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

Metallic two-dimensional *b*-BS_2 monolayer for superior Na/K-ion batteries anodes

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The particle swarm optimization (PSO) method within the evolutionary algorithm as implemented in the Crystal structure AnaLYsis by Particle Swarm Optimization (CALYPSO) code was employed to find the lowest energy structures of BS_x (x = 0.5, 1, 1.5, 2) monolayers. In the first step, random structures with certain symmetry are constructed in which atomic coordinates are generated by the crystallographic symmetry operations.

Up to now, a few BS_x (e.g. B_2S, BS, and B_2S_3) monolayers have been reported. To determine the relative stability of our predicted *b*-BS_2 monolayer, we fully relaxed the other known BS_x monolayers and built the convex hull, as shown in Fig. S1. The *b*-BS_2 monolayer, sitting on the solid line, is thermodynamically stable with respect to decomposition into B and S elements.

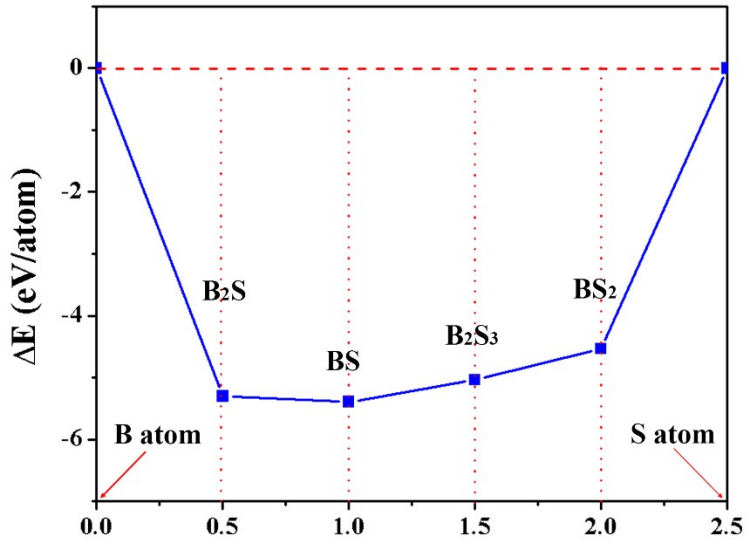

Fig. S1. (a) Relative formation energy of BS_x (x = 0.5, 1, 1.5, 2) monolayers with respect to B and S atoms at 0 K.

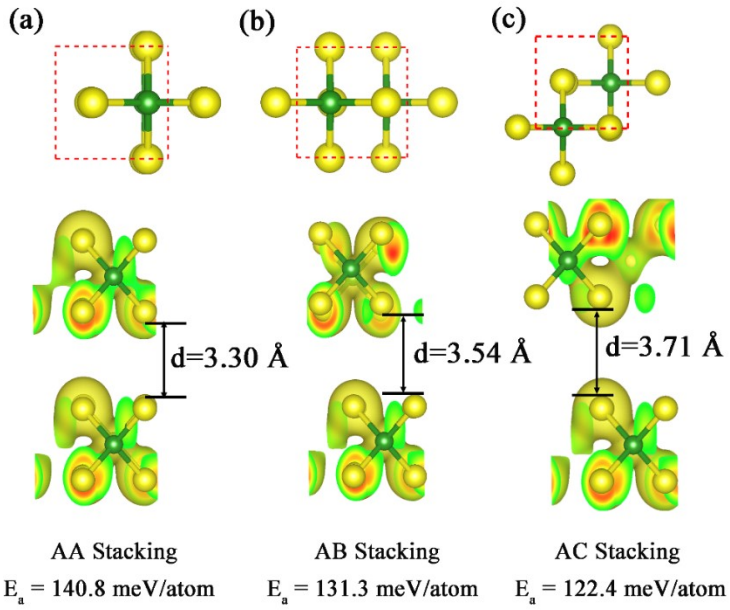

Fig. S2. (a)-(c) Geometries of the BS_2 bilayer with AA, AB, and AC stacking patterns, corresponding their interlayer distances and interaction energies.

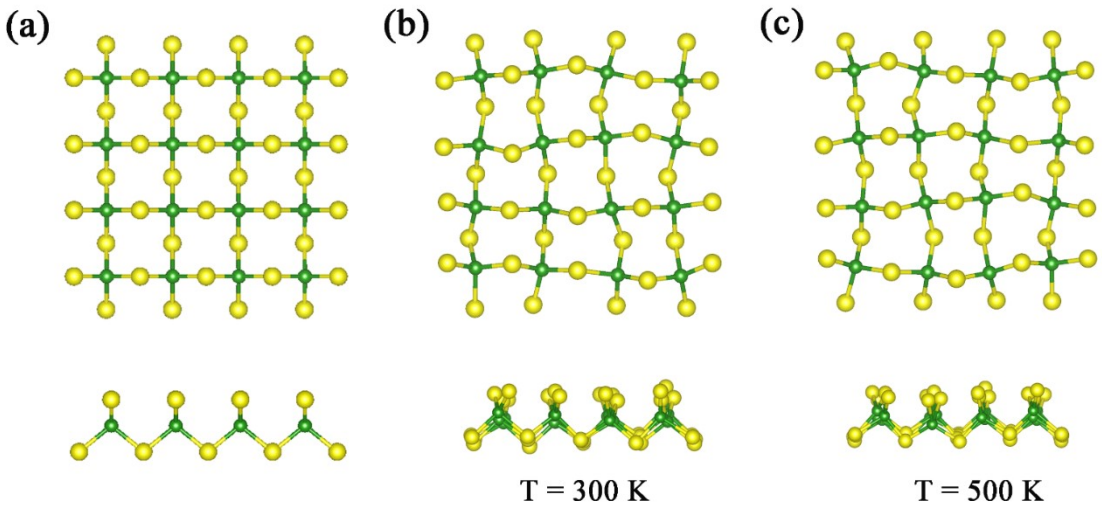

Fig. S3. The BS_2 monolayer structures of (a) original, (b) 300 K, and (c) 500 K at the end of 5 ps with a time step of 1.0 fs AIMD simulations.

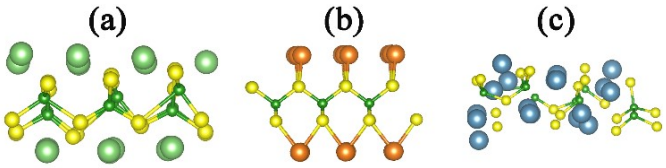

Fig. S4. Geometric structures for (a) Li, (b) Mg, and (c) Ca adsorption on the BS_2 monolayer of side views.

Table S1 Comparison of capacity of previously reported 2D materials with *b*-BS_2 monolayer for NIBs and KIBs.

	Na	K
PC_6	1301.07[1]	781[2]
PC_3	1200 [3]	1200[4]
Si_3C	1115[5]	836[5]
BC_3	572[6]	858[6]
B_2C	1596	
BC_7	870.25[7]	
B_3P	1706	
Penta-BN_2	690.23[8]	690.23[8]
B_2S	831.48[9]	
b-BS_2	2146.08	715.36

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