Theoretical prediction and experimental evidences of 2D monolayered transition metal oxide films family

Dmitry G. Kvashnin[a,c]*, Konstantin V. Larionov[b], Leonid A. Chernozatonskii[c] and Pavel B. Sorokin[a,b,c]

a. *National University of Science and Technology MISiS, Moscow, Russian Federation*
b. *Technological Institute for Superhard and Novel Carbon Materials, Moscow, Russian Federation*
c. *Emanuel Institute of Biochemical Physics RAS, Moscow, Russian Federation*

* dgkvashni@phystech.edu

2D and quasi-2D materials have attracted attention since the discovery of graphene, which can maintain its structure due to strong covalent bonding within a layer, whereas the weak van der Waals forces acting between the layers allow its isolation. Like graphene hexagonal boron nitride (h-BN) and quasi-2D sheets of transition metal dichalcogenides have been found so far, and reported to exhibit unique and attractive properties. These materials have their bulk counterparts with layered structures.

In contrast to the above reports, non-layered materials with wurtzite and cubic crystal structures were theoretically predicted to form 2D layers, and this possibility is important as it significantly widens the range of potential 2D materials. Recently, graphene-like 2D zinc oxide clusters and 2D iron clusters with a square lattice have been observed by aberration-corrected transmission electron microscopy. In both cases, the 2D layers were in the small pores in graphene, and their edges can be stabilized by bonding with carbon, whereas such geometry limits the size and properties of 2D materials.

Here we report the structure and properties of a novel family of 2D material, transition metal oxides (TMO), studied by theoretical methods which data perfectly supported by available experimental results. In particular, observed atomic structure of 2D CuO sheets agrees very well with our predictions.

Density functional theory allowed to elucidate the nature of the stability of observed metal nanofilms. It was defined a critical role of the oxygen impurity atoms in the formation of stable 2D CuO cluster with unexpected orthogonal crystal lattice. It was found that the structure and stability of 2D CuO clusters strongly depends on the concentration and relative arrangement of oxygen impurities. Number of oxygen configurations was analyzed and the stable configuration was found corresponded well with experimental data.

We predict that 2D TMO sheets have unusual electronic and magnetic properties depending on the composition. We study of stability of such films and its stabilization in the graphene 2D matrix. We combine crystal growth theory and atomistic computations for the prediction of the energy favorable structure of 2D TMO/graphene composite.

Results of this investigations were published in Nanoscale journal and submitted to The Journal of Physical Chemistry Letters.

Authors acknowledge the financial support of the RSF according to the research project № 17-72-20223. D.G.K. also acknowledges grant RFBR № 18-32-00682.