In this work, we adopt a first-principles study to evaluate the potential of boron phosphide (BP) monolayer as an anode material for alkali metal-based (e.g., Li, Na and K) batteries. It is found that the BP monolayer shows negative adsorption energies of −0.202, −0.160 and −0.681 eV, respectively, for Li, Na and K. During loading, when any of the three alkali metal atoms reaches a critical position (~6 Å), the adsorption energy increases dramatically with no energy barrier. It is also shown that after adsorbing Li, Na or K, the semiconducting BP monolayer is transformed to a metallic state, becoming an electrical conductor. More importantly, the alkali metal atoms show high diffusivities on the BP monolayer, with low energy barriers of 0.364, 0.217 and 0.155 eV for Li, Na and K, respectively. Finally, the BP monolayer has high theoretical specific capacities of 1283 and 570 mA h g⁻¹ for Li and K storages, which are among the highest values of the anode materials reported in the literature, and multiple times higher than that of graphite anode materials in use. The above-mentioned results suggest that the BP monolayer is a promising anode material not only for Li-ion and K-ion batteries, but also for other lithium-based and potassium-based batteries.

**1. Introduction**

With a wide range of applications from portable electronic devices to electric vehicles, and to large-scale power grid, secondary batteries are considered to be promising energy storage technologies that power the world. Particularly, rechargeable lithium-ion (Li-ion) batteries have attracted much attention since their first commercialization by Sony in 1991, ascribed to the combination of satisfied reversible capacity, power density and cycle life.1–9 Presently, the specific energy of commercialized Li-ion batteries is limited to approximately 250 Wh kg⁻¹, which is only half of the goal for a family car to travel 300 miles without recharging,9 in part due to the low theoretical specific capacity (372 mA h g⁻¹) of the anode material graphite. Other investigated anode materials for next-generation Li-ion batteries such as metal oxides, oxysalts and silicon also suffer from critical issues including poor reversibility, low lithium diffusivity and large volume change.10–13 Therefore, there is a substantial need to develop new anode materials with high specific capacity and high rate capability. In addition to Li-ion batteries, recently, sodium-ion (Na-ion) and potassium-ion (K-ion) batteries have attracted increasing research interest as large-scale electronic storage systems, motivated by the much more natural abundance of Na (23 000 ppm) and K (17 000 ppm) than Li (20 ppm) in the earth’s crust.14 In spite of the similarities between alkali metals, Na and K systems present different kinetic and thermodynamic properties due to the larger ionic radii of Na and K than Li, limiting the applications of conventional Li storage materials for Na and K storages. In this regard, developing potential anode materials for Na-ion and K-ion batteries is also in urgent demand.

In this regard, two-dimensional (2D) materials have attracted increasing attention and are believed to be promising candidates for the anode in metal-ion batteries due to their advantages of large surface-to-volume ratio and unique electronic properties. Until now, numerous 2D materials have been identified as potential anode materials with enhanced specific capacity and ion diffusivity for Li-ion, Na-ion and K-ion batteries.15–17 For example, phosphorene was found to have a theoretical specific capacity of 863 mA h g⁻¹ for both Li and Na. In addition, the Li and Na diffusions on it were very fast with the energy barriers of 0.12 and 0.04 eV.18,19 Ti₃C₂ MXene was also predicted to be the potential anode material for Li-ion, Na-ion and K-ion batteries with the specific capacities of 447.8, 351.8 and 191.8 mA h g⁻¹ as well as ion diffusion barriers of 0.068, 0.096 and 0.103 eV, respectively.20 Borophene was recently discovered to be an outstanding anode material for Li-ion batteries with a specific capacity of 1860 mA h g⁻¹ and a lithium diffusion barrier as low as 2.6 meV. And its further applications in Na-ion and K-ion batteries were also speculated.21

