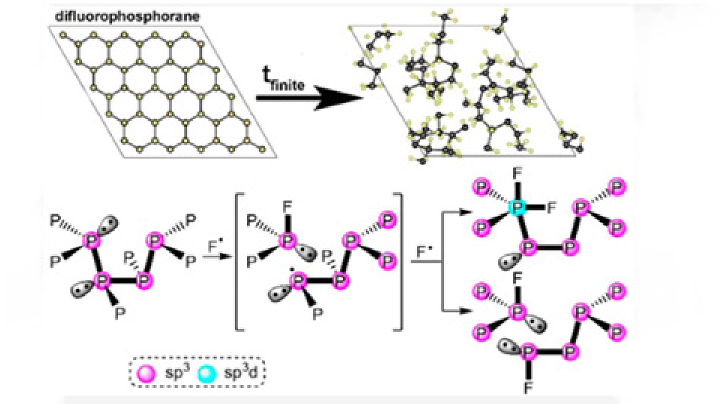
Chemists have managed to stabilize the "capricious" phosphorus

An international team of Russian, Swedish and Ukrainian scientists has identified an effective strategy to improve the stability of two-dimensional black phosphorus, which is a promising material for use in optoelectronics.



The most effective mechanism of fluorination has been revealed. In addition to increased stability compared to previously proposed structures, the materials predicted by the researchers showed high antioxidative stability. The main results of the work have been presented in The Journal of Physical Chemistry Letters.

Black phosphorus is obtained from white phosphorus under conditions of high pressure and elevated temperature. The material has a layered structure and resembles graphite in appearance and properties. However, unlike graphite, it is a good semiconductor.

> *“Phosphorene is a monolayer of black phosphorus with interesting physical properties (high anisotropic electrical and thermal conductivity, flexible band gap variability depending on the number of layers), which makes it a promising material for use in various fields of optoelectronics (transistors, inverters, flexible electronics, solar panels). Unfortunately, one of its main problems is instability in the environment. Unlike its volumetric analogue, which is almost immune to external conditions, phosphorene quickly begins to attach oxygen from the air and degrades within a few hours. As one of the strategies for improving the stability of phosphorene, mechanism of fluorination was proposed. Over the past five years, scientists have proposed several theoretically possible options for such a “coupling”. An experiment was conducted that showed a significant increase in the stability of phosphorus in ambient conditions after fluorination. However, the features of the obtained material structure remained unexplained.*
>
> *Using various theoretical approaches, my colleagues and I showed that the previously proposed structures of “stabilized” phosphorus were actually unstable. It is known that phosphorus is able to form compounds with 3 or 5 fluorine atoms. Our calculations also confirmed that the characteristic coordination of the phosphorus atom in the PF system is 3 or 5. By sequential addition of atoms, it was possible to identify the most effective and really working mechanism by which fluorine atoms should attach to the surface of phosphorene. Thus, we have determined the type of structures that are likely to have been obtained by our predecessors in the above-mentioned experiment,"* — said **Artem Kuklin**, a research fellow of SibFU.

Scientists note that the materials formed by the predicted mechanism are really stable and have increased antioxidant ability (that is, they are not quickly degradable) and their electronic properties, which do not differ much from the properties of pure phosphorus, provide the possibility of their practical application in optoelectronic devices, i.e. transistors, solar panels, flexible electronics, LEDs, photosensors, biomedical devices, optical devices for storing and transmitting information, etc.

Apart from the scientists from Siberian Federal University, researchers from the Royal Institute of Technology (Sweden), Henan University (China) and Khmelnitsky Cherkassy National University took part in this research.

The study was supported by the Ministry of Science and Higher Education of the Russian Federation and the Siberian Federal University (Grant No. 16.1455.2017 / ПЧ).

6 december 2019