

A DFT study of alkali metal intercalation in two-dimensional heterostructures towards ion battery applications

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Two dimensional (2D) materials are very promising structures for battery applications since their high surface area and capability of higher charging rates as metal ions do not need to diffuse in a 3D lattice. Hence, interest in electrochemical energy storage applications of 2D materials is growing rapidly. MXenes, as the newest family of 2D materials, offer great potential in a wide range of technological applications including alkali-ion battery. MXenes ($M_{n+1}C_nTx$) offer an unusual combination of conductivity and hydrophilicity, and attractive electrochemical properties since the presence of a metal carbide core ($M_{n+1}C_n$) together with termination groups (Tx). In recent years, by considering the superior properties of MXenes and outstanding electrical conductivity of graphene, we have proposed several different heterostructures possessing unique potential in battery applications [1-6]. Our results show that the MXene systems are appropriate for battery applications in terms of adsorption energies, full coverage capacity, and low-diffusion energy barriers. For practical battery applications, a balance between the storage capacity and kinetics is needed and our results show that selected heterostructures offer a compromise between capacity and kinetics due to the low diffusion energy barriers and strong ion binding strengths.

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