Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Promising application of SiC_2/C_3B heterostructure as a new platform for lithium-ion batteries

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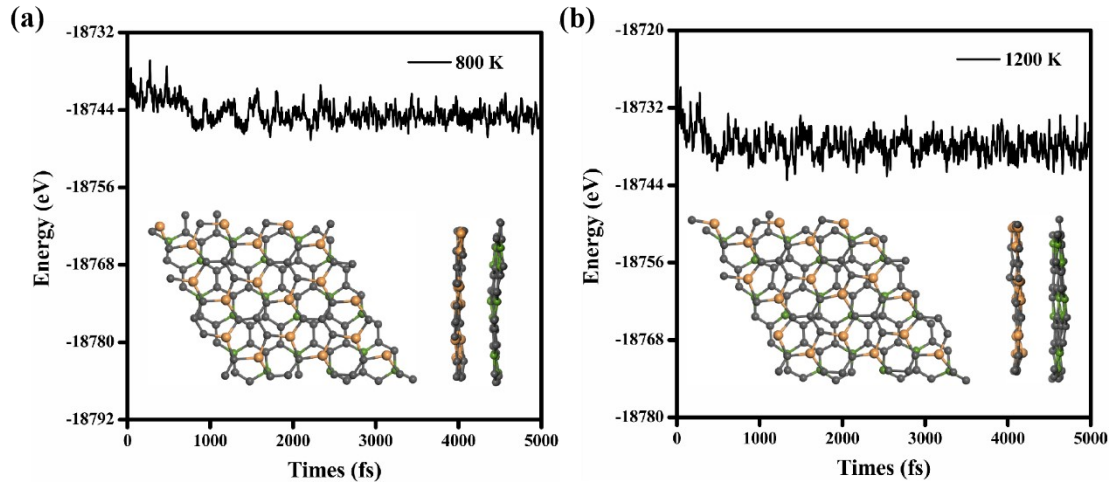

Fig. S1 Total energy fluctuation and structure of the SiC_2/C_3B heterostructure during the AIMD simulations at (a) 800 K and (b) 1200 K after 5 ps.

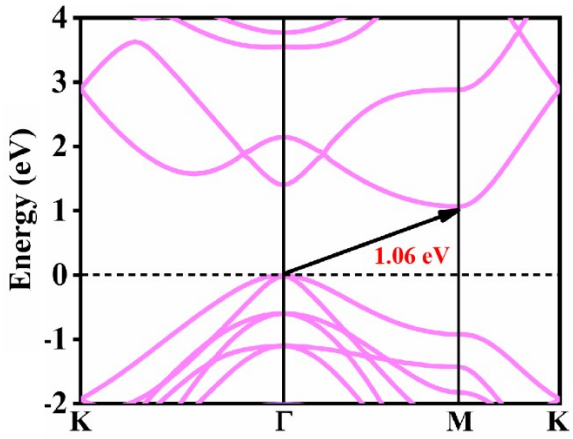

Fig. S2 Quasi-particle band structure of the SiC_2/C_3B heterostructure.

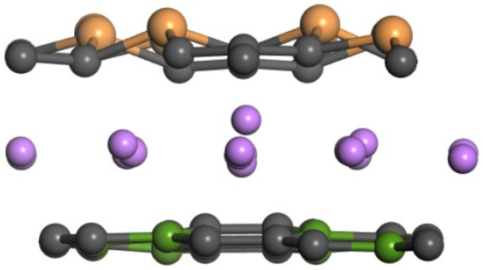

Fig. S3 Side views of lithiated SiC_2/C_3B heterostructure with 17 Li atoms.

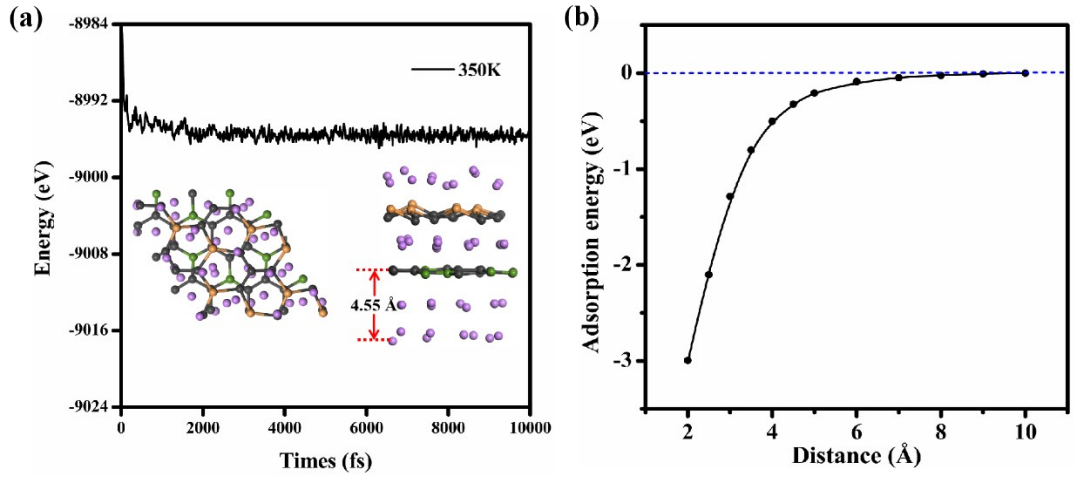

Fig. S4 (a) Total energy fluctuation and structure of $Li_{44}C_{40}B_8Si_8$ during the AIMD simulations at 350 K after 10 ps. (b) The adsorption energy changing along with the distance between Li atom and the outside surface of C_3B layer.

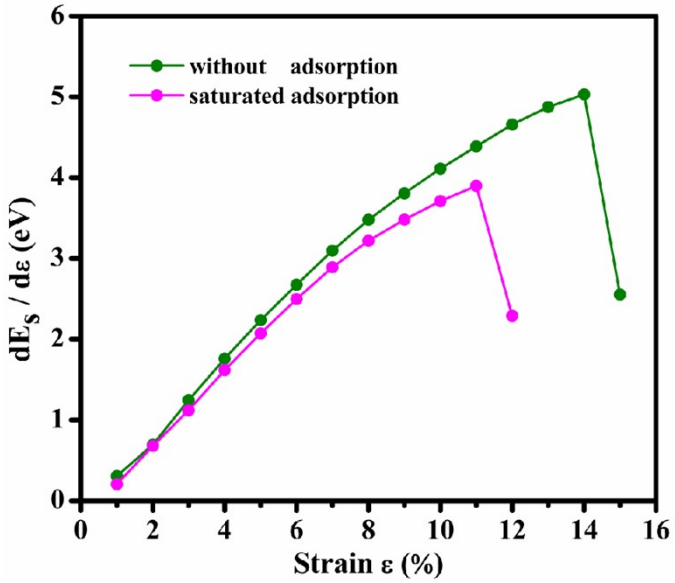

Fig. S5 The variation in the derivative of strain energy (E_s) of the SiC_2/C_3B heterostructure without adsorption (green solid line) and with saturated adsorption (pink solid line).