Electronic Properties and Shuttle Effect Inhibition in Two-Dimensional Mo_2CT_2 (T = S, O) MXenes for Sodium-Sulfur Batteries: A Density Functional Theory Study

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Sodium-sulfur (Na-S) batteries have gained considerable attention in recent years as a viable solution for large-scale energy storage, primarily due to their high energy density, low cost, and the abundance of sodium and sulfur resources. However, the shuttle effect hinders the practical implementation of Na-S batteries, leading to irreversible capacity loss and reduced performance. In response to this challenge, two-dimensional (2D) materials, particularly Mo_2CT_2 (T=S, O) MXene, have emerged as promising candidates to mitigate the shuttle effect by anchoring sodium polysulfides and improving electrode stability. This study employs density functional theory (DFT) to investigate the mechanism by which Mo_2CT_2 (T=S, O) MXene inhibits the shuttle effect in Na-S batteries. DFT calculations provide insights into the atomic-level interactions between sodium polysulfides and the MXene surface, highlighting the role of functional groups and structural properties in immobilizing polysulfides and enhancing battery performance. The findings demonstrate that Mo_2CT_2 (T=S, O) MXene effectively reduces the diffusion of polysulfides, leading to improved cycling stability and efficiency. This work offers a theoretical foundation for the development of high-performance Na-S batteries with enhanced durability and stability, contributing to the advancement of renewable energy storage technologies.

Keywords: Sodium-sulfur batteries, shuttle effect, sodium polysulfides, MXene, DFT