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Supporting Information

Blue Phosphorene/Graphene Heterostructure as a Promising Anode for Lithium-Ion Batteries: A First-Principles Study with Vibrational Analysis Techniques

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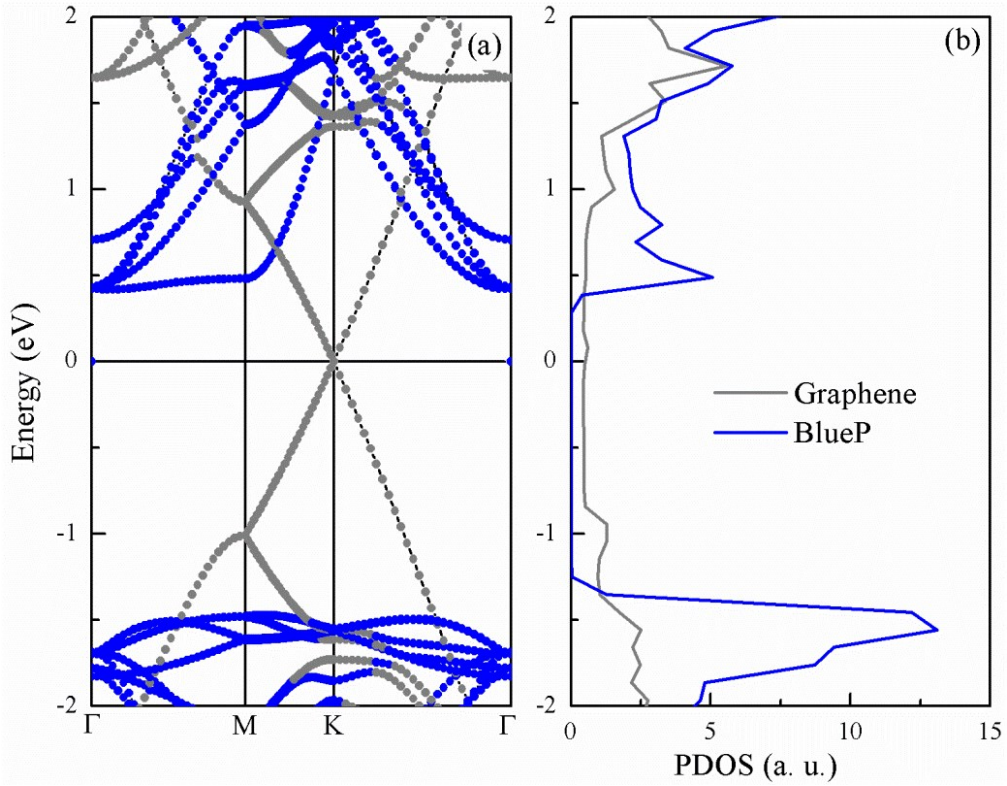

Fig. S1 (a) Band structure and (b) Partial density of states (PDOS) of BlueP/G heterostructure calculated based on D2 method. The Fermi level is set to 0. The blue and grey solid circles represent the projected weight of BlueP and graphene, respectively.

