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New method enables synthesis of hundreds of new 2D materials

March 14 2024

Jie Zhou, assistant professor at Linköping university. Credit: Olov Planthaber

Materials that are incredibly thin, only a few atoms thick, exhibit unique properties that make them appealing for energy storage, catalysis and water purification. Researchers at Linköping University, Sweden, have now developed a method that enables the synthesis of hundreds of new 2D materials. Their study has been published in the journal *Science*.

Since the discovery of graphene, the field of research in extremely thin materials, so-called 2D materials, has increased exponentially. The reason is that 2D materials have a large surface area in relation to their volume or weight. This gives rise to a range of physical phenomena and distinctive properties, such as good conductivity, high strength or heat resistance, making 2D materials of interest both within fundamental research and applications.

"In a film that's only a millimeter thin, there can be millions of layers of the material. Between the layers there can be a lot of chemical reactions and thanks to this, 2D materials can be used for energy storage or for generating fuels, for example," says Johanna Rosén, professor in Materials physics at Linköping University.

The largest family of 2D materials is called MXenes. MXenes are created from a three-dimensional parent material called a MAX phase. It consists of three different elements: M is a transition metal, A is an (A-group) element, and X is carbon or nitrogen. By removing the A element with acids (exfoliation), a two-dimensional material is created. Until now, MXenes has been the only material family created in this way.

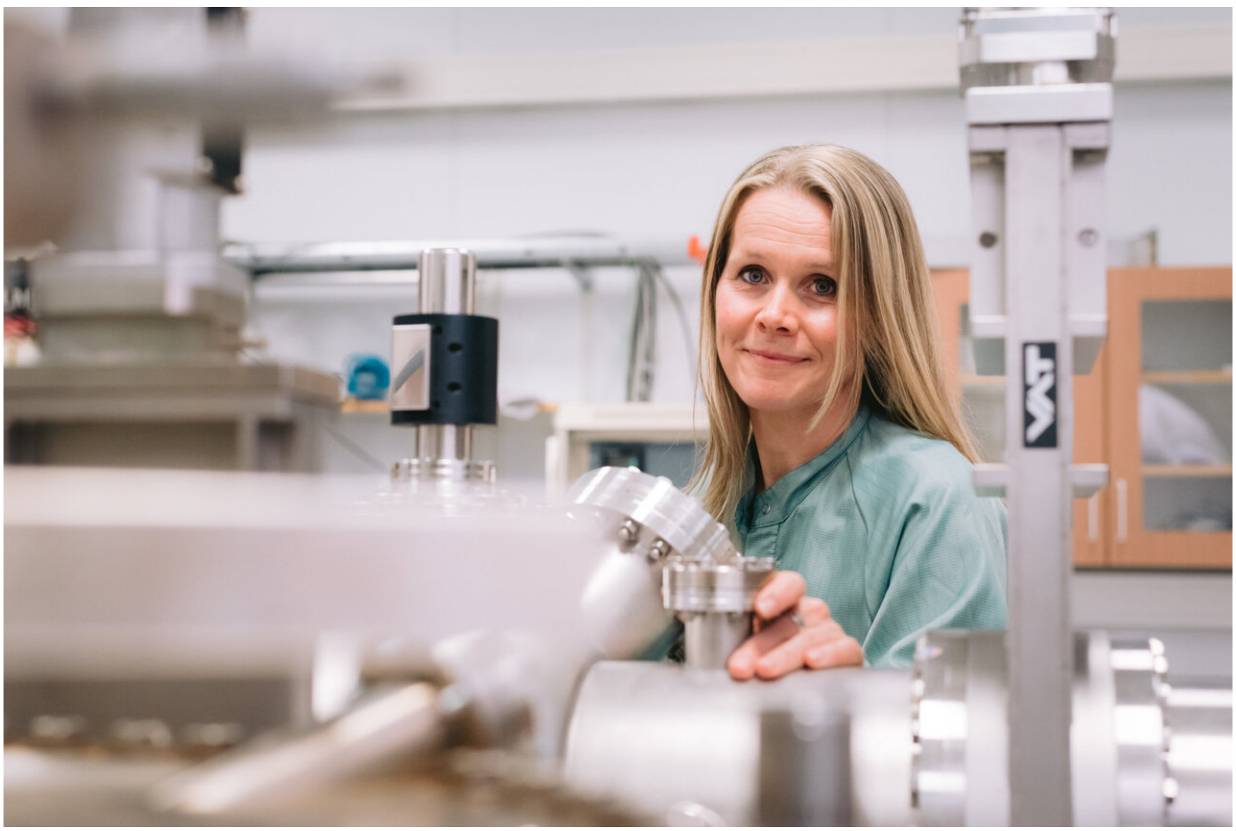
Jonas Björk, associate professor at Linköping University. Credit: Thor Balkhed

The Linköping researchers have introduced a theoretical method for predicting other three-dimensional materials that may be suitable for conversion into 2D materials. They have also proved that the theoretical model is consistent with reality.

To succeed, the researchers used a three-step process. In the first step, they developed a theoretical model to predict which parent materials would be suitable. Using large-scale calculations at the National Supercomputer Center, the researchers were able to identify 119 promising 3D materials from a database and a selection consisting of 66,643 materials.

The next step was to try to create the material in the lab.

"Out of 119 possible materials, we studied which ones had the chemical stability required and which materials were the best candidates. First, we had to synthesize the 3D material, which was a challenge in itself. Finally, we had a high-quality sample where we could exfoliate and etch away a specific atom layers using hydrofluoric acid," says Jie Zhou, assistant professor at the Department of Physics, Chemistry and Biology.



Johanna Rosén, professor at Linköping University. Credit: Anna Nilsen

The researchers removed yttrium (Y) from the parent material YRu_2Si_2, which resulted in the formation of two-dimensional $Ru_2Si_xO_y$.

But to confirm success in the lab, verification is necessary—step three. The researchers used the scanning transmission electron microscope Arwen at Linköping University. It can examine materials and their structures down at the atomic level. In Arwen it is also possible to investigate which atoms a material is made up of using spectroscopy.

"We were able to confirm that our theoretical model worked well, and that the resulting material consisted of the correct atoms. After exfoliation, images of the material resembled the pages of a book. It's amazing that the theory could be put into practice, thereby expanding the concept of chemical exfoliation to more materials families than MXenes," says Jonas Björk, associate professor at the division of Materials design.

The researchers' discovery means that many more 2D materials with unique properties are within reach. These, in turn, can lay the foundation for a plethora of technological applications. The next step for the researchers is to explore more potential precursor materials and scale up the experiments. Rosén believes that future applications are almost endless.

"In general, 2D materials have shown great potential for an enormous number of applications. You can imagine capturing carbon dioxide or purifying water, for example. Now it's about scaling up the synthesis and doing it in a sustainable way," says Rosén.

More information: Jonas Björk et al, Two-dimensional materials by large-scale computations and chemical exfoliation of layered solids, *Science* (2024). DOI: 10.1126/science.adj6556. www.science.org/doi/10.1126/science.adj6556

Provided by Linköping University

Citation: New method enables synthesis of hundreds of new 2D materials (2024, March 14) retrieved 27 April 2024 from https://phys.org/news/2024-03-method-enables-synthesis-hundreds-2d.html