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

Supplementary Information

Metallic two-dimensional BP_2: A high-performance electrode material for Li- and Na-ion batteries

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I. Phonon density of states

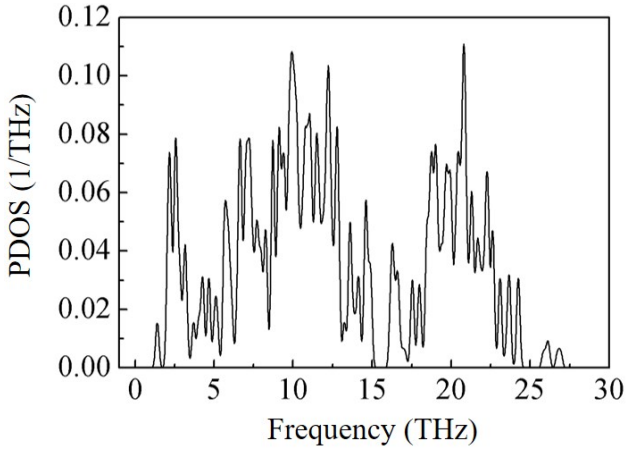


Fig. S1 Phonon density of states of the BP_2 monolayer.

II. Change of the total energy profile under uniaxial strains

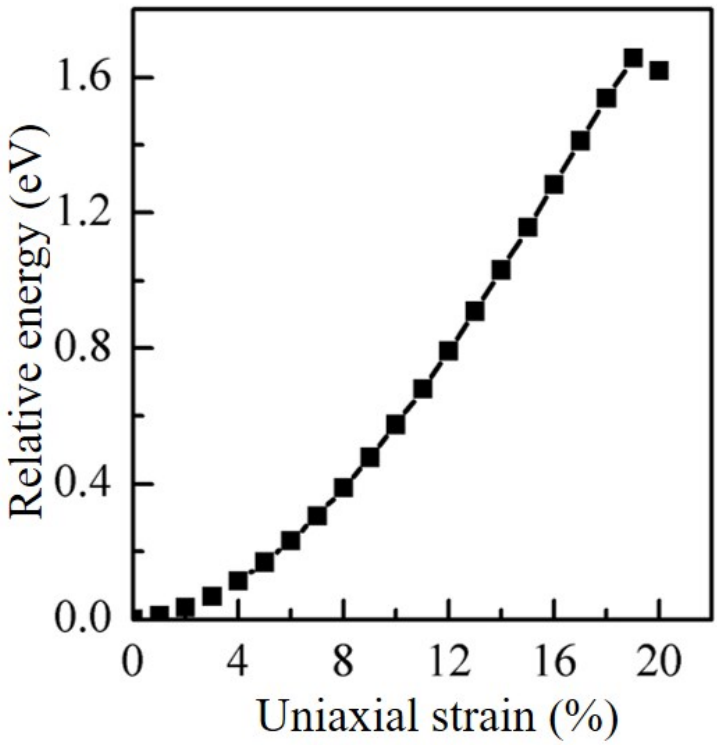


Fig. S2 Change of the total energy profile with respect to tensile strain along the *x* direction. The trend with the tensile strain along *y* direction is the same as that along *x* direction.

III. Phonon dispersion under uniaxial strains

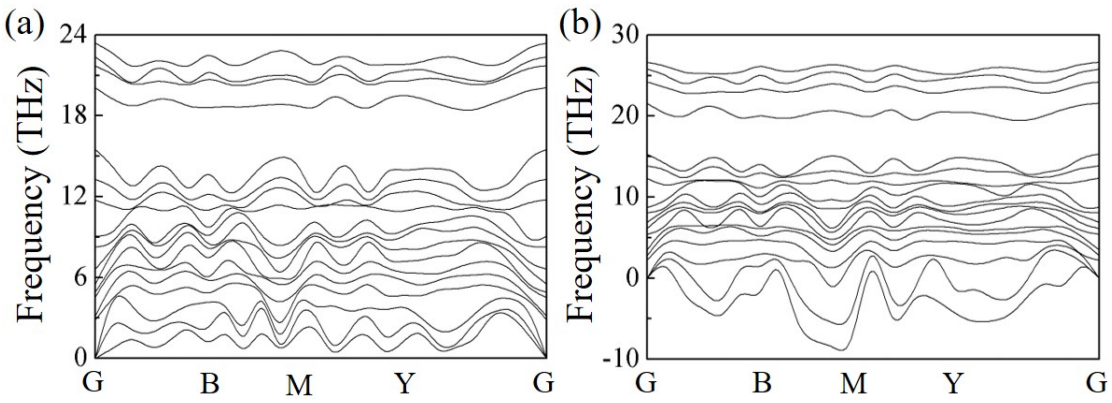
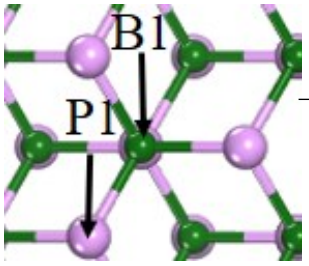


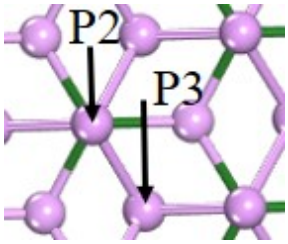
Fig. S3 Phonon dispersion of the BP_2 monolayer under the tensile strain of (a) 19% and (b) 20%.

IV. The Hirshfeld charge for B/P atoms

Table S1. The electrons transferred from Li/Na to the neighboring B or P atoms.



	T_B (Li/Na)	T_{P1} (Li/Na)
B1 (*e*)	-0.13 / -0.13	-0.12 / -0.12
P1 (*e*)	-0.02 / -0.03	-0.02 / -0.03



	H_2 (Li/Na)	T_{P2} (Li/Na)
P2 (*e*)	-0.05 / -0.05	-0.05 / -0.05
P3 (*e*)	0.08 / 0.07	0.08 / 0.07

V. The electrons for BP_2 back-donates to Li/Na

Table S2. The electrons for BP_2 back-donates to the empty Li-2*p* (Na-3*p*) orbitals.

	T_B	T_{P1}	H_2	T_{P2}
Li-2*p* (*e*)	-0.23	-0.19	-0.18	-0.16
Na-3*p* (*e*)	-0.07	-0.06	-0.02	-0.02

VI. The computing time for calculating the diffusion barrier

Table S3. The computing time (in minutes) for calculating the diffusion barrier of a Li (Na) atom on the monolayer BP_2 using LST/QST and NEB methods.

	LST/QST	NEB
Li-BP_2	3935	5005
Na-BP_2	4392	5732