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Supplementary Information

Prediction of SiS_2 and $SiSe_2$ as the Promising Anode Materials for Sodium-ion Batteries

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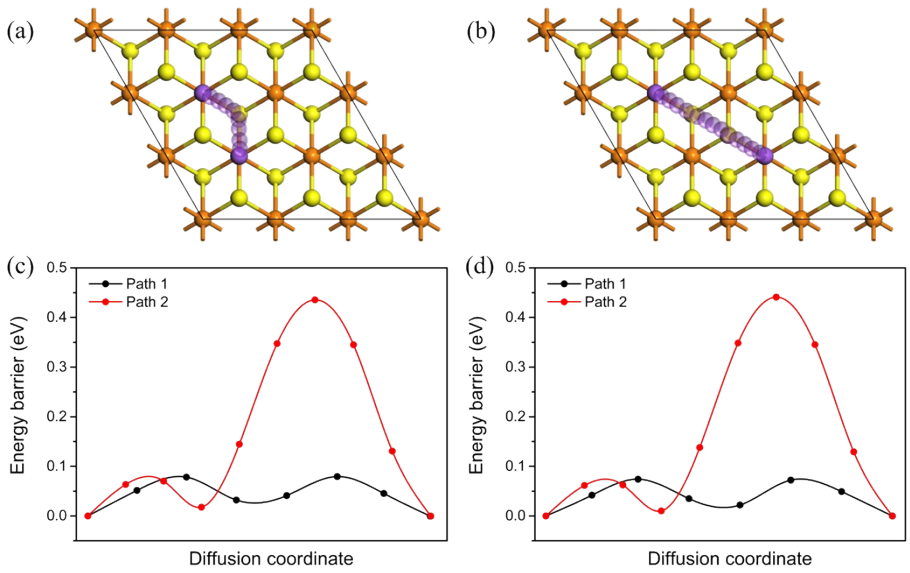

Figure S1. (a)-(b) Two possible Na diffusion paths on SiX_2 surface, and the diffusion barriers for (c) SiS_2 and (d) $SiSe_2$.

The adsorption and diffusion of single Na ion on the Na_1SiSe_2 surface

We investigate the Na diffusion barrier on the first adsorbed Na layer by using the CI-NEB method, and plotted in Figure S2. Four adsorption sites (S1, S2, S3, H1) are considered on the Na_1SiSe_2 surface (Figure S2a-b), and H1 is the most favorable adsorption site. There are two different diffusion paths for Na on the Na_1SiSe_2 surface, namely, path 1 and path 2. As shown in Figure S2c, path 1 is the Na ion migrates from the most stable H1 site to the adjacent H1 site, passing through a metastable S1 site. Path 2 is the Na ion diffuses along the H1→S2→S3→H1 path.

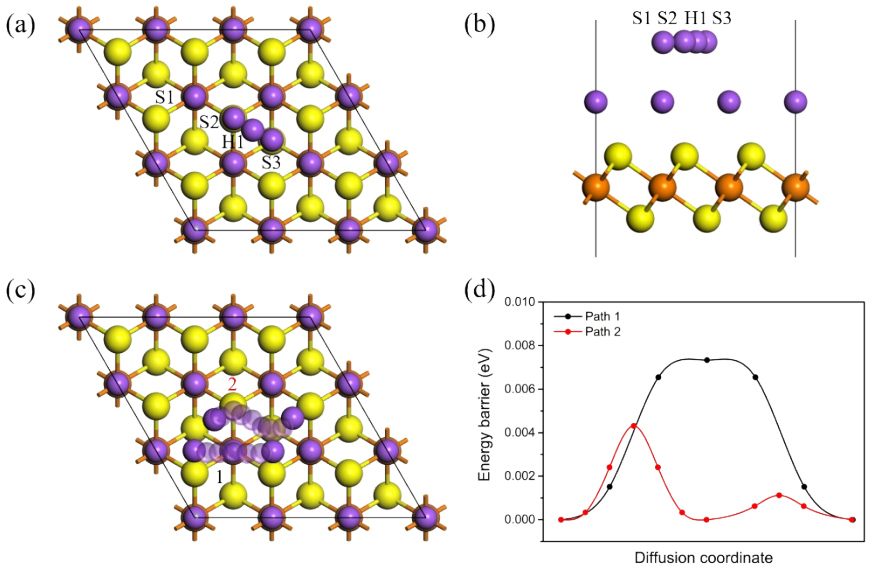

Figure S2. (a) Top view and (b) side view of Na_1SiSe_2 with four possible adsorption sites denoted by S1, S2, S3, and S4; (c) two different diffusion paths of Na ion and (d) the corresponding diffusion barriers.