Covalent heterostructure based on self-decorated MoS_2 and graphene

Dmitry G. Kvashnin[1,2], Gotthard Seifert[3], Leonid A. Chernozatonskii[1]

[1]Emanuel Institute of Biochemical Physics RAS, 119334, 4 Kosigina st., Moscow, Russia
[2]National University of Science and Technology MISiS, 4 Leninskiy prospekt, Moscow, 119049, Russian
[3]Technische Universität Dresden, 01069 Dresden, Germany
dgkvashnin@gmail.com

Investigations of two dimensional materials are the most promising and developing areas in science and technologies nowadays. Graphene and MoS_2 are the two intensive study materials. Graphene is semimetal with zero band gap displays amazing electronic, mechanical and optical properties. MoS_2 belongs to the family of transition metal dichalcogenides with semiconductor bulk band gap about 1.6 eV depending of the thickness. Complementary physical properties of graphene and MoS_2 naturally allow combining these materials to create heterostructures with unusual properties.

Set of numbers of the layers of various compounds allows us to create heterostructures by combining the layers between each other. Only the drawback of obtained heterostructure is the weak van der Waals interaction between the layers. To improve a weak interaction an individual metal atoms could be adsorbed on the layers surface before the creation of the heterostructure.

Here the detailed investigation of novel covalent heterostructures based on graphene and MoS_2 was carried out using *ab initio* calculations. Firstly the decoration process of MoS_2 by Mo adatoms (self-decoration) was studied. It was found the strong binding between the MoS_2 layer and molybdenum adatoms which states about energy favorability of adsorption onto MoS_2 surface.

Further investigation of step by step decoration process and migration barrier of adatom on the MoS_2 surface to understand the origin of strong binding with taking into account inertness nature of MoS_2 layer was carried out. Electronic properties were also studied during the decoration process.

Finally the electronic properties of covalent heterostructure were studied. It was found that d_z^2 orbitals of Mo adatoms between the graphene and MoS_2 surfaces are responsible for the formation of the conduction channel.

We are grateful to the 'Chebishev' and 'Lomonosov' supercomputers of Moscow State University and the Joint Supercomputer Center of the Russian Academy of Sciences for the possibility of using a cluster computer for our quantum-chemical calculations. LAC acknowledges Russian Scientific Foundation (project no 14-12-01217). DGK acknowledges the financial support of the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST "MISiS" (No. K2-2015-033).