Contribution ID: **42** Type: **Poster**

Binding of antibiotic drug molecules to the surface of silver nanoparticles: tight-binding DFT study

Monday, 23 December 2019 18:25 (5 minutes)

Enhancement of therapeutic activity of organic drug molecules bound to nanoparticle surface has recently been highlighted as a possible way to overcome resistance of bacteria towards traditional antibiotics [1]. Investigation of the physical interactions responsible for such complexation, however, becomes challenging when nanoparticle is formed by transition metal atoms due to the need of accurate treatment of the nanoparticle polarizability [2]. Purely ab initio approaches, on the other hand, are typically ruled out by the number of atoms in such systems and consequent demands for computational resources. In the variety of molecular modeling approaches available nowadays, the density-functional based tight-binding (DFTB) method is unique in combining the clear hierarchy of physically sound approximations with high computational efficiency [3], thus, being ideal for treating the systems of hundreds of atoms in reasonable time.
In the present contribution we report the applications of DFTB-based automated conformational searching algorithms [4] to obtain the energetically most stable complexes formed by organic drug molecules Ceftriaxone and Doxorubicin with silver nanoparticles (ca. 1 nm diameter) of different shapes.

[1] A. Panáček, M et al., Molecules (2016), Vol. 21, P. 26.
[2] F. Iori, S. Corni. J. Comput. Chem.(2008), 29(10), 1656-1666.
[3] J. Cuny, N. Tarrat, F. Spiegelman, A. Huguenot, M. Rapacioli. J. Phys. Condens. Matter (2018), Vol. 30, p. 303001.
[4] S. Grimme. J. Chem. Theory Comput (2019), 15(5), 2847-2862.

Primary authors: Ms HUSAK, Olha (Faculty of Physics of Taras Shevchenko National University of Kyiv); Dr NIKOLAIENKO, Tymofii (Faculty of Physics of Taras Shevchenko National University of Kyiv); Dr PAVLENKO, Olena (Faculty of Physics of Taras Shevchenko National University of Kyiv)

Presenter: Ms HUSAK, Olha (Faculty of Physics of Taras Shevchenko National University of Kyiv)

Session Classification: Poster session

Track Classification: Physics of Biological Macromolecules