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

C12B2

|                | C   | B   |
|----------------|-----|-----|
| 11.8467556014048103 | 0.0000000000000000 | 0.0000000000000000 |
| 5.9233778007024069  | 10.2595913032290600 | 0.0000000000000000 |
| 0.0000000000000000  | 20.0000000000000000 | 0.0000000000000000 |

|                | C   | B   |
|----------------|-----|-----|
| 0.4070313359871207 | 0.1859316676351952 | 0.5000000000000000 |
| 0.4672120785149971  | 0.0655705418981327  | 0.5000000000000000 |
| 0.3333313296681197  | 0.6666641611622097  | 0.5000000000000000 |

Direct

|                |      |      |      |
|----------------|------|------|------|
| 0.4070313102567411 | 0.4070303586203110 | 0.5000000000000000