ТЕЗИСЫ ДОКЛАДОВ

INTERNATIONAL WORKSHOP

«Multiscale Biomechanics and Tribology of Inorganic and Organic Systems»

МЕЖДУНАРОДНАЯ КОНФЕРЕНЦИЯ

«Перспективные материалы с иерархической структурой для новых технологий и надежных конструкций»

VIII ВСЕРОССИЙСКАЯ НАУЧНО-ПРАКТИЧЕСКАЯ КОНФЕРЕНЦИЯ С МЕЖДУНАРОДНЫМ УЧАСТИЕМ, ПОСВЯЩЕННАЯ 50-ЛЕТИЮ ОСНОВАНИЯ ИНСТИТУТА ХИМИИ НЕФТИ

«Добыча, подготовка, транспорт нефти и газа»

Томск
Издательский Дом ТГУ
2019

DOI: 10.17223/9785946218412/7

BIO – INORGANIC INTERFACES: FROM SIMULATIONS TO APPLICATIONS

[1]Alexey A. Tsukanov, [1]Sergey G. Psakhie
[1]*Institute of Strength Physics and Materials Science, SB RAS, Tomsk, Russia*

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).

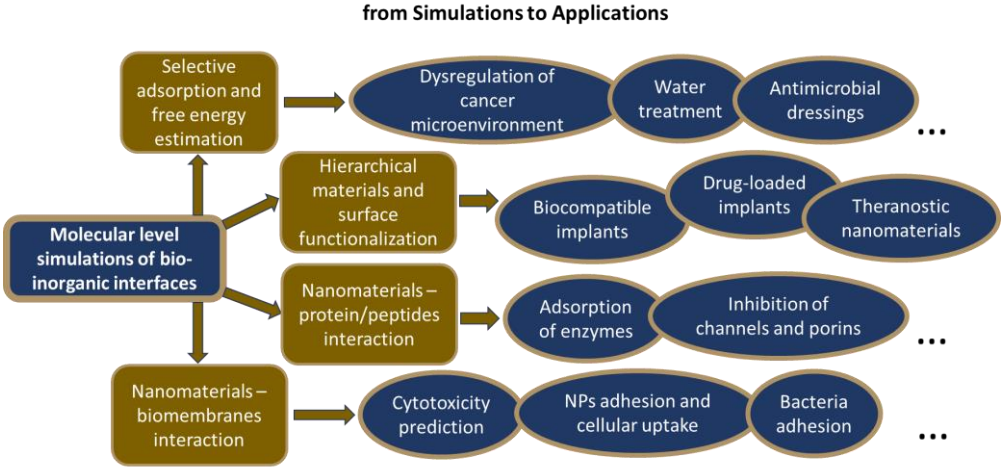

Fig. 1. Molecular-level computer simulations of effects and phenomena, taking place within bio-inorganic interfaces, provide important data for such practical fields as biomedicine, implantology, environmental and materials sciences.

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 aloohene – 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 aloohene causes the tumour microenvironment dysregulation, which allows the aloohene 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.

1. Dolgonos G., Tsukanov A., Psakhie S. G., Lukin O., Gurbych O., Shivanyuk A. Theoretical studies of capsular complexes of C2V-symmetrical resorcin[4]arene tetraesters with tetramethylammonium cation. // Comp. and Theor. Chem., 2019. V. 1159. P. 12–17.
2. Psakhie S. G. et al. Movable cellular automata method as a tool for physical mesomechanics of materials. // Phys. Mesomech, 1998. V. 1(1). P. 89–101.
3. Lozhkomoev A. S., et al. On the possibility of soft matter nanostructure formation based on mesoporous aluminum hydroxide. Prospects for biomedical applications. // Phys. Mesomech., 2017. V. 20(2). P. 134–141.
4. Lozhkomoev A. S., Kazantsev S. O., Lerner M. I., Psakhie S. G. Acid-base and adsorption properties of the AlOOH 2D nanostructures as factors for regulating parameters of model biological solutions. // Nanotech. in Russia, 2016. V. 11(7-8). P. 506–511.
5. Lerner M. I. et al. Crumpled Aluminum Hydroxide Nanostructures as a Microenvironment Dysregulation Agent for Cancer Treatment. // Nano Letters, 2018. V. 18(9). P. 5401–5410.
6. Bernstein M. et al. Low Temperature Fabrication of β-TCP–PCL Nanocomposites for Bone Implants. // Adv. Engineering Mater., 2010. V. 12(8). P. B341–B347.
7. Sharipova A., Swain S. K., Gotman I., Starosvetsky D., Psakhie S. G., ..., Gutmanas E. Y. Mechanical, degradation and drug-release behavior of nano-grained Fe-Ag composites for biomedical applications. // J. mech. behavior of biomed. mater., 2018. V. 86. P. 240–249.
8. Mikhaylov G. et al. Ferri-liposomes as an MRI-visible drug-delivery system for targeting tumours and their microenvironment. // Nature nanotech., 2011. V. 6(9). P. 594.
9. Tsukanov A. A., Psakhie S. G. Adhesion effects within the hard matter–soft matter interface: molecular dynamics. Facta Universitatis, Series: Mechanical Engineering, 2016. V. 14(3). P. 269–280.
10. Tsukanov A. A., Psakhie S. G. From the soft matter-hard matter interface to bio-self-organization and hybrid systems. // Phys. Mesomech., 2017. V. 20(1). P. 43–54.
11. Tsukanov A., Psakhie S. G. Energy and structure of bonds in the interaction of organic anions with layered double hydroxide nanosheets: A molecular dynamics study. Sci. rep., 2016. V. 6. P. 19986.
12. Tsukanov A. A., Psakhie S. G. Adsorption of charged protein residues on an inorganic nanosheet: Computer simulation of LDH interaction with ion channel. // AIP Conference Proceedings, 2016. V. 1760(1). P. 020066.
13. Tsukanov A. A., Psakhie S. G. Two-dimensional Al hydroxide interaction with cancerous cell membrane building units: Complexed free energy and orientation analysis. // AIP Conference Proceedings, 2017. V. 1882(1). P. 020076.
14. Tsukanov A., Psakhie S. G. Potential of mean force analysis of short boron nitride and carbon nanotubes insertion into cell membranes. // Adv. Biomater. and Dev. in Med., 2016. V. 3(1). P. 1–9.