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


# Supporting Information for

# Black Phosphorous/Blue Phosphorous van der Waals Heterostructure: A Potential Anode Material for Lithium-Ion–Batteries

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**Supporting figures:**

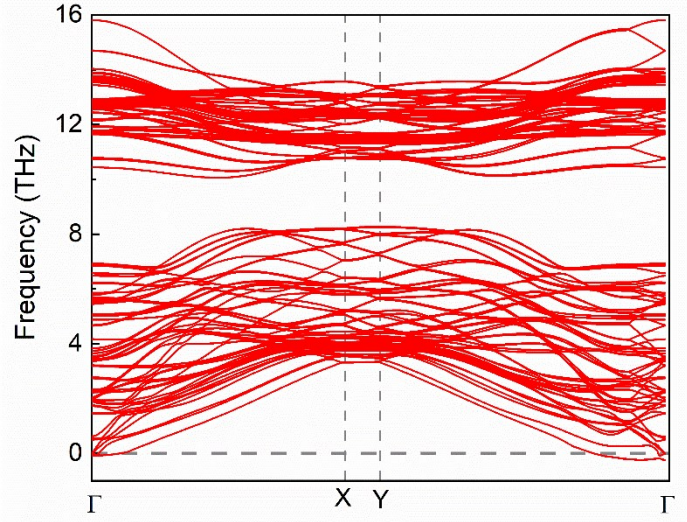


Fig. S1. Phonon spectra of BLK-P/BLE-P vdW heterostructure calculated with the DFT method.

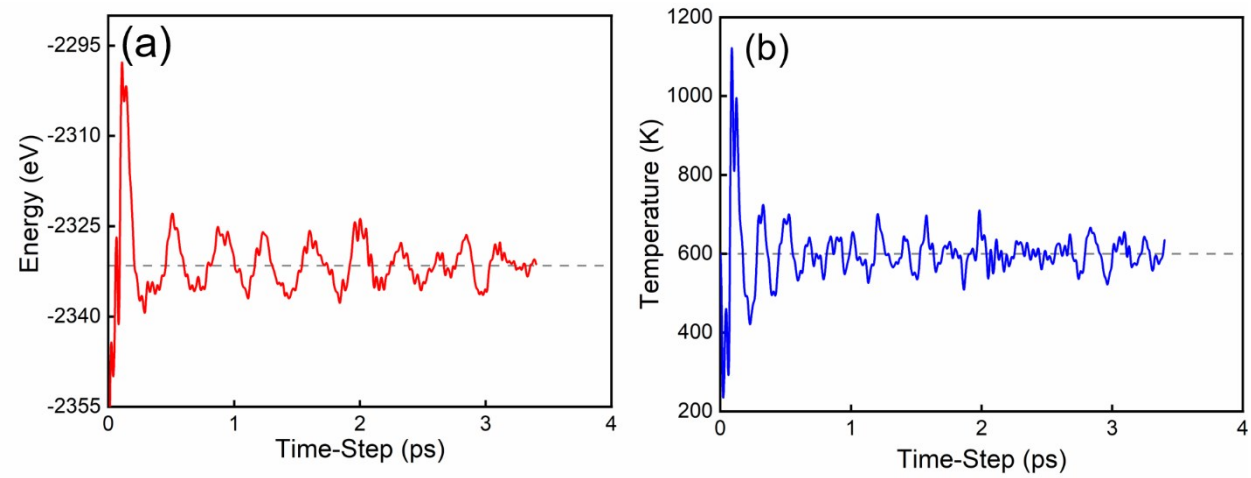


Fig. S2. Evolutions of the (a) total energy and (b) temperature of a BLK-P/BLE-P heterostructure during the AIMD simulations at 600 K and up to 3.5 ps. These results indicate that BLK-P/BLE-P vdW heterostructure is thermodynamically stable.

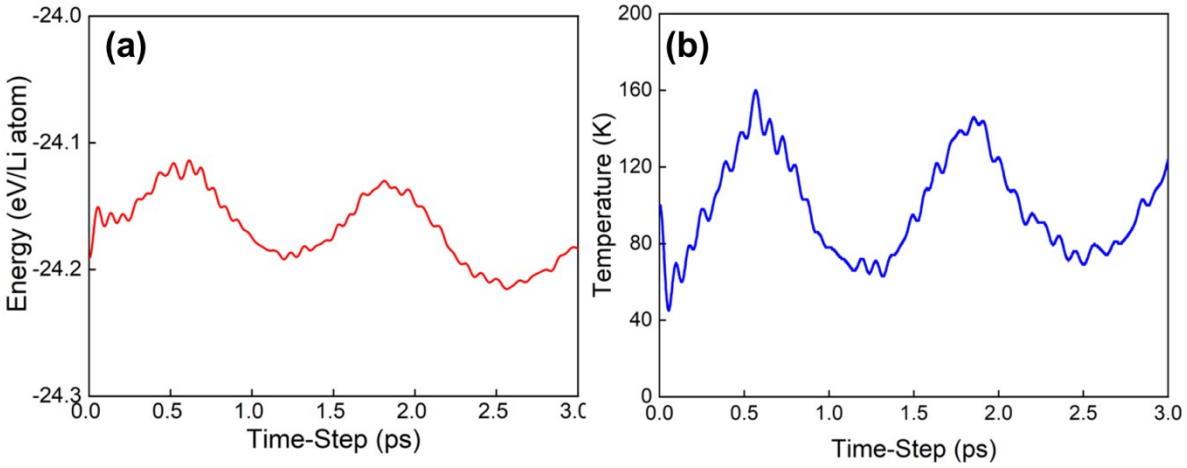


Fig. S3**.** Evolutions of the (a) total energy and (b) temperature of a lithiated BLK-P/BLE-P vdW heterostructure during the AIMD simulations at 100 K and up to 3.0 ps. These results indicate that the lithiated BLK-P/BLE-P vdW heterostructure is thermodynamically stable at least up to 100 K.