Although substantial progress has been reported, the efforts of designing new 2D materials with enhanced battery...
performance are never diminished. In the past decade, the successful synthesis of monolayer hexagonal III–V binary compounds\textsuperscript{22–26} has aroused enormous interest in this system.\textsuperscript{27–32} In particular, hexagonal boron nitride (h-BN) is the most investigated one due to its potential applications as the dielectric material for flexible nanoelectronics,\textsuperscript{23} oxidation-resistant coating\textsuperscript{44} and ultraviolet optical material.\textsuperscript{25} However, its further utilization to be the electrode materials for metal-ion batteries is hindered by the large band gap\textsuperscript{36} and weak adsorption to metal ions.\textsuperscript{37} For example, h-BN has a band gap of 4.06 eV and would not transform from semiconducting to metallic states after adsorbing Li atoms.\textsuperscript{35,38} In addition, its adsorption energy to Li atoms is even lower than the Li cohesive energy.\textsuperscript{37} Another III–V binary compound monolayer, BP, though has not been successfully synthesized, also attracts much attention recently owing to its structural similarity to graphene and BN.\textsuperscript{39–42} The calculated phonon spectrum shows that no imaginary frequencies exist in the BP monolayer and its in-plane Young modulus and Poisson’s ratio are comparable with those of the MoS\textsubscript{2} monolayer, ensuring a satisfied mechanical stability.\textsuperscript{43} In addition, the predicted band gap of the BP monolayer is much smaller than that of h-BN\textsuperscript{46} with the value of 0.91 eV,\textsuperscript{44} indicating a greatly enhanced electrical conductivity when substituting N atoms in h-BN by P atoms. This small band gap is comparable to that of some potential anode materials for alkali metal-ion batteries, such as phosphorene (1.0 eV),\textsuperscript{44} GeS (1.61 eV)\textsuperscript{44} and SiS (1.40 eV).\textsuperscript{45} In fact, for alkali metal-based batteries, the requirements for anode materials are similar. To be specific, an anode material with high specific capacity and high rate capacity is needed to ensure a high battery performance. Inspired by its structural similarity to graphene and good electrical conductivity, one may naturally wonder whether it is possible to use the BP monolayer as a potential anode material for alkali metal-based batteries. However, until now, hardly any experimental or theoretical efforts of research on the energy storage application of BP monolayer have been reported.

To respond to this clearly identified need, in this work, density functional theory (DFT) based first-principles calculations were adopted to evaluate the potential of a free-standing BP monolayer as the anode material in alkali metal-based batteries. We first optimized the structures of the BP monolayer and compared the results with previous studies. Then, the adsorption energies of Li, Na and K on representative high-symmetry sites were calculated. Third, the electronic properties of Li (Na, K)–BP nanostructures were investigated by analyzing the electron density of states (DOS). Fourth, the Li, Na and K diffusion barriers in representative directions of the BP monolayer were calculated and compared. Finally, the effects of Li, Na and K concentrations were clarified and the theoretical specific capacities of the BP monolayer as the anode material in alkali metal-based batteries were obtained.

2. Computational methods

DFT based first-principles calculations were performed by using ABINIT\textsuperscript{46,47} code. The exchange–correlation functional was coped with by the generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) type\textsuperscript{48} and the electron–ion interactions were considered by projector-augmented-wave (PAW) potentials.\textsuperscript{49} To ensure a satisfied convergence for wave-basis expansion, the energy cutoff was set to 24 Ha. A vacuum layer of 20 Å was added in the slab model to avoid image–image interactions. A $3 \times 3 \times 1$ supercell with a BP monolayer was adopted in all calculations and the Brillouin zone was sampled using $5 \times 5 \times 1$ Monkhorst–Pack grids.\textsuperscript{50} The force convergence criteria for self-consistent-field (SCF) cycles and structural relaxation were set to $4.0 \times 10^{-5}$ and $6 \times 10^{-4}$ Ha per bohr, respectively.

The adsorption energy of alkali metal atoms on the BP monolayer was calculated by:

$$E_{\text{ads}} = (E_{\text{AM+BP}} - n\mu_{\text{AM}} - E_{\text{BP}})/n$$

where $E_{\text{AM+BP}}$ and $E_{\text{BP}}$ are the DFT energies of the BP monolayer with and without alkali metal atoms; $\mu_{\text{AM}}$ is the chemical potential of Li, Na and K, which are obtained from their body centered cubic bulk structures; $n$ indicates the number of alkali metal atoms.

The temperature-dependent molecular transition rate ($D$) was investigated by using the Arrhenius equation:

$$D \sim \exp \left(\frac{-E_{\text{k}}}{k_B T}\right)$$

where $E_{\text{k}}$, $k_B$ and $T$ are the diffusion barrier, Boltzmann’s constant and temperature, respectively.

