Supporting Information

Metallic VS$_2$/graphene heterostructure as an ultra-high rate and high-specific capacity anode material for Li/Na-ion batteries

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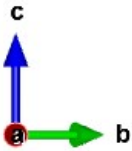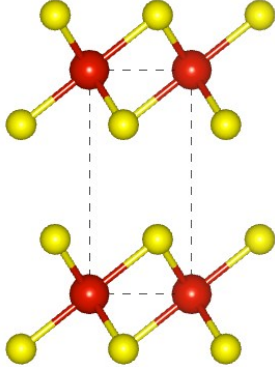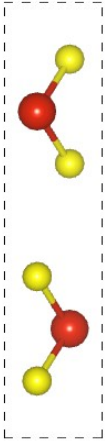**Table S1.** Two different phases with the same VS_2 formula and their total energies (in eV/f.u.)
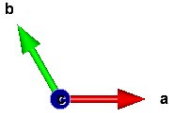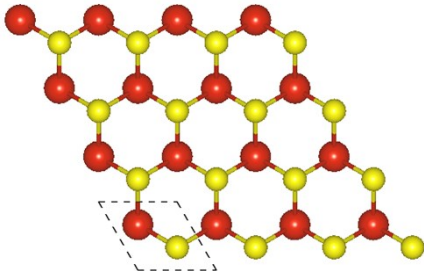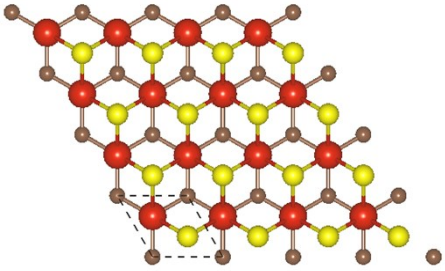

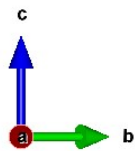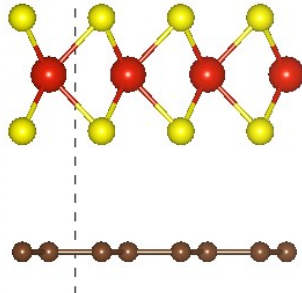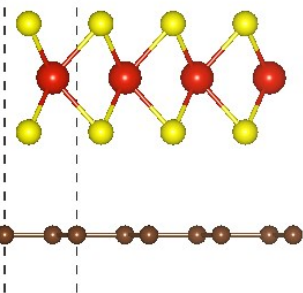| Phase	1T	2H
Total energy(eV/f.u.)	-20.318	-20.337

Table S2. Two different stacking patterns with the same VS_2/Graphene formula and their total energies (in eV/f.u.)

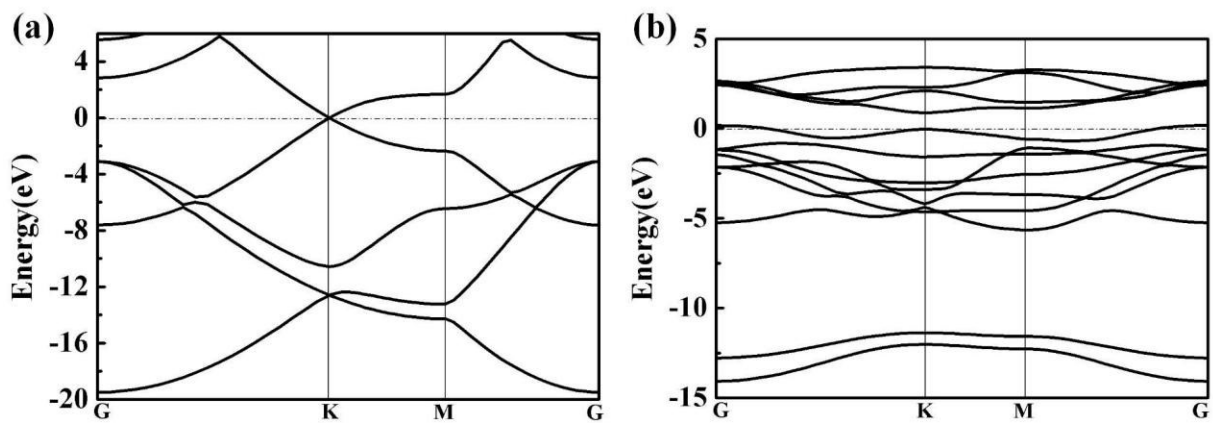| Stacking patterns	AA	AB
Total energy(eV/f.u.)	-36.229	-36.261

