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Supplementary - A new extraordinary high capacity cathode material for Li/Na-ion batteries: Dihafnium sulfide (Hf_2S)†

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Table 1 Magnetic moments on each atom of Hf_2S monolayer under the different values of strain

Strain ratio	Hf1 (μ_B)	Hf2 (μ_B)	S (μ_B)	Total (μ_B)
-18	0.357	0.357	0.078	0.792
-16	0.239	0.239	0.022	0.5
-14	0.445	0.455	0.029	0.93
-12	0.31	0.309	0.013	0.632
-10	0.423	0.41	0.007	0.839
-8	0.31	0.311	0.004	0.625
-6	0.271	0.271	-0.002	0.54
-4	0.313	0.315	-0.004	0.624
-2	0.348	0.35	-0.005	0.693
0	0.415	0.415	-0.009	0.822
2	0.285	0.287	-0.009	0.563
4	0.274	0.273	-0.008	0.539
6	0.115	0.114	-0.003	0.226
8	0	0	0	0
10	0.179	-0.179	0	0
12	-0.001	0.002	0	0
14	0.373	0.341	0.014	0.728
16	0.027	0.026	0.002	0.055
18	0.028	0.03	0.002	0.06

Electronic band structure of Hf_2S monolayer included spin-orbit interaction was presented in FigS1. It can be seen that spin-orbit calculation has no significant effect on the band structure when compared with the PBE band structure as shown in the main text.

Because F-termination changed the band structure of Hf_2S monolayer, spin-orbit calculation (SOC) was performed in electronic structure of F-terminated system. While PBE band structure has metallic effect, the band gap of 0.18 eV was opened when spin-orbit interaction was included as shown in FigS2.

The band structures of one Li or Na atom adsorbed to 4×4 supercell Hf_2S monolayer was presented in FigS3. It is seen that the system maintains its metallic property after Li/Na adsorption.

Li atoms were increased one by one on 4×4 supercell Hf_2S monolayer up to eight atom and preferable sites of each Li atom were shown in FigS4. The atoms that choose a site other than the hollow according to the increase of the atoms, when they reach the number of eight atoms, are perfectly arranged in the hollow site.

The adsorption energy (E_{ads}) of the Li atoms increased one by one on Hf_2S monolayer was shown in FigS5. This E_{ads} was calculated as below:

$$E_{ads} = E_{Hf_2S} + n \times E_{Li_{bulk}} - E_{Total} \quad (1)$$

Here $E_{Hf_2}S$ is the energy of bare Hf_2S monolayer, $E_{Li_{bulk}}$ is the energy per atom in bulk Li form, and E_{total} is the energy of total system of Li adsorbed to Hf_2S monolayer.

Linear increase of E_{ads} was remarkable.

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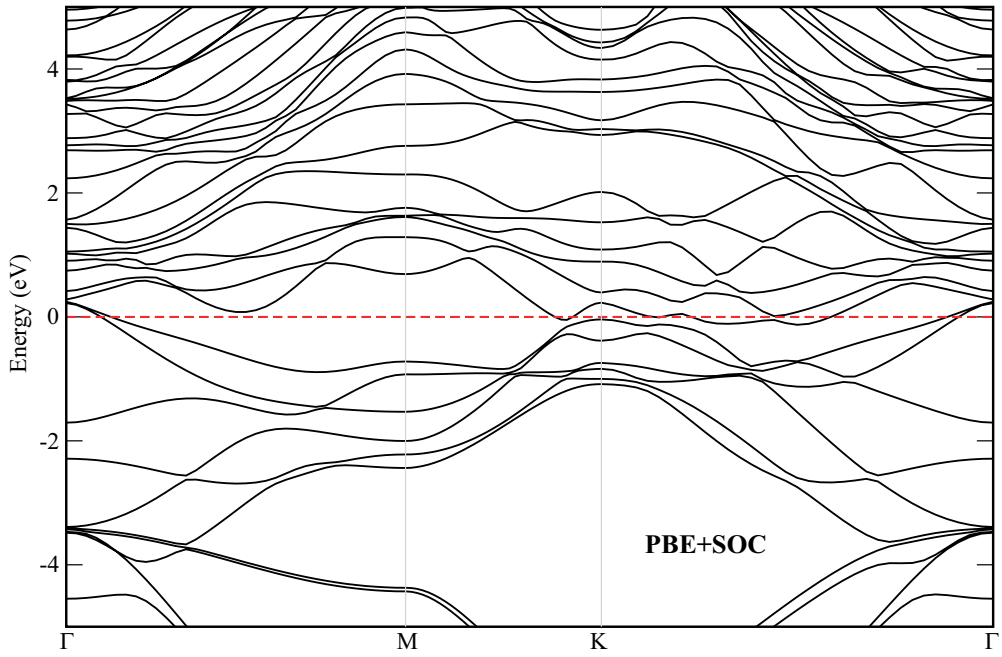

Fig. S1 Electronic band structure of bare Hf_2S monolayer with spin-orbit interaction. Fermi level was shifted to zero and shown by dashed line.

