Discovery of Two-dimensional Hexagonal MBene HfBO

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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.

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Keywords: 2D materials, DFT calculations, high-throughput screening, lithium-ion batteries

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