Figure S1. Calculated band structure of (a) graphene and (b) VS$_2$. The Fermi level is set to 0 eV, and is indicated with a black dotted line.
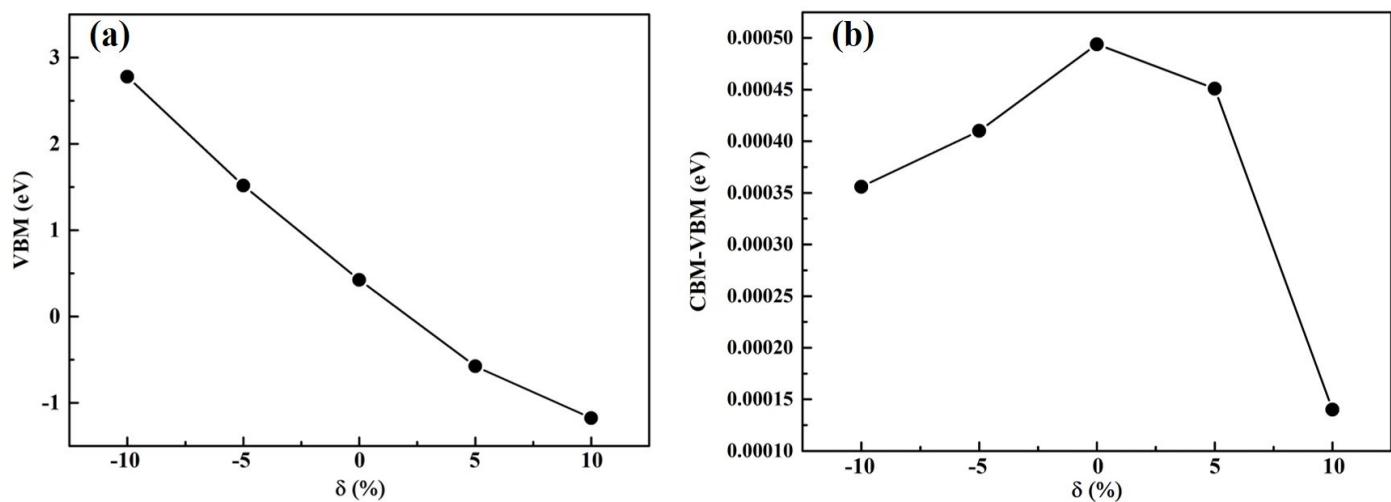

Figure S2. Evolution of the VBM and CBM-VBM value as a function of the tensile or compressive strain (δ), taking the origin at the lowest energy configuration.