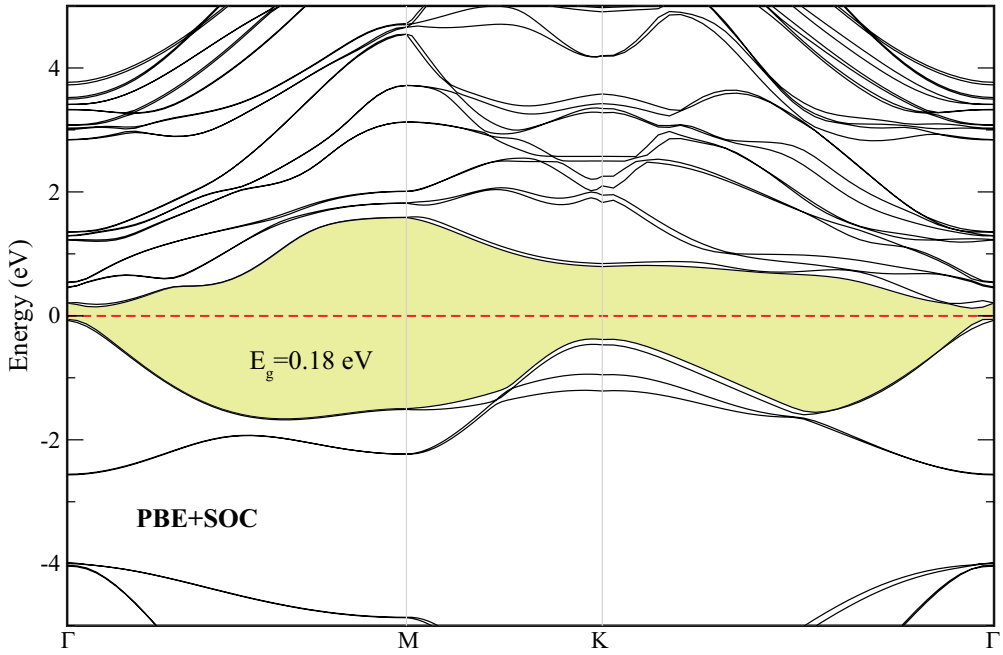

Fig. S2 Electronic band structure of F-terminated Hf_2S monolayer with spin-orbit interaction. Fermi level was shifted to zero and shown by dashed line.

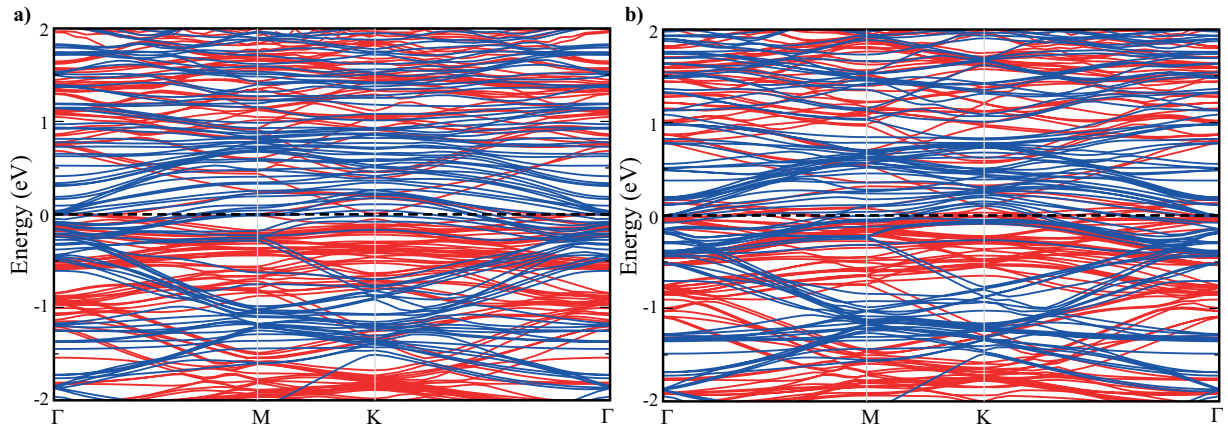

Fig. S3 Electronic band structure of a) one Li and b) one Na atom adsorbed to Hf_2S monolayer with spin-orbit interaction. The red and blue lines indicate spin up and spin downs states.

