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# Tuning the electrochemical performance of $Cr_2B_2$ MBene anodes for Li and Na-ion batteries through F and Cl-functionalization: A DFT and AIMD study

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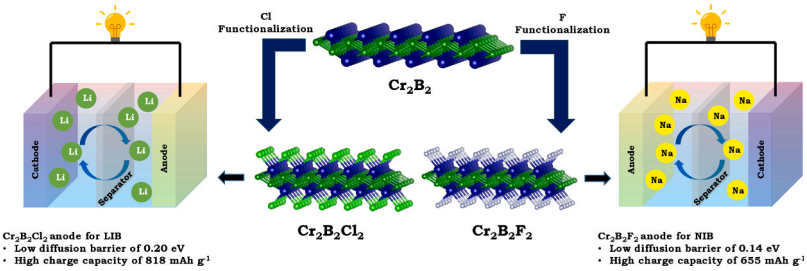
## HIGHLIGHTS

- $Cr_2B_2Cl_2$ and $Cr_2B_2F_2$ are both mechanically, thermally, and dynamically stable auxetic materials.
- Surface functionalization of Cr-MBene by Cl/F significantly lowers the diffusion barrier of Li/Na-ions.
- $Cr_2B_2Cl_2$ has a high charge storage capacity of 818 mAh $g^{-1}$ for Li-ion battery.
- $Cr_2B_2F_2$ is an outstanding candidate for Na-ion battery with an ultra-high storage capacity of 655 mAh $g^{-1}$.

## GRAPHICAL ABSTRACT




## ARTICLE INFO

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## ABSTRACT

In an era in which sustainable energy sources and electric vehicles are prevalent, the development of efficient anode materials is paramount to address the pressing demand for improved energy storage technologies. After the graphene revolution, many other 2D materials such as graphene, MXene (atomically thin layer of Transition Metal Carbide/Nitride/Carbonitride), TMDC (Transition Metal Dichalcogenide), and MBene (atomically thin layer of Transition Metal Borides) have emerged as potential high-performance anode materials. A recent study demonstrated the possibility of synthesizing chromium-based MBenes for the first time, and the electrochemical performance of $Cr_2B_2$ as a potential anode material has also been studied theoretically. Inspired by this, the current study utilized density functional theory and *ab initio* molecular dynamics simulations to probe the role of Cl and F-functionalization of $Cr_2B_2$ MBenes as anode materials for rechargeable lithium-ion batteries (LIB) and sodium-ion batteries (NIB). The electronic structure, adsorption, diffusion, and storage capacity of Li (Lithium) and Na (Sodium) were systematically investigated. This study revealed that $Cr_2B_2F_2$ and $Cr_2B_2Cl_2$ exhibit excellent conductivity due to their intrinsic metallic properties. In addition, they have low diffusion energy barriers for Li and Na ions (0.13/0.14 and 0.20/0.20 eV for $Cr_2B_2F_2$ and $Cr_2B_2Cl_2$, respectively) facilitating rapid charge/discharge rates. The calculations further unveiled a notable Li-ion storage capacity of 818 mAh g-1 for 2D $Cr_2B_2Cl_2$, accompanied by a moderate open-circuit voltage (OCV) range of 0.38 V to 0.98 V, illustrating its potential as a superior anodic material for LIBs. Similarly, $Cr_2B_2F_2$ demonstrated a substantial Na-ion storage

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