## Supporting Information

## A stable metallic 3D porous BPC<sub>2</sub> as a universal anode material for Li, Na, and K ion batteries with high performance

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Figure S1 (a, b, c) The partial density of states (PDOS) for Lithium-ion adsorption at site  $S_{1}$ ,  $S_{2}$ , and  $S_{3}$  respectively.



Figure S2 (a, b, c) The partial density of states (PDOS) for sodium-ion adsorption at site  $S_{1}$ ,  $S_{2}$ , and  $S_{3}$  respectively.



**Figure S3** (a, b, c) The partial density of states (PDOS) for potassium ion adsorption at site  $S_{1}$ ,  $S_{2}$ , and  $S_{3}$  respectively.



**Figure S4** The side views of the following five different concentrations of Li-ions in 3D-BPC<sub>2</sub> (a) 0.031 (b) 0.0625 (c) 0.125 (d) 0.1875 (e) 0.25.



**Figure S5** The side views of the following five different concentrations of Na-ions in 3D-BPC<sub>2</sub> (a) 0.031 (b) 0.0625 (c) 0.125 (d) 0.1875 (e) 0.25.



**Figure S6** The side views of the following four different concentrations of K-ions in 3D-BPC<sub>2</sub> (a) 0.031 (b) 0.0625 (c) 0.125 (d) 0.1875.



**Figure S7** (a) The AIMD simulation at 300 K for low-medium-high (0.031-0.125-0.25) concentration of Li-ions.



**Figure S8** (a) The AIMD simulation at 300 K for low-medium-high (0.031-0.125-0.25) concentration of Na-ions.



**Figure 9** (a) The AIMD simulation at 300 K for low-medium-high (0.031-0.125-0.187) concentration of K-ions.