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Supporting Information

Boron-graphdiyne: superstretchable semiconductor with low thermal conductivity and ultrahigh capacity for Li, Na and Ca ions storage

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1. Atomic structure of boron-graphdiyne unit-cell

2. Most stable adsorption sites for Li, Na, Mg and Ca atoms over B-graphdiyne.

1. Atomic structure of B-graphdiyne unit-cell

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C12B2
   1.00000000000000
    11.8467556014048103    0.0000000000000000    0.0000000000000000
     5.9233778007024069   10.2595913032290600    0.0000000000000000
     0.0000000000000000    0.0000000000000000   20.0000000000000000
   C    B
    12     2
Direct
  0.4070313359871207  0.1859316676351952  0.5000000000000000
  0.4672120785149971  0.0655705418981327  0.5000000000000000
  0.4070313102567411  0.4070303586203110  0.5000000000000000
  0.4672113650511491  0.4672112185712862  0.5000000000000000
  0.5327836106014843  0.5327839635983835  0.5000000000000000
  0.5929637664429919  0.5929648549585735  0.5000000000000000
  0.5929638727348205  0.8140640368300751  0.5000000000000000
  0.5327845410920844  0.9344251783120043  0.5000000000000000
  0.1859315430662534  0.4070331135330179  0.5000000000000000
  0.0655704174789662  0.4672136888685117  0.5000000000000000
  0.8140642497539758  0.5929627139400750  0.5000000000000000
  0.9344251513708954  0.5327831630738729  0.5000000000000000
  0.3333313296681197  0.3333314582972733  0.5000000000000000
  0.6666641611622097  0.6666642439564683  0.5000000000000000
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2. Most stable adsorption sites for Li, Na, Mg and Ca atoms over B-graphdiyne.

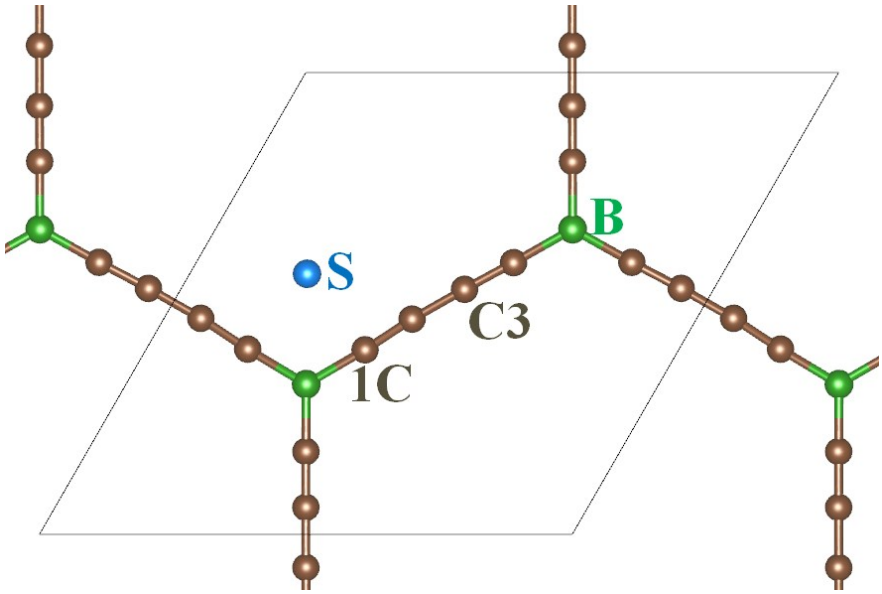

Fig. S1, Atomic structure of B-graphdiyne monolayer.

Table S1, Predicted most stable adsorption sites for the single Li, Na, Mg and Ca adatoms over the single-layer B-graphdiyne. Here, E_{ad}, L_{x-y}, Z and ΔQ depict, respectively, the corresponding adsorption energy, distance between the closest x and y atoms, the out-of-plane movement of an adatom at the "S" adsorption site (shown in Fig. S1) and the charge transfer from a single adatom to the B-graphdiyne monolayer predicted by the Bader charge analysis.

Most stable adsorption sites	Li	Na	Mg	Ca
First	S site	S site	S site	S site
	E_{ad}= -1.7 eV	E_{ad}= -1.75 eV	E_{ad}= 0.65 eV	E_{ad}= -1.22 eV
	L_{B-Li}= 2.453Å, Z=0.0 Å	L_{B-Na}= 2.9 Å, Z=0.0 Å	L_{B-Mg}= 2.5 Å, Z=1.38Å	L_{B-Ca}= 2.627 Å, Z=1 Å
	ΔQ= 0.994 |e|	ΔQ= 0.993 |e|	ΔQ= 1.467 |e|	ΔQ= 1.469 |e|
Second	1C top	B top	B top	C3-C3 bridge
	E_{ad}= -1.22 eV	E_{ad}= -1.34 eV	E_{ad}= 0.73 eV	E_{ad}= -0.94 eV
	L_{1C-Li}= 2.054 Å	L_{B-Na}= 2.431 Å	L_{B-Mg}= 2.388 Å	L_{C3-Ca}= 2.33 Å
	ΔQ= 0.988 |e|	ΔQ= 0.992 |e|	ΔQ= 1.252 |e|	ΔQ= 1.4 |e|
Third	B top	1C top		B top
	E_{ad}= -1.19 eV	E_{ad}= -1.32 eV		E_{ad}= -0.85 eV
	L_{B-Li}= 2.106 Å	L_{1C-Na}= 2.45 Å		L_{B-Ca}= 2.343 Å
	ΔQ= 0.989 |e|	ΔQ= 0.992 |e|		ΔQ= 1.44 |e|