When the volume and entropy effects during the alkali metal loading process are neglected, the average open circuit voltage can be obtained by calculating the average voltage in the concentration range of $x_1 < x < x_2$,\textsuperscript{51–53}

$$V \approx \frac{E_{\text{AM+BP}} - E_{\text{AMx_BP}} + (x_2 - x_1)E_{\text{AM}}}{(x_2 - x_1)e}$$

where $E_{\text{AM+BP}}$, $E_{\text{AMx_BP}}$ and $E_{\text{AM}}$ are the total energies of AM$_x$BP, AM$_2$BP and alkali metal atoms, respectively.

To calculate the alkali metal diffusion barriers, the simplified string method\textsuperscript{54,55} was used.

3. Results and discussion

The optimized structures (top and side views) of the free-standing BP monolayer are shown in Fig. 1. It is seen that the BP monolayer has a graphene-like planar structure with all atoms located in the same layer. The optimized lattice constants are $a = b = 3.18$ Å and $\alpha = 120^\circ$, consistent with previous theoretical results.\textsuperscript{29} In addition, the B and P atoms alternately appear, with each B/P atom bonded to three P/B atoms, and finally form a honeycomb structure. The calculated B–P bond length is 1.83 Å, which is larger than the B–N bond length of 1.45 Å in h-BN,\textsuperscript{46} attributed to the larger atomic radius of P than N.

To be a promising anode material for alkali metal-based batteries, a relatively strong adsorption energy with alkali metal atoms is a necessary prerequisite. In this regard, we firstly
calculate the adsorption energies of the BP monolayer towards single Li, Na and K atoms. Considering the high symmetry of the BP monolayer, three representative adsorption sites are chosen, as shown in Fig. 1c. Here, we define the symbols H, TB and TP as (a) H site: above the hollow site of the B–P hexagon, (b) TB site: above the top site of boron atoms, and (c) TP site: above the top site of phosphorus atoms. The calculated adsorption energies are summarized in Fig. 2a, with the red, blue and brown lines representing the adsorption of single Li, Na and K atoms, respectively. It is found that the adsorption energy decreases in the sequence of H site > TB site > TP site for Li and Na atoms, and decreases in the sequence of H site > TP site > TB site for K atom. In particular, the H site has the highest adsorption energies for all Li, Na and K atoms. The Li adsorption energy on the H site is $-0.202$ eV, thereby attracting Li atoms here. On the contrary, the adsorption energies on TB and TP sites have positive values of $0.096$ and $0.183$ eV, indicating that both of them would not be the Li adsorption sites for Li-based batteries. Interestingly, a similar adsorption tendency for Na is obtained to that of Li. Results show that the Na adsorption energies on H, TB and TP sites are $-0.160$, $0.001$ and $0.051$ eV, respectively, which means only the H site benefits the Na storage for Na-based batteries, owing to its negative adsorption energy. More importantly, it is seen that K atom shows larger adsorption energies than Li and Na atoms and have all negative values on high-symmetric adsorption sites. The K adsorption energies on H, TB and TP sites are $-0.681$, $-0.565$ and $-0.556$ eV, respectively, indicating that all these three sites are applicable for K storage in K-based batteries. On the most stable H site, the distances of Li, Na and K atoms to the BP surface are 1.73, 2.24 and 2.69 Å, consistently with the atomic radii increasing tendency of Li < Na < K. Then, we move the alkali metal atoms vertically away from the BP surface by a distance of 16 Å to 17.73, 18.24 and 18.69 Å for Li, Na and K atoms. The changes in potential energy with respect to the distance between alkali metal atoms and the BP monolayer ($d_{M-BP}$) are presented in Fig. 2b, and the embedded figures show the adsorbed structures on the most stable site. Here, the chemical potentials of Li, Na and K atoms are obtained from isolated atoms instead of bulk phases. Clearly, it is seen that the energy is maintained constant when the distance is larger than 8 Å, indicating that the total energies of the systems do not change for the distance beyond 8 Å. In this case, the alkali metal atoms have no interaction with the BP monolayer and can be regarded as isolated atoms. On the contrary, when the distance is within 6 Å, the energy increases dramatically, showing that strong interactions exist between alkali metal atoms and the BP monolayer. Therefore, it is expected that when alkali metal atoms reach a critical position on the BP monolayer (~6 Å), the atoms will be rapidly adsorbed and there is no energy barrier during loading.

