World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:18, No:05, 2024

Open Science Index, Chemical and Materials Engineering Vol:18, No:05, 2024 publications.waset.org/abstracts/181936.pdf

Discovery of Two-dimensional Hexagonal MBene HfBO

Authors : Nanxi Miao, Junjie Wang

Abstract : The discovery of 2D materials with distinct compositions and properties has been a research aim since the report of graphene. One of the latest members of the 2D material family is MXene, which is produced from the topochemical deintercalation of the A layer from a laminate MAX phase. Recently, analogous 2D MBenes (transitional metal borides) have been predicted by theoretical calculations as excellent alternatives in applications such as metal-ion batteries, magnetic devices, and catalysts. However, the practical applications of two-dimensional (2D) transition-metal borides (MBenes) have been severely hindered by the lack of accessible MBenes because of the difficulties in the selective etching of traditional ternary MAB phases with orthorhombic symmetry (ort-MAB). Here, we discover a family of ternary hexagonal MAB (h-MAB) phases and 2D hexagonal MBenes (h-MBenes) by ab initio predictions and experiments. Calculations suggest that the ternary h-MAB phases are more suitable precursors for MBenes than the ort-MAB phases. Based on the prediction, we report the experimental synthesis of h-MBene HfBO by selective removal of in from h-MAB Hf2InB2. The synthesized 2D HfBO delivered a specific capacity of 420 mAh g-1 as an anode material in lithium-ion batteries, demonstrating the potential for energy-storage applications. The discovery of this h-MBene HfBO added a new member to the growing family of 2D materials and provided opportunities for a wide range of novel applications.

Keywords : 2D materials, DFT calculations, high-throughput screening, lithium-ion batteries
Conference Title : ICC 2024 : International Conference on Chemistry
Conference Location : London, United Kingdom
Conference Dates : May 23-24, 2024