenomena within the HSI.

The presentation is devoted to the use of numerical molecular models to study the interaction between biological nanoobjects and low-dimensional metal hydroxide nanostructures, which lay the basis for the development of multifunctional hierarchical nanoparticles for biomedical applications. The report consists of two parts, including an introductory review on soft matter systems, nanoceramics, hierarchical nanoparticles, and hybrid systems with the HSI. The second part is a discussion of the computer simulation outcomes obtained by our scientific group for organic-inorganic heterogeneous systems with the HSI using unbiased and steered molecular dynamics.

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Speaker Biography

Alexey A Tsukanov graduated from of the Physics Faculty (Dept. of Computer Methods of Physics) of Lomonosov Moscow State University (MSU) in 2007. In 2006-2007 he participated in international project at the International Material Institute for New Functionality in Glass, Lehigh (PA, USA). He completed his PhD at the MSU and IPE RAS in 2010. After that he had a five-year long experience in the oil&gas industry. In 2014-2016 he continued his researches as postdoc at the Skolkovo Institute of Science and Technology (Skoltech), Skolkovo, Russia. Since 2016 Alexey Tsukanov is scientific researcher at the Institute of Strength Physics and Materials Science (ISPMS) SB RAS, Tomsk, Russia. He has over 40 publications that are cited about 200 times. He serves as an editorial board member of ABioDeM journal.

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