To have a more intuitively clear view on the charge transfer of alkali metal atoms adsorbed on the most stable site, the charge difference is calculated and expressed by:

![Fig. 1](image1.png)

(a) Top and (b) side views of the free-standing BP monolayer. (c) Considered representative adsorption sites on the BP monolayer surface.

![Fig. 2](image2.png)

Fig. 2 (a) The calculated adsorption energies of Li, Na and K on the BP monolayer. (b) The changes in potential energy with respect to the distance between alkali metal atoms and the BP monolayer ($d_{M-BP}$). The red, blue and brown lines represent the adsorption of single Li, Na and K atoms, respectively.
where \( \rho_{AM-BP}, \rho_{AM} \) and \( \rho_{BP} \) are the charge densities of alkali metal–BP systems, isolated alkali metal atoms and the BP monolayer, respectively. The charge difference plots of Li, Na and K atoms adsorbed on the BP monolayer are shown in Fig. 3a–c, with blue and yellow areas representing the electron loss and gain. In the case of Li, since the electronegativities of B and P are larger than that of Li, an obvious net loss of charges around the Li atom and a net gain of charges above the BP monolayer are found, indicating a significant charge transfer from Li to the BP monolayer. A similar tendency can also be observed in the cases of Na and K. However, one thing needed to be mentioned is that due to the electronegativity decrease in the sequence of Li > Na > K, the yellow area (i.e., electron gain) increases in the sequence of Li < Na < K, indicating enhanced charge transfers from alkali metal atoms to the BP monolayer.

In addition to the adsorption behaviors, it is essential to understand the electronic properties of anode materials. Unlike graphene, Mo\(_2\)C and borophene, the BP monolayer has low electrical conductivity due to its semiconducting behavior. Therefore, there is an imperative need to examine the electronic properties of the BP monolayer with Li, Na and K intercalations. The DOS of the pristine BP monolayer is shown in Fig. 4a. It is found that the pristine BP monolayer has a band gap of 0.87 eV, consistent with previous theoretical results. However, when alkali metal atoms are adsorbed, as shown in Fig. 4b and c for Li, Na and K, the Fermi levels are shifted and the alkali metal–BP systems are changed from semiconducting to metallic states, indicating much enhanced electrical conductivity. This phenomenon is also observed in other potential anode materials for alkali metal-based batteries, such as phosphorene, \( \alpha \)-Si\(_3\)S\(_8\) and Se\(_2\), which is attributed to the electron-denoting behavior of alkali metal atoms. In this regard, the BP monolayer anode can ensure a satisfied electrical conductivity during battery cycling.

Another fundamental characteristic to evaluate the suitability of an anode material for rechargeable batteries is the rate capability, which largely depends on the mobility of alkali metal atoms. In this regard, we investigate the diffusion pathways and calculate the energy barriers of Li, Na and K atoms on the BP monolayer, as shown in Fig. 5. Considering the highly symmetric structure of the BP monolayer, two representative diffusion pathways are chosen: path 1 goes through the midpoint of the B–P bond, and path 2 goes through the top of P and B atoms. Results show directional anisotropies for all Li, Na and K atoms, with energy barriers along path 1 smaller than along path 2. In the case of Li, the diffusion barriers along path 1 and 2 are 0.364 and 0.421 eV, respectively. On the basis of Arrhenius equation, the Li diffusivity along path 1 is 9 times larger than along path 2. A similar phenomenon is observed for Na diffusion, with the energy barriers of 0.217 eV along path 1 and 0.257 eV along path 2, indicating a 5 times larger Na diffusivity along path 1 than 2. For K diffusion, the diffusion barrier is 0.155 eV along path 1 and 0.177 eV along path 2, which means K diffuses 2 times faster along path 1 than 2. More importantly, from our calculation and comparison, two interesting facts are found for alkali metal atoms: one is that the alkali metal diffusion barrier decreases as the atomic number increases, and the other is that the directional anisotropy becomes weaker as the atomic number increases, both of which are consistent with the increasing atomic radii of Li < Na < K. When compared with other anode materials, the BP monolayer also shows higher alkali metal diffusivity with lower energy barrier. In the case of Li, the Li diffusion barrier (0.364 eV) on the BP monolayer is much smaller than that on other high specific capacity anode materials, such as Si (0.58 eV)\(^{55}\) and Sn (0.39 eV),\(^{29}\) and is comparable with that on graphene (0.33 eV).\(^{29}\) Moreover, since the diffusion barriers of Na and K are lower than that of Li, Na and K atoms show faster diffusions than Li on the BP monolayer. Therefore, the BP monolayer facilitates a faster transport not only for Li but also for other alkali metal elements (e.g., Na and K), indicating an enhanced rate capability for alkali metal-based batteries.