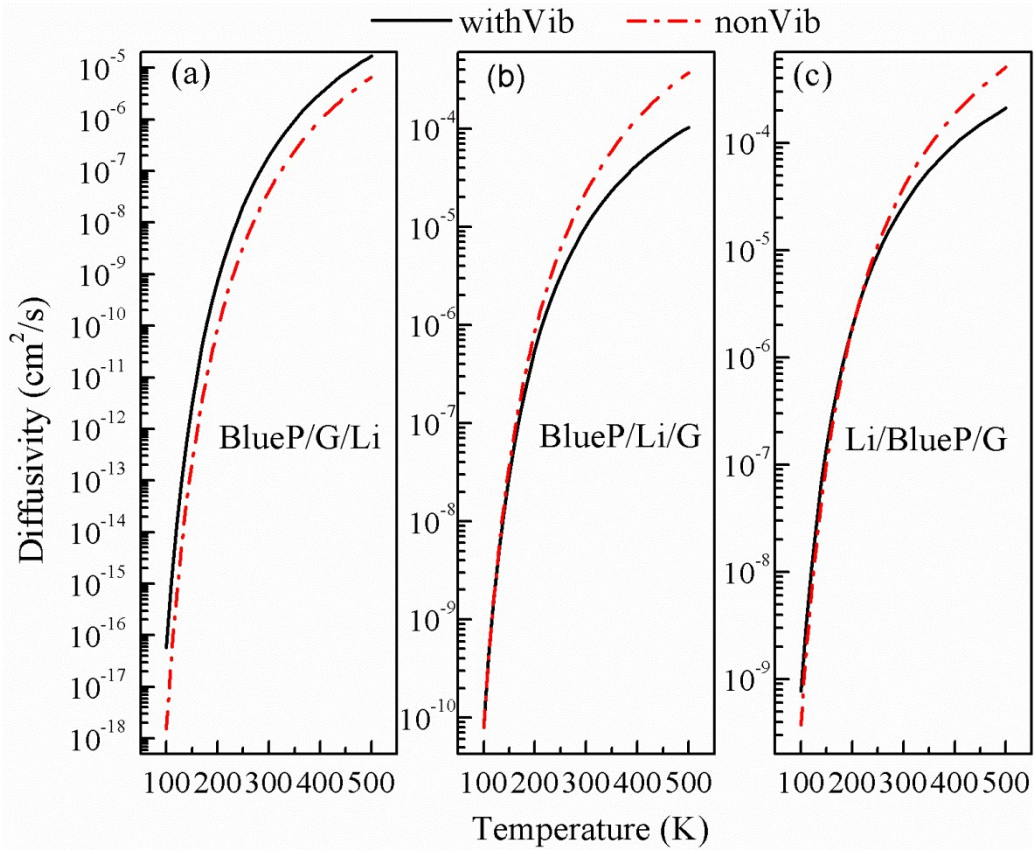

Fig. S2 Diffusivity of Li (a) on outside surface of graphene (BlueP/G/Li), (b) through the interlayer of BlueP/G heterostructure (BlueP/Li/G) and (c) on outside surface of BlueP (Li/BlueP/G). The solid black lines and the dashed red lines denote the diffusivity with and without the vibrational contribution, respectively.

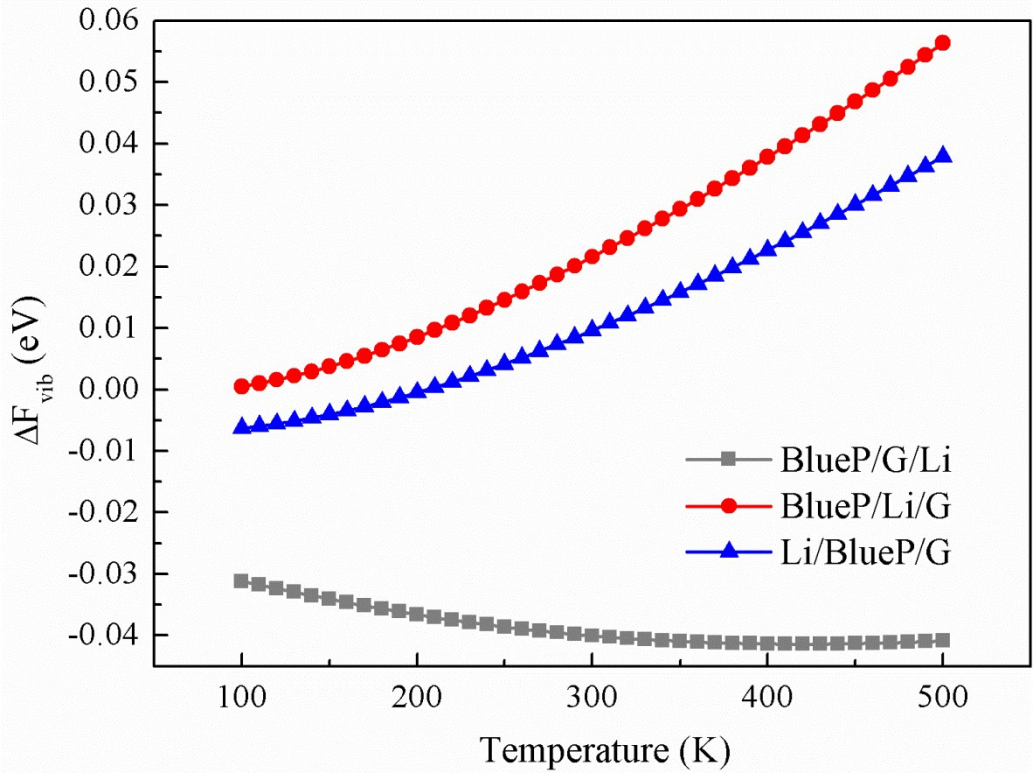

Fig. S3 Evolution of the change in the vibrational Helmholtz free energy ($^{\Delta F_{vib}}$) in the temperature range of 100 to 500 K.

