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First-principles analysis of potassium and magnesium adsorption on an innovative VC4 monolayer
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Abstract
Mg-ion batteries (MgIBs) and K-ion batteries (KIBs) are considered excellent energy storage options due to their affordability and similarity to Li-ion batteries (LIBs) regarding the rocking chair mechanism. Nevertheless, a significant challenge exists in the form of a shortage of suitable electrode materials that can provide high performance for KIBs and MgIBs. Our study utilized first-principles calculations based on density functional theory (DFT) to evaluate the potential of the VC4 monolayer as an anode material for MgIBs and KIBs. The results indicate that Mg and K adsorption on the surface of VC4 is associated with negative favorable energies. Moreover, the VC4 monolayer can effectively achieve double-layer adsorption for K/Mg on both sides of its surface. The VC4 exhibits a remarkably high theoretical capability of 812 mA h/g for KIBs and 1624 mA h/g for MgIBs. These exceptional capacities for KIBs and MgIBs primarily arise from the minimal Coulombic repulsion forces between the VC4 sheet and K/Mg. Moreover, K and Mg portray large diffusivity on VC4, illustrated by low energy barriers of 0.15 eV and 0.09 eV, respectively. Moreover, the open circuit voltages (OCV), measuring 0.28 V for MgIBs and 0.49 V for KIBs, are notably lower than in previous studies. Despite the relatively large size of K+/Mg+ ions, the maximum alteration in VC4 lattice parameters stands at 6.01 % and 6.8 %, respectively. This observation highlights the material's structural stability, ensuring robust cycling performance for KIBs and MgIBs. These results underscore the potential of the VC4 monolayer as a novel candidate for KIBs and MgIBs.

Author Keywords
Diffusion barrier; First-principles calculations; K-ion batteries; Mg-ion batteries; VC4 monolayer

Index Keywords
Energy, First principle calculations, First principles, Ion batteries, K-ion battery, Mg-ion battery, Principle analysis, Rocking chair, VC4 monolayer; Lithium-ion batteries

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