For practical applications, anode materials should also have a high storage capacity. Therefore, the effects of Li, Na and K concentrations on the adsorption energies are further investigated and the highest theoretical specific capacities are evaluated accordingly. The adsorbed atoms are gradually increased on the BP monolayer and the criteria to find the highest concentration are the same as the previous work.\(^{23}\) The adsorption energy changes as the function of Li, Na and K concentrations in Li\(_x\)BP, Na\(_x\)BP and K\(_x\)BP are summarized in Fig. 6a–c, respectively, and the embedded figures show the optimized structures (top view) of representative intermediates. The optimized structures from the side view of Li, Na and K
adsorbed on the BP monolayer at the highest concentration are shown in Fig. S1.† For Li storage shown in Fig. 6a, the concentration of $x = 0.1111$ corresponds to the case of single atom adsorption, with the adsorption energy of $-0.202$ eV. Then as the Li concentration increases, the adsorption energy decreases due to the increased repulsion forces between neighboring Li atoms, and finally reaches the lowest one of $-0.081$ eV at the concentration of $x = 0.6667$. After that, the Li adsorption energy gradually increases as the Li concentration increases, attributed to the structural changes of the BP.

![Fig. 4](image)

**Fig. 4** The density of states of (a) pristine BP monolayer, (b) Li$_{0.111}$BP, (c) Na$_{0.111}$BP and (d) K$_{0.111}$BP. The Fermi levels have been shifted to zero.

![Fig. 5](image)

**Fig. 5** Energy profiles of Li diffusion on (a) path 1 and (b) path 2, Na diffusion on (c) path 1 and (d) path 2, K diffusion on (e) path 1 and (f) path 2. The embedded figures are the corresponding diffusion pathways. The green, red and purple balls represent Li, Na and K atoms, respectively.
monolayer induced by added atoms. The highest Li concentration is found to be \( x = 2.0 \), corresponding to \( \text{Li}_2\text{BP} \), at which both sides of the BP monolayer are fully covered by Li atoms with the average adsorption energy of \(-0.185\) eV. A similar tendency to Li adsorption energy changes has also been found in other 2D anode materials, such as GeS, SnS, GeSe and SnSe.\(^{60}\)

Generally, for Li adsorption on the anode material, there are two kinds of competitive effects existing: one is the repulsion force between neighboring atoms (Effect 1), which decreases the adsorption energy; the other is the induced substrate structural changes (Effect 2), which increases the adsorption energy. In the case of Li adsorption on the BP monolayer, initially, Effect 1 is the dominant one and the overall adsorption energy decreases as the Li concentration increases (\( 0 < x < 0.6667 \)). Then, as the adsorbed Li atom further increases, the structural changes become more and more important, which makes, finally, Effect 2 become the dominant one and the adsorption energy increases as the lithium concentration increases (\( 0.6667 < x < 2 \)).

Interestingly, from our results, it is also found that at the final state of \( x = 2.0 \) when both sides are fully covered, the BP monolayer transforms from a planar structure to a puckered structure (Fig. S1a†), which can lead to the increased charge transfer and decreased distance, thus enhancing the adsorption energy, consistent with the observed adsorption energy increasing tendency caused by structural changes. For Na storage shown in Fig. 6b, the adsorption energy decreases dramatically as the Na concentration increases, indicating strong repulsion forces between neighboring atoms. Finally, at the Na concentration of \( x = 0.3333 \), the adsorption energy decreases to a positive value, indicating the end of the adsorption process and a low concentration for Na storage. Fig. 6c shows the adsorption energy changes of K atoms on the BP monolayer. It is seen that the adsorption energy continuously decreases from \(-0.681\) to \(-0.277\) eV as the K concentration increases, indicating Effect 1 is the dominant one during the whole process. At the highest K concentration of \( x = 0.89 \), both sides of the BP monolayer are fully covered by K atoms. Unlike the phenomenon in Li adsorption that Li atoms all locate at H sites, the K atoms adsorb on the BP monolayer with no definite site at high concentrations, which is attributed to the much larger radius of K than Li. Moreover, the calculated average open circuit voltages of the BP monolayer for Li, Na and K storages are 0.185, 0.056 and 0.277 V, indicating that the BP monolayer is suitable to be used as the anode material, which leads to a high output voltage of the batteries.

