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Two-Dimensional SnS and SnSe as Hosts of K-Ion Storage: A First-Principles Prediction

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Abstract

Potassium ion batteries (KIBs) have attracted remarkable consideration due to their intrinsic safety and huge availability of potassium. However, the large size of the K ion and low charge-discharge efficiency are the main obstacles to the progress of KIBs. To overcome these hurdles, we chose SnS and SnSe

monolayers as K anodes for KIBs due to their layered structural assemblies, wider surface area to accommodate more K content, and high thermal stabilities. First-principles simulations were carried out to study the electronic properties and K storage capability of SnS and SnSe monolayers as anode materials for KIBs. We found that K adsorption enhances the electrical conductivity of both SnS and SnSe monolayers, which become metallic after the adsorption of a very minor concentration of K. The outcomes of the ab initio molecular dynamic simulations display the thermal stability of the host materials for KIBs. According to our calculations, the theoretical capacities of SnS and SnSe monolayers are 355 and 271 mA h/g, respectively. Consequently, we obtain very low average voltages of 0.45 V for SnS and 0.36 V for SnSe monolayers. In addition, the low diffusion barriers for the K-ion on SnS and SnSe monolayers are 0.14 and 0.16 eV, correspondingly, illustrating the fast ion transfer rate with rapid potassiation and depotassiation. These intriguing results suggest that SnS and SnSe monolayers could be promising anode materials for KIBs. © 2023 American Chemical Society.

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