Supporting information

Atomic Insight into the Structural Transformation and Anionic/Cationic Redox Reactions of VS_2 Nanosheets in Sodium-Ion Batteries

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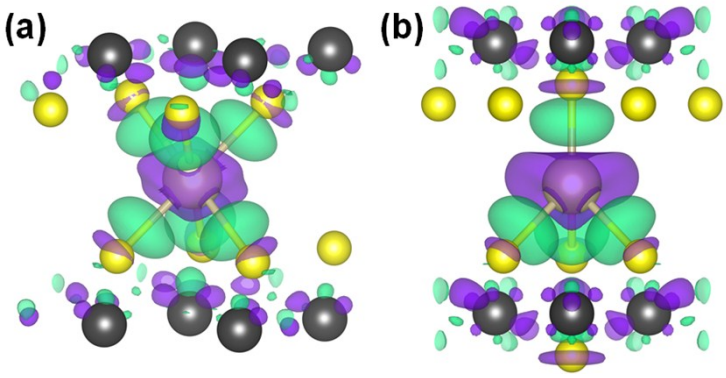

Fig. S1. Charge density difference of VS_2 with an isolated Na in an octahedral site (a) and in a tetrahedral site (b). Green, accumulation of electron density and blue, depletion of electron density.

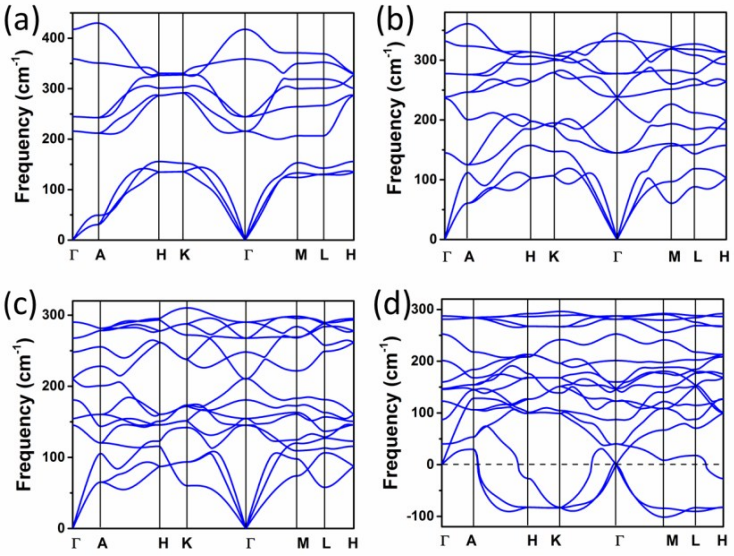

Fig. S2. Phonon band dispersions of VS_2 (a), $Na_{1.0}VS_2$ (b), $Na_{2.0}VS_2$ (c), and $Na_{3.0}VS_2$ (d).

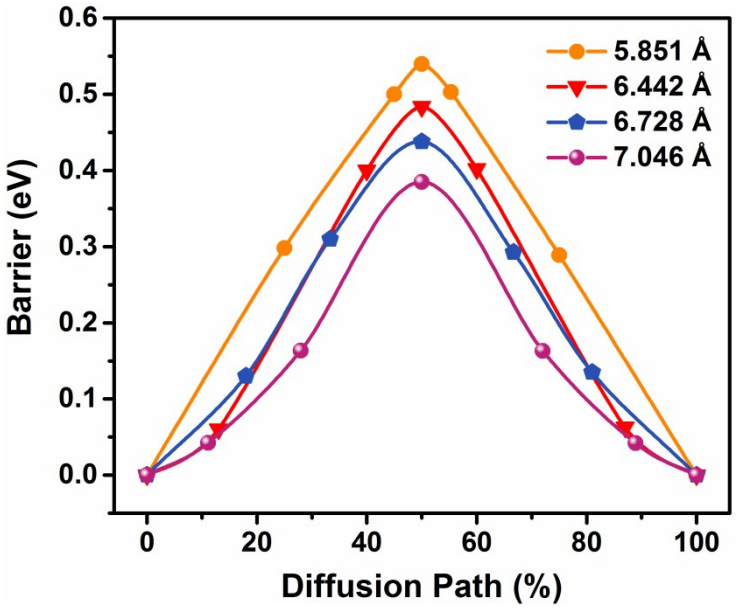

Fig. S3. Calculated diffusion barriers of Na in VS_2 along the O→O' pathway with different interlayer spacing.

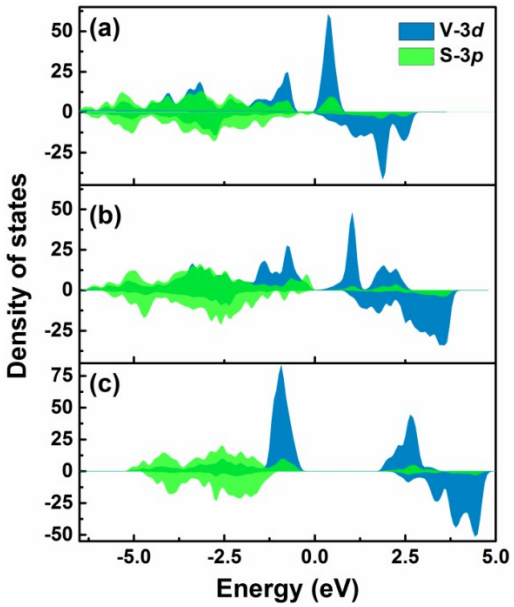

Fig. S4. Partial density of states (PDOS) of V-3*d* and S-3*p* in VS_2 (a), $Na_{1.0}VS_2$ (b) and $Na_{2.0}VS_2$ (c).