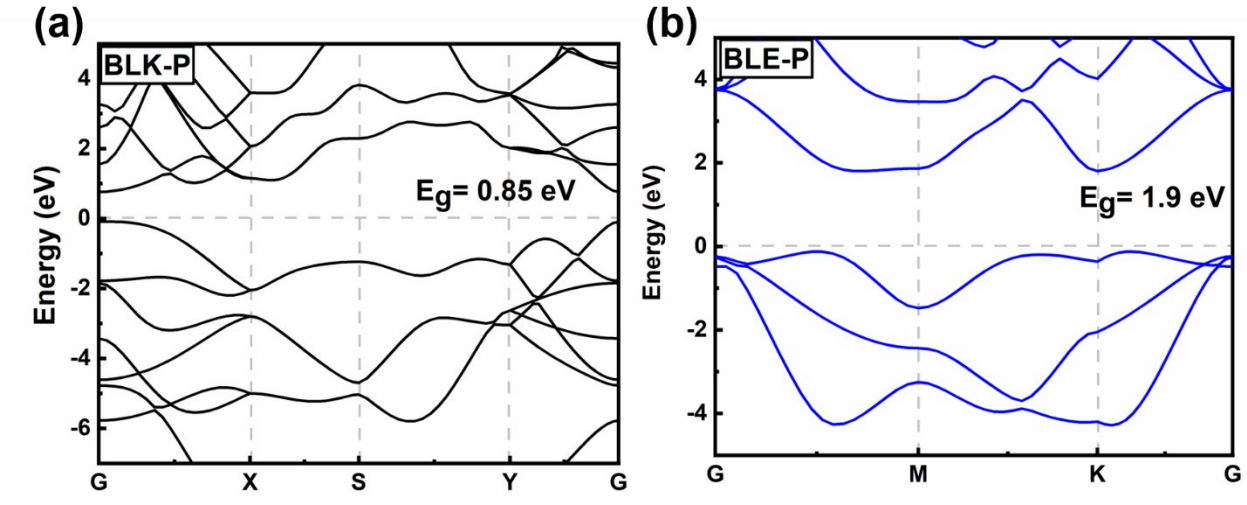


Fig. S4. The electronic band structures of the (a) pristine BLK-P and (b) BLE-P monolayers. The Fermi level is set to zero.

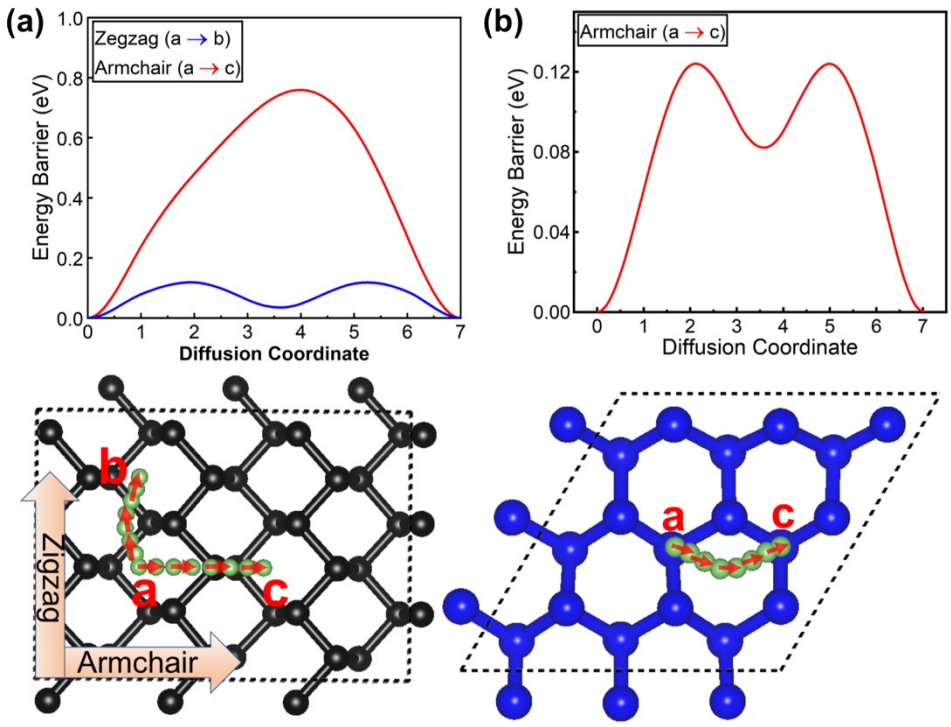


Fig. S5**.** Energy profiles for Li diffusion on (a) BLK-P and (b) BLE-P monolayers. The corresponding schematic representations are given in the lower panels.