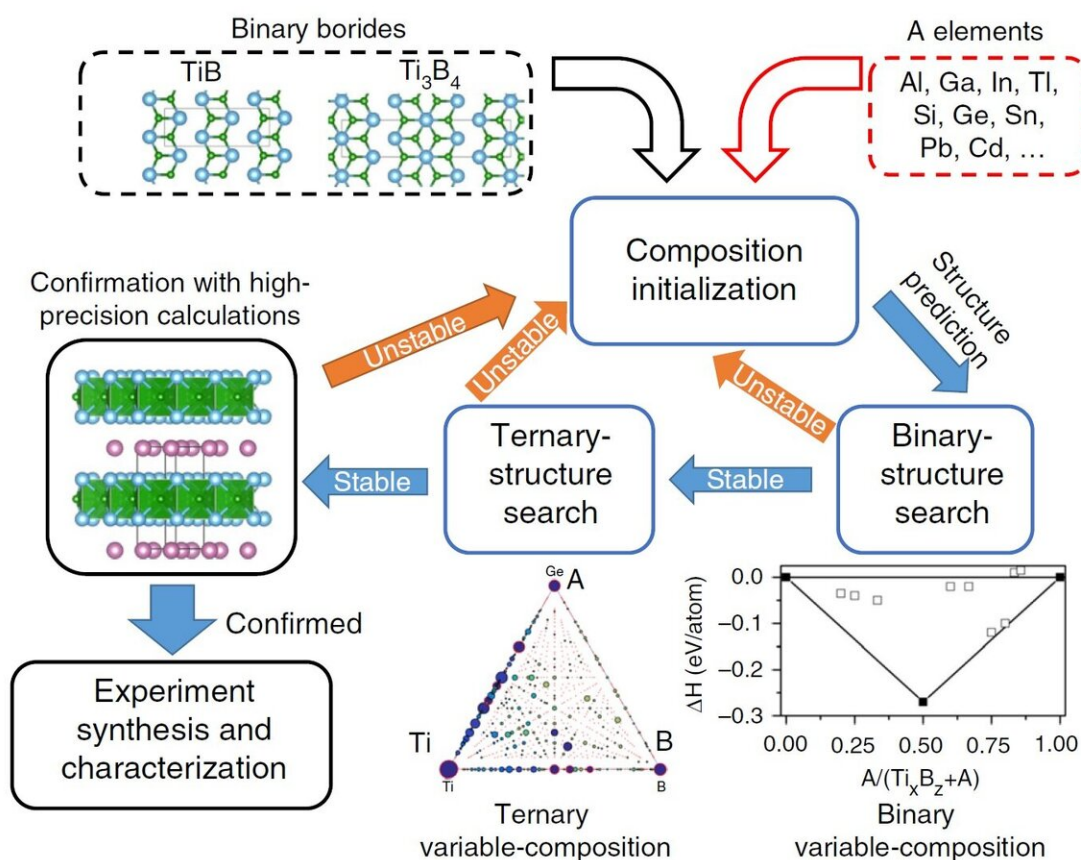


Finding a needle in a haystack: Discovery of Ti_2InB_2 for synthesizing layered TiB

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With the strategy depicted, it was possible to conduct a theoretical search with thousands of initial candidates to finally obtain the best two MAX phases for the potential synthesis of TiB MXenes, which have promising applications in fields such as nanoelectronics. Credit: Nature Communications

Scientists at Tokyo Institute of Technology (Tokyo Tech) have used boron as the X element in a family of materials called MAX phases, for which only carbon and nitrogen could previously be used. A clever search strategy allowed them to avoid resorting to trial and error to design this novel material, from which layered TiB can be obtained for applications in Li- or Na-ion batteries.

Considering that there are dozens of elements in the [periodic table](#) and thousands of possible combinations, it is no surprise that researchers resort to ingenious ways to predict which [compounds](#) can be synthesized in practice and would have favorable properties. One class of useful materials is referred to as "MAX phases." These are ternary compounds consisting of three elements represented by M, A and X that exhibit ceramic and metallic properties.

These compounds form layered structures from which the "A-layer" can be etched, leaving behind what is known as 2-D MXenes. MXenes have attracted a lot of attention because they can take a number of forms and structures and offer excellent chemical and mechanical stability. This makes them applicable in a wide variety of fields, such as batteries and catalysis.

Until now, MAX compounds have been limited to using carbon or nitrogen for the X element. A research team from Tokyo Tech, led by Prof. Hideo Hosono, studied the possibility of synthesizing MAX phases composed of titanium, indium and boron: Ti_2InB_2 . Motivated by the fact that borides have promising applications in nanoelectronics, the team ultimately sought to synthesize TiB-based MXenes.

Because direct synthesis of layered TiB is impossible, the team first had to determine an A-element for synthesizing a MAX phase (that is, the middle element in Ti-A-B). Then they would have to find a way to etch the A-layer from the MAX phase to obtain the coveted layered TiB. In

order to determine which elements were suitable for the A in the MAX phase, they employed a clever automated search strategy through computer-assisted calculations. They first analyzed the "binary" structures formed between each of the candidates for A and either TiB or Ti₃B₄. Those that proved stable were subjected to "ternary" calculations for determining the global stability of the ternary compound.

A final verification with high-precision structural calculations was carried out for the best candidates, which finally pointed at Ti₂InB₂ as the best option. With this strategy, they reduced the computational cost of their search and demonstrated a clever approach for finding desired ternary compounds. "A feasible strategy to simplify the search for ternary compounds based on the available domain knowledge is in high demand," explains Hosono.

The team demonstrated that Ti₂InB₂ could be effectively synthesized, and then explored the possibility of removing In from the MAX phase to obtain the desired MX phase. Although the team did manage to obtain layered TiB from the MAX [phase](#), its structure was not exactly compatible with that of existing 2-D MXenes. However, by tuning the necessary conditions of their approach, the researchers believe that it will be possible to obtain TiB MXene in the future. Thus, they carried out a number of calculations demonstrating its superior electrical properties, hinting at its potential application as an excellent anode material for lithium- or sodium-ion batteries. "The present research will extend the fascinating class of MAX phases and MXenes," concludes Hosono.

More information: Junjie Wang et al, Discovery of hexagonal ternary phase Ti₂InB₂ and its evolution to layered boride TiB, *Nature Communications* (2019). [DOI: 10.1038/s41467-019-10297-8](https://doi.org/10.1038/s41467-019-10297-8)

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