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Strain effects on alkali metal ion adsorption mechanisms on ZrS_2 monolayer for efficient sodium and potassium-ion batteries: A DFT study

In the pursuit of advanced energy storage systems with high energy and power densities, two-dimensional materials like zirconium disulfide (ZrS_2) are being investigated as potential anode candidates for alkali metal-ion batteries due to their exceptional properties. However, there is limited information regarding the application of ZrS_2 monolayers as electrode materials specifically in sodium and potassium-ion batteries.

In this work, density functional theory with Hubbard (U) parameter implemented in Quantum ESPRESSO, was used to investigate the effects of strain on sodium and potassium-ion adsorption mechanisms on ZrS_2 monolayer. Our results revealed that when sodium is present on a ZrS_2 surface at low coverage, it favors a more tightly bound structure, with sodium ions strongly adsorbing at −1.213 eV under compression and −0.848 eV under stretching, compared to an energy of −1.055 eV at normal distances. For potassium ions, the corresponding energies are −1.113 eV (compressed) and −0.748 eV (stretched), with an unstrained value of −0.940 eV.

Although both ions exhibit attraction to adatoms, the repulsion between them intensifies as additional adatoms are incorporated, resulting in energy levels that stabilize at approximately −0.5 eV across various strains. Furthermore, the inclusion of Na and K adatoms introduces additional energy levels within the band gap, enhancing electronic conductivity. When the material is compressed, the band gap reduces to 1.071 eV, whereas stretching increases it to as much as 2.002 eV, also influencing the spin orientation. In terms of the diffusion behavior of adatoms on the ZrS_2 surface, we found that the hollow site serves as the preferred location for adatom diffusion. The energy barriers for hopping to adjacent sites were found to be between 0.256 to 0.270 eV (path-1) and 0.920 to 0.950 eV (path-2) for sodium, while for potassium, they ranged from 0.312 to 0.330 eV (path-1) and 1.020 to 1.045 eV (path-2). Notably, these low energy barriers signify rapid ionic diffusion, which is crucial for the electrochemical processes in energy storage systems. Ultimately, this study reveals the significant impact of strain on the structural and electronic properties of monolayer ZrS_2, positioning it as a promising electrode material for next-generation sodium and potassium-ion batteries.

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