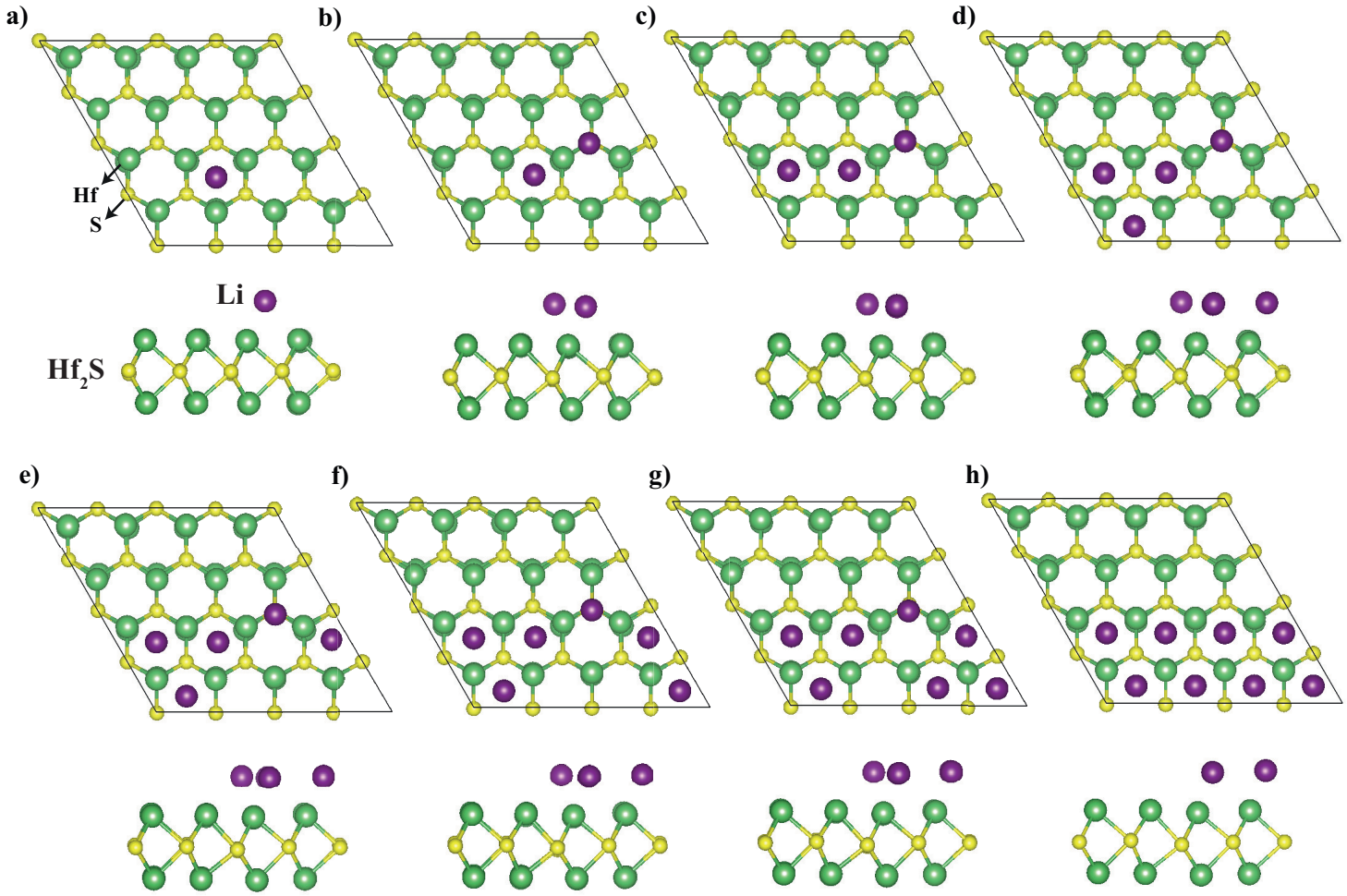

Fig. S4 a-h) Top and view sides of the structures obtained by increasing Li atoms one by one on the Hf_2S monolayer.

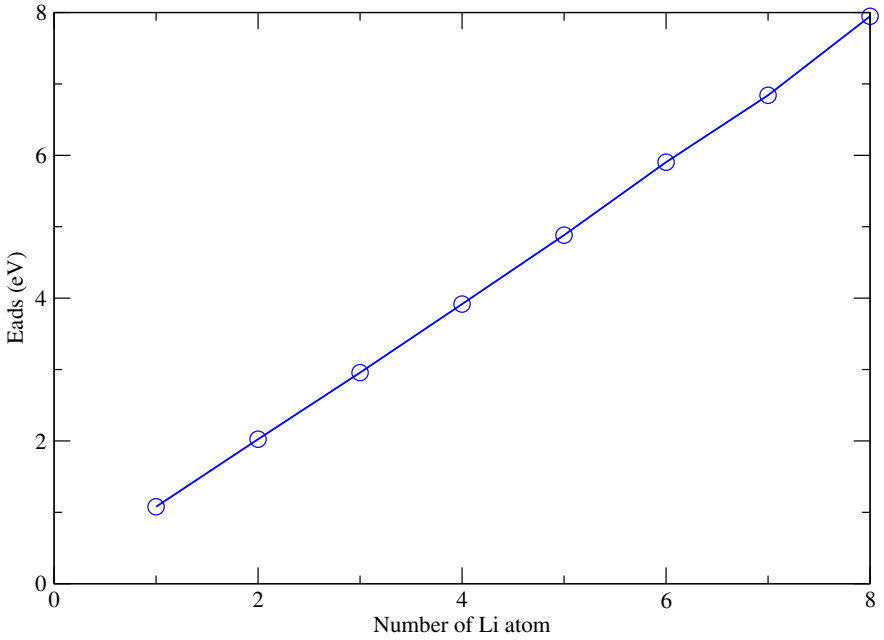

Fig. S5 The adsorption energy of the Li atoms increased one by one on Hf_2S monolayer.