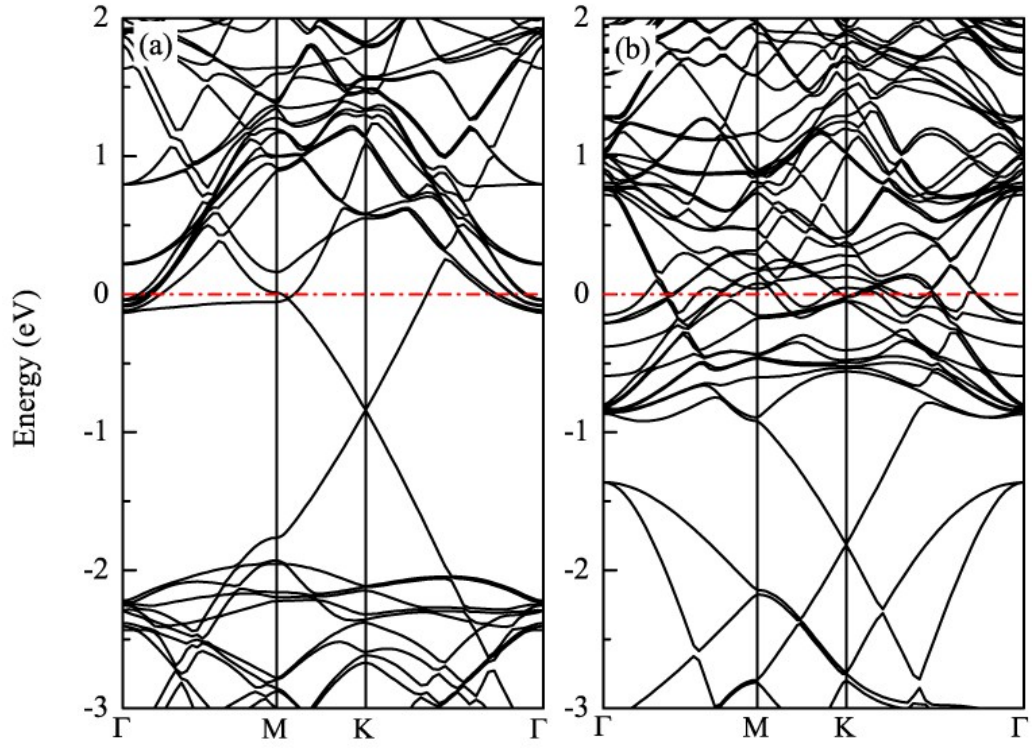

Fig. S4 Band structures of (a) $Li_3P_{18}C_{32}$ and (b) $Li_{22}P_{18}C_{32}$. The fermi level is set to zero.

Table SI Li Adsorption Site, Binding Energy E_b, Charge Transfer of Li, P, C Atoms, ΔQ_{Li}, ΔQ_P , ΔQ_C, respectively, Equilibrium Interlayer Distance *d*, calculated based on D2 level.

System	Li site	E_b (eV)	ΔQ_{Li} (e)	ΔQ_P(e)	ΔQ_C(e)	*d* (Å)
BlueP/Li	V_P	-2.07	-0.89	0.89	-	-
G/Li	H_C	-1.56	-0.91	-	0.91	-
Li/BlueP/G	V_P	-2.11	-0.89	0.78	0.11	3.48
BlueP/G/Li	H_C	-1.71	-0.91	0.15	0.76	3.46
BlueP/Li/G	V_I	-2.79	-0.87	0.52	0.35	3.60

Table SII Li Adsorption Site, Binding Energy E_b, Charge Transfer of Li, P, C Atoms, ΔQ_{Li}, ΔQ_P , ΔQ_C, respectively, Equilibrium Interlayer Distance *d*, calculated based on D3-BJ level.

System	Li site	E_b (eV)	ΔQ_{Li} (e)	ΔQ_P(e)	ΔQ_C(e)	*d* (Å)
BlueP/Li	V_P	-2.00	-0.88	0.88	-	
G/Li	H_C	-1.23	-0.90	-	0.90	
Li/BlueP/G	V_P	-2.07	-0.88	0.77	0.11	3.52
BlueP/G/Li	H_C	-1.33	-0.90	0.16	0.74	3.50
BlueP/Li/G	V_I	-2.32	-0.87	0.53	0.34	3.62

Table III Diffusion Barrier of Li on different substrates calculated based on D2, D3 and D3-BJ methods.

System	Barrier (eV)		
	D2	D3	D3-BJ
BlueP/Li	0.148	0.129	0.119
G/Li	0.380	0.303	0.293
Li/BlueP/G	0.150	0.135	0.124
BlueP/Li/G	0.340	0.147	0.156
BlueP/G/Li	0.387	0.296	0.283