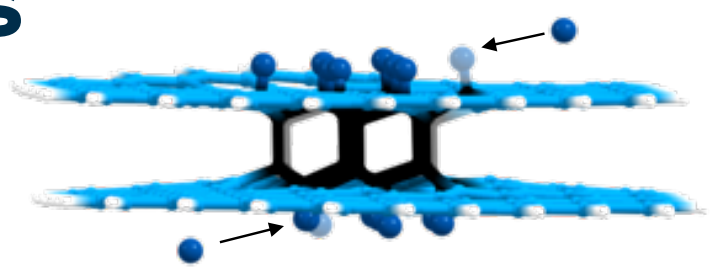
When: February 14, 16:00-17:00
Where: Skoltech, Blue Bldg, room 402

Skoltech
Skolkovo Institute of Science and Technology

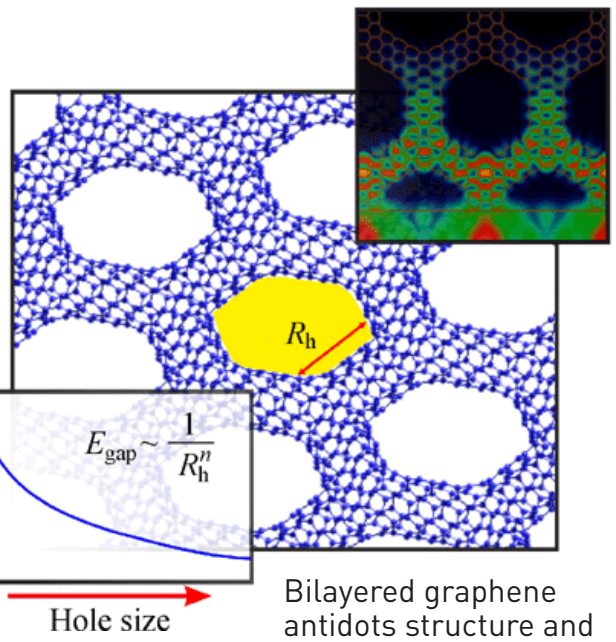
Computational Materials Science
Seminar

2D CARBON NANOSTRUCTURING

Several examples of new nanostructures formation with promising properties



Diamond film formation



Bilayered graphene antidots structure and properties

Speaker:
Pavel B. Sorokin
National University of Science and Technology MISiS, Moscow, Russian Federation

ABSTRACT

The control of atomic structure of ultrathin films on the atomic level is one of the key issues in the rapidly developed field of the 2D films. Here I will present our recent results in the field of theoretical analysis of the already experimentally obtained carbon nanomaterials and our predictions of perspective structures with specific properties.

I will show how a few-layer graphene can undergo phase transformation into ultrathin diamond film under reduced or no pressure, if the process is facilitated by hydrogenation or fluorination of the surfaces. Such "chemically induced phase transition" [1] is inherently nanoscale phenomenon, when the surface conditions directly affect thermodynamics, and the transition pressure depends greatly on film thickness. Ab initio computation of Gibbs free energy of the subsequent adsorption of reference atoms allows to directly observe a nanoscale diamondization process and estimate a nucleation barrier. We show that diamond formation considerably depends on graphene layers number, their packing, type and arrangement of adatoms as well as external parameters and therefore requires they fine tuning in the further experiments [2].

I will present a study of new nanostructures based on the bilayered graphene with periodically arranged holes (bilayered graphene antidots). Our ab initio calculations show that fabrication of holes in bigraphene leads to connection of the neighboring edges of the two graphene layers with formation of a hollow carbon nanostructure sheet which displays wide range of electronic properties (from semiconductor to metallic), depending on the size of the holes and the distance between them [3] whereas multilayered graphene irradiation with high-energy heavy ions allows to observe the formation of such pores in the upper layers of the films [4].

BIOGRAPHY

Dr. Pavel Sorokin graduated from Krasnoyarsk State University with honors in 2005. He defended PhD thesis in 2007 in condensed matter physics at Lebedev Physical Institute of RAS, Moscow. After the defense, Dr. Sorokin worked in position of senior lecturer in Siberian Federal University and as a post-doctoral researcher in Rice University, Houston, TX, US. In 2014 Pavel Sorokin defended Doctor of Science thesis (Habilitation) at Karpov Institute of Physical Chemistry, Moscow.

From 2011 Pavel Sorokin works in Technological Institute for Superhard and Novel Carbon Materials (Moscow, Russia) in the position of senior researcher (from 2015 as a head of the Laboratory of new materials simulation). Dr. Sorokin is leading a research group in MISiS doing quantum mechanical and classical atomistic simulations of ultrathin films and superhard materials, and has the position of visiting researcher in Quantum Beam Science Research Directorate, National Institutes for Quantum and Radiological Science and Technology (Japan). He is author of more than 100 publications among which number of papers were published in such high-impact journals as Nature Chemistry, Nature Physics, Advanced Materials, Nature Communications, Nano Letters, ACS Nano etc.

LOOKING FORWARD TO SEEING YOU!

References

[1]. Kvashnin A.G. et al. Phase diagram of quasi-two-dimensional carbon // Nano Lett. 2014. Vol. 14, № 2. P. 676–681.

[2]. Erohin S.V. et al. Nanothermodynamics of diamond films with atomic thickness // submitted. 2019.

[3]. Kvashnin D.G. et al. Bilayered semiconductor graphene nanostructures with periodically arranged hexagonal holes // Nano Res. 2015. Vol. 8, № 4. P. 1250–1258.

[4]. Chernozatonskii L.A. et al. Bilayer graphenes with antidots: structures, properties and applications // J. Phys. Conf. Ser. 2018. Vol. 1092, № 1. P. 012018.