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## Bi-metallic MXenes $\text{Mo}_2\text{V}_2\text{C}_3\text{T}_2$ (T = O, F, OH) for energy storage devices. Atomisitics insights on ion-adsorption process

MXenes materials have shown good electrochemical properties for energy storage such as metallic behavior, high electrical conductivity and low energy barriers for ions diffusion. Recent studies have shown that bi-metallic MXenes, such as  $\text{Ti}_2\text{Ta}_2\text{C}_3$ , exhibit superior electrochemical behavior compared to monometallic counterparts, offering potential for extended lifespan in energy storage systems, as Maldonado-Lopez reports in 2022 [1]. This study reports the functionalization of bi-metallic MXene  $\text{Mo}_2\text{V}_2\text{C}_3$  with O, F, and OH. Moreover, highlights the significance of bi-metallic MXenes and surface functionalization in advancing energy storage technologies, suggesting avenues for improving cycling stability and energy efficiency in next-generation energy storage devices. Our results suggest that the oxidized phase grants a better performance as anode in batteries, and the Li-ion offers a higher gravimetric capacity.

### Keywords

MXenes Materials

### Reference

Maldonado-Lopez, Daniel; et al., Atomic-Scale Understanding of Li Storage Processes in the  $\text{Ti}_4\text{C}_3$  and Chemically Ordered  $\text{Ti}_2\text{Ta}_2\text{C}_3$  MXenes: A Theoretical and Experimental Assessment ACS Appl. Energy Mater. 2022, 5, 2, 1801–1809

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### Author approval

I confirm

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