Clever simulation scheme helps identify the most promising compositions of two-dimensional materials

January 16 2018

A high-throughput scan of possible compositions for a new class of materials known as MXenes gives researchers invaluable direction for picking the best candidate from the millions of possible material recipes. The simulation study by researchers from the A*STAR Institute of High Performance Computing is a significant advancement in the field of MXenes, which have exciting potential in next-generation energy storage applications.

Two-dimensional (2-D) materials are a relatively new class of materials that display a wide range of unusual properties associated with their ability to constrain the movement of electrons and energy in a 2-D plane. The MXene alloys are a very recently discovered class of 2-D materials, which could conceivably consist of any of millions of possible arrangements of transition metals (like molybdenum or titanium), carbon and nitrogen. These characteristics are reflected in the name 'MXene'—the 'M' represents metal atoms, the 'X' denotes carbon and nitrogen, while the 'ene' suffix signals the materials' 2-D atomic structure .

"Since MXenes are new, there's still much to be learned about their structure and properties," says Teck Leong Tan from A*STAR. "As MXene alloys are formed by mixing different types of transition elements at different compositions, the alloying possibilities in MXenes are huge. So we developed a high-throughput computational method to

predict the probable structures and stable phases of different MXene alloys across all compositional ranges and temperatures."

Although there are many possible MXene alloy compositions, most will not be stable. The challenge faced by material scientists has been how to efficiently sweep through the huge number of alloy configurations to identify those with the lowest formation energy and hence highest stability. Conventional 'first principles' calculation approaches are too computationally intensive for such a scan to be feasible.

"Our approach uses what's called a cluster expansion method to 'learn' the effective interactions between atoms, thus enabling quick evaluation of the formation energies of millions of MXene alloy structures," says Tan.

The scan, conducted in collaboration with Drexel University in the US, revealed that molybdenum-based MXenes mixed with vanadium, tantalum, niobium or titanium, appear to form the most stable ordered structures. Titanium however tends to form stable 'asymmetric' ordered structures that were previously not considered viable.

"Our scan allows us to predict the structures of MXene alloys that are yet to be fabricated and estimate the likelihood of their fabrication from a thermodynamics viewpoint. And for known MXene alloys, our predicted structures are consistent with experimental results."

More information: Teck Leong Tan et al. High-Throughput Survey of Ordering Configurations in MXene Alloys Across Compositions and Temperatures, *ACS Nano* (2017). DOI: 10.1021/acsnano.6b08227

Provided by Agency for Science, Technology and Research (A*STAR),

Singapore