The maximum theoretical specific capacities (\( C \)) of Li, Na and K atoms on the BP monolayer are expressed by:

\[
C = \frac{1}{M_{BP}} \left( z \times x_{\text{max}} \times F \times 10^3 \right) \tag{5}
\]

where \( z \) is the valance number (\( z = 1 \) for Li, Na and K), \( x_{\text{max}} \) is the highest concentration of Li, Na and K on the BP monolayer, \( F \) is the Faraday constant (26.810 A h mol\(^{-1}\)), and \( M_{BP} \) is the atomic mass of the BP monolayer. From Fig. 6, it is found that the highest concentrations of Li, Na and K on the BP monolayer are 2.0, 0.2222 and 1.0, corresponding to the chemical formulae of \( \text{Li}_2\text{BP} \), \( \text{Na}_{0.2222}\text{BP} \) and \( \text{K}_{0.89}\text{BP} \). Therefore, the theoretical specific capacities of the BP monolayer for Li, Na and K storages are 1283, 143 and 570 mA h g\(^{-1}\), respectively. To further validate the fact that the BP monolayer can be a promising anode material for alkali metal-based batteries, we compare the theoretical specific capacities with other widely investigated materials. In the case of Li, the theoretical specific capacity of 1283 mA h g\(^{-1}\) is among the highest ones in existing anode materials, which is higher than that of phosphorene (433 mA h g\(^{-1}\)),\(^{63}\) siliconene (954 mA h g\(^{-1}\)),\(^{62}\) Sn (994 mA h g\(^{-1}\)),\(^{64}\) and Ti\(_3\)C\(_2\) (320 mA h g\(^{-1}\)).\(^{65}\) However, for Na storage, the theoretical specific capacity is relatively low, indicating that the BP monolayer is not suitable to be used as the anode material in Na-based batteries. In addition, the K storage capacity also shows a high value of 570 mA h g\(^{-1}\), much larger than that of

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**Fig. 6** The adsorption energy changes as the function of (a) Li, (b) Na and (c) K concentrations in Li\(_2\)BP, Na\(_{0.2222}\)BP and K\(_{0.89}\)BP. The embedded figures are the optimized structures (top view) of representative intermediates.
Thus, the BP monolayer can be a promising anode material for Li-based and K-based batteries with high specific capacity.

4. Conclusion

In summary, a DFT based first-principles study is carried out to investigate the potential of BP monolayer as the anode material for alkali metal-based batteries. It is found that the BP monolayer shows negative adsorption energies for Li, Na and K of $-0.202$, $-0.160$ and $-0.681$ eV, respectively, at the most stable H site. During loading, when the alkali metal atoms reach a critical position ($\sim 6 \text{ Å}$), the energy increases dramatically, indicating a rapid adsorption with no energy barrier. From charge difference plots, since electronegativities of B and P are larger than that of alkali metal atoms, an obvious net loss of charges around alkali metal atoms and a net gain of charges above the BP monolayer are found, showing charge transfer from the alkali metal to the BP monolayer. To analyze the electronic properties, the DOS of pristine BP and alkali metal–BP systems is calculated. Although the BP monolayer has a bandgap of $0.87$ eV, it transforms from a semiconducting behavior to metallic states after Li, Na and K interactions, ensuring a satisfied electrical conductivity as the anode material. Furthermore, Li, Na and K atoms show fast diffusions on the BP monolayer, with the energy barriers of $0.364$, $0.217$ and $0.155$ eV. Interestingly, the alkali metal diffusion barrier decreases and the directional anisotropy becomes weaker as the atomic number increases, consistent with the increasing atomic radii of Li $<$ Na $<$ K. Finally, by gradually increasing the number of adsorbed atoms on the BP monolayer, the theoretical specific capacities for Li and K storages are found to be $1283$ and $570$ mA h g$^{-1}$, which are among the highest values in the anode materials investigated to date, and substantially higher than that of the commercial graphite anode material. Given these advantages, it is expected that the BP monolayer is a promising anode material, offering high energy density and high power density, not only for Li-ion and K-ion batteries, but also for other lithium-based and potassium-based batteries.

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Notes and references

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