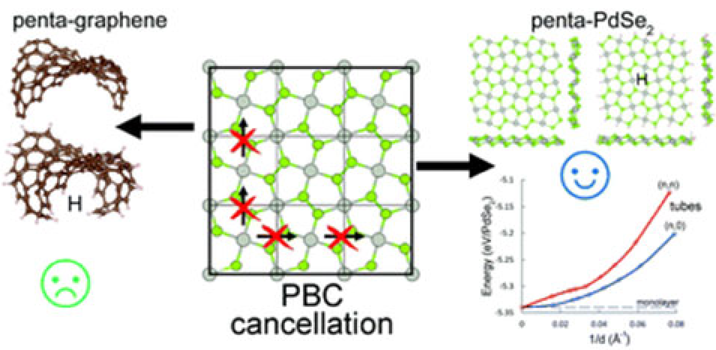
Scientists devise a way to determine the viability of predicted 2D materials



An international team of researchers from Russia, Sweden and South Korea has proposed a new way to test the structural stability of predicted 2D materials. The testing revealed a number of materials erroneously proposed earlier. The scholars believe that the use of the new method will further help to avoid mistakes in the development of two-dimensional nanomaterials that are in high demand in the modern world. The results were published in the international journal Physical Chemistry Chemical Physics.

The existence of two-dimensional structures, which are the thinnest films consisting of one layer of the crystal lattice of atoms, has been widely discussed since the mid 20th century. Scientists had been heatedly discussed for several decades until such possibility was proved by theoretical conclusions and confirmed experimentally later by the synthesis of graphene — crystalline carbon with a thickness of one atom. Since then, attention to two-dimensional materials with unexpected properties — high strength (hundreds of times stronger than metal), lightness, thermal conductivity — has grown significantly, and today the number of experimentally obtained 2D materials comes in dozens.

It is worth noting that most of the early materials were discovered mainly by trial and error. With the advent of sufficient computer power and theoretical methods of prediction, however, scholars now are discovering materials even before their synthesis. Modern high-performance algorithms and methods can be used for mass scanning of new 2D materials among already known compounds. Moreover, with their help, we can create previously unknown materials with designed properties. Nevertheless, it is necessary to calculate the stability of such predicted materials in order to make them desired for the production and have future prospects for adopting into the reality.

> *'We discovered that the existing and widely used methods for checking the stability of theoretically-known 2D materials have a serious drawback, which allows bypassing the generally accepted criteria and, virtually, in some cases leads to a false prediction of the stability of a 2D material. To put it simpler, such materials merely should not exist, there is practically no chance to get them experimentally, and the discovery of such materials is just an error of the method used,'* said **Artyom Kuklin**, a research engineer at the Laboratory for Fundamental Scientific Research, Department of Science and Innovation, SibFU.

The scholar explained that the main disadvantage of the common method applied nowadays is the model of representation of the material.

> *'When modelling, researchers use conditional material of some kind, which is an infinitely repeating pattern consisting of the so-called unit cells — minimal fragments of the structure. It looks like cells recurring on a notebook sheet. Moreover, information about one cell gives information about the entire sheet. The model assumes that all these cells are rigidly interconnected and that they cannot be bent along this connection. In other words, we knowingly get a perfectly even infinite sheet, which, of course, lines up weakly with the reality,'* explained **Artyom Kuklin**.

The authors of the study propose to disregard an infinite model of a material, but instead, to consider its portion of a finite size as an additional criterion for the stability of two-dimensional nanomaterials, as this part has no strict restrictions on the connection between separate fragments of the structure. If under these conditions, the material remains the same as it was in the periodic model, then there are no internal stresses in it. If the material significantly distorts (for example, folds up), then the internal stress in such structure will become a marker of instability, and hence realizability of this material will be dubious in reality.

> *'Using the proposed method, our team demonstrated the structural stability of the recently synthesized 2D material of Palladium diselenide (PdSe2) and the instability of several previously proposed two-dimensional materials with a similar structure. We consider this approach effective enough to theoretically study materials which are promising for the future technology. By the way, as for another criterion for assessing the absence of internal stresses in a 2D material, we have proposed to study its stability with respect to nanotubes of the same material. In this case, a two-dimensional material should be more stable than nanotubes.*
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> *We hope that the scientific community will turn their attention to the mentioned problem and improve the existing algorithms to avoid similar errors in the future,'* summed up the **researcher**.

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