A Whole New Universe of 2D Materials Is Emerging

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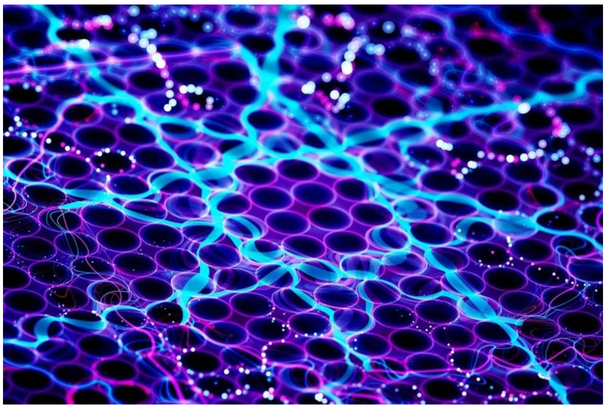

Courtesy of SynEvol

Extremely thin materials, only a few atoms thick, have special qualities that make them desirable for water purification, catalysis, and energy storage. Now, scientists at Sweden's Linköping University have created a technique that makes it possible to create hundreds of novel 2D materials.

The field of study for incredibly thin materials, or 2D materials, has grown rapidly since the discovery of graphene. The explanation for this is that, compared to their volume or weight, 2D materials have a significant surface area. As a result, 2D materials exhibit a variety of unique characteristics and physical phenomena, including high strength, heat resistance, and superior conductivity, which are valuable for both fundamental research and practical applications.

Courtesy of SynEvol
Credit: Thor Balkhed

Millions of layers of the material can exist in a sheet as thin as one millimeter. Many chemical reactions can occur between the layers, which makes 2D materials useful for producing fuels or storing energy, for example, according to Johanna Rosén, a professor of materials physics at Linköping University.

MXenes is the name of the largest family of 2D materials. A three-dimensional parent material known as the MAX phase is used to make MXenes. It is made up of three distinct elements: X is either carbon or nitrogen, A is an element of the (A-group), and M is a transition metal. A two-dimensional substance is produced by exfoliating, or eliminating the A element with acids. As of right now, MXenes is the only material family produced in this manner.

A theoretical technique for forecasting further three-dimensional materials that would be appropriate for transformation into two-dimensional materials has been presented by the Linköping researchers. Additionally, they have demonstrated the consistency of the theoretical model with reality.

The researchers employed a three-step procedure to be successful. To determine which parent materials would be appropriate, they first created a theoretical model. From a database and a selection of 66,643 materials, the researchers were able to discover 119 interesting 3D materials using large-scale simulations at the National Supercomputer Centre.

Trying to make the substance in the lab was the next step. "We looked at 119 different materials to see which ones were the greatest options and which ones had the necessary chemical stability. The 3D material had to be synthesized first, which presented its own set of difficulties. The hydrofluoric acid we used to etch away certain atom layers was finally a high-quality sample," according to Jie Zhou, an assistant professor in the Department of Physics, Chemistry, and Biology.

Two-dimensional $Ru_2Si_xO_y$ was formed when the researchers extracted yttrium (Y) from the parent material YRu_2Si_2.

However, step three, verification, is required to validate success in the lab. The Arwen scanning transmission electron microscope at Linköping University was utilized by the researchers. It is capable of analyzing materials and their atomic structures. Using spectroscopy, one can also look at the individual atoms that make up a material in Arwen.

We were able to verify that the substance produced had the right atoms in it and that our theoretical model performed as predicted. Images of the material after exfoliation resembled book pages. "It's incredible that the theory can be implemented, broadening the scope of chemical exfoliation beyond MXenes to include more material families," says associate professor Jonas Björk of the Materials Design division.

Thanks to the researchers' discovery, a large number of additional 2D materials with distinctive features are now feasible. They can then serve as the basis for an endless number of technical applications. The researchers' next course of action is to expand the experimentation and investigate more promising precursor materials. Future uses, in Johanna Rosén's opinion, are practically limitless.

All things considered, 2D materials have demonstrated tremendous promise for a plethora of uses. Consider removing carbon dioxide or cleaning water, for instance. According to Johanna Rosén, the current focus is on increasing the synthesis while maintaining sustainability.

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