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BIO – INORGANIC INTERFACES: FROM SIMULATIONS TO APPLICATIONS

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The study of interfacial effects and phenomena, occurring in the molecular scale at bio-inorganic interfaces, are important in many practical and scientific fields such as nanomedicine, theranostics, bio-nanotechnology, implantology, environmental and materials sciences. Besides the growth of computational power of supercomputers and the efficiency of parallel technologies, the development of computational methods in the chemistry and materials sciences has allowed the computer simulations to become a powerful tool to study the complicated molecular systems and to predict their behavior or properties at the levels from quantum-mechanical [1] to mesoscale one [2]. The present work is a review of studies conducted by the scientific group of Dr. Sergey G. Psakhie, related to the phenomena on the bio – inorganic (soft matter – hard matter) interfaces at the molecular scale, and the use of molecular dynamics simulations to obtain the quantitative and qualitative characteristics of these systems.

The computer simulations of heterogeneous systems with a bio-inorganic interfaces can improve the understanding of molecular-level mechanisms related to the practically essential problems such as the selective adsorption of biomolecules and the ions of biological medium, the formation and stability of functionalized and hierarchical nanomaterials and coatings, the interaction of nanomaterials with cells and bacteria, including the impact to the plasma membrane integrity and the functioning of proteins. Four types of problems are considered, each of which is important for several practical applications. Some of them are depicted at the scheme (see Fig.1).

Fig. 1. Molecular-level computer simulations of effects and phenomena, taking place within bio-inorganic interfaces, provide important data for such practical fields as biomedicine, implantology, environmental and materials sciences.

Due to the high specific surface area, amphoteric properties and high surface density of active groups the low-dimensional aluminum (oxy)hydroxide nanostructures are very prospective for the range of biomedical applications [3, 4]. The results of classical unbiased simulations demonstrate that the presence of the alooehene – aluminum oxyhydroxide based nanomaterial – leads to the selective adsorption and redistribution of the bio ions in the proximity of the cell membrane [5]. Such an action of the alooehene causes the tumour microenvironment dysregulation, which allows the alooehene to be the adjuvant and the base for the development an efficient anticancer agent [5].

Investigations of the formation and the stability of bio-inorganic complexes can provide us with the data necessary for the design and development of functional coatings, bio-inorganic composites [6], drug-loaded implants [7] and the hierarchically composed theranostics agents for the medical imaging and targeted drug delivery [8]. Molecular simulations can provide a deep inside into mechanism of intermolecular interaction between subsystems, estimate the free energy as well as assist in choosing of the functional groups with stronger binding energy or inorganic material with certain type of irregularities and defects [9, 10]. For instance, the outcomes of MD simulations shown that the formation of bio-

inorganic multi-molecular complexes of amino acid anions on the surface of Al-Mg layered double hydroxide is possible and is driven by hydrogen bonding and electrostatic attraction [11].

Interactions at bio-inorganic interface between nanomaterial and the fragments of protein may, in principle, disrupt the functioning of this protein. Using the classical and steered molecular dynamics it was shown that the free energy of adsorption of glutamic residues is sufficiently large to bind the entire protein loop, carrying these residues, with the metal hydroxide nanosheet [12]. Such an interaction may cause the deformation of the protein structure, inhibiting its functioning.

We also face the bio-inorganic interface in the problem of the nanomaterials' cytotoxicity assessment. The computer simulations can be used for this problem as well. In particular, MD simulations of nanoparticles interaction with the plasma membrane as well as interaction between the nanomaterial surface and the membrane building units may shed a light on the possible mechanisms of cell membrane disruption [13, 14].

In summary, the present review demonstrates the versatility of the systems with bio-inorganic interfaces at the same time with an opportunity we have of comprehensive studying of such systems at the nanometer scale using the direct computer simulations with a molecular dynamics approach.

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