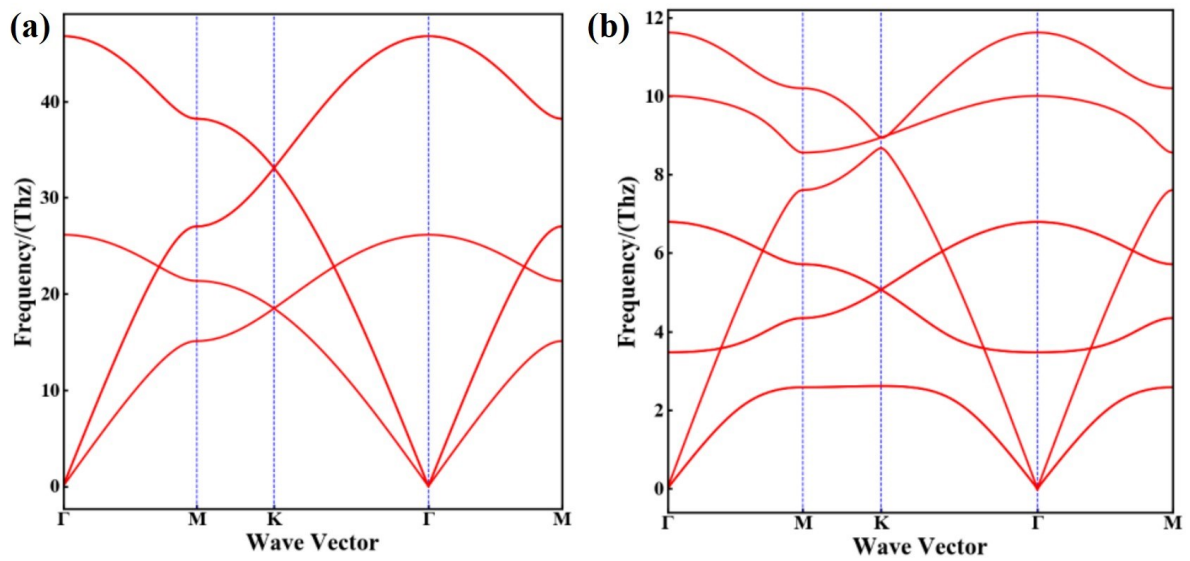**Figure S3**. Calculated phonon dispersion curves for the structures of (a) graphene and (b) VS$_2$ monolayer.
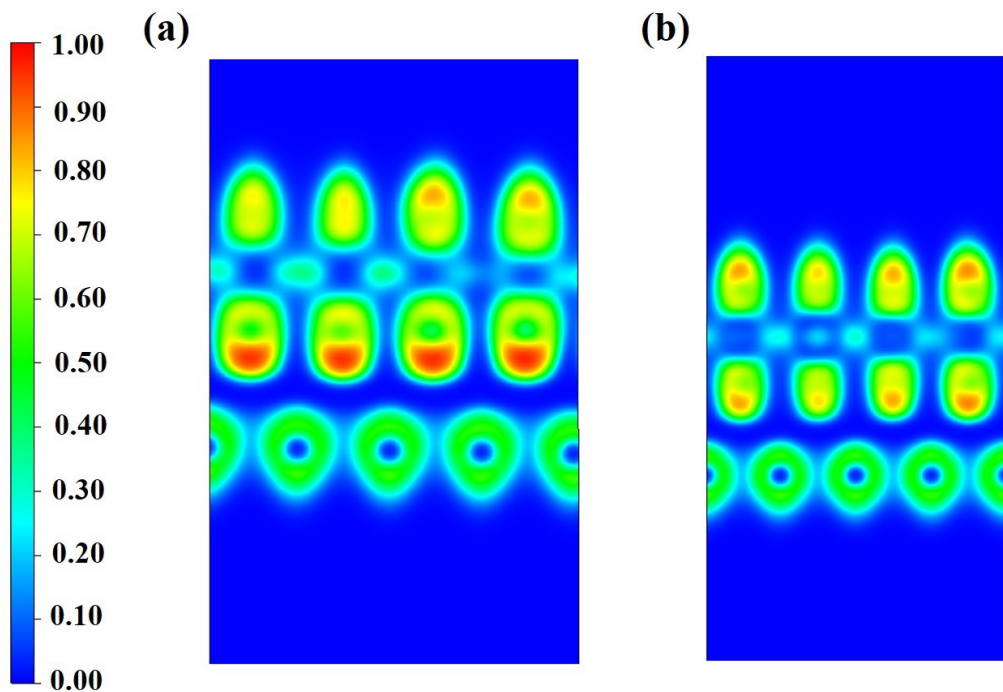

Figure S4. Electron localization functions of the (100) slice of VS$_2$/Graphene system with the stable (a) Li and (b) Na adsorption site.

Table S3. Diffusion distances, energy barriers, and diffusion coefficients at 300 K for Li/Na Migration in the VS_2/Graphene heterostructure.

Path	Diffusion distance	Energy barriers (eV)	Diffusion coefficients (cm^2/s)
Li@I_T-I_T	2.98	0.03	2.78×10^{-3}
Li@T_v-T_v	3.14	0.15	2.98×10^{-5}
Li@H_c-H_c	2.86	0.53	1.02×10^{-11}
Na@I_c-I_c	4.54	0.37	1.25×10^{-8}
Na@T_T-T_T	3.31	0.08	4.96×10^{-4}
Na@H_c-H_c	3.19	0.36	9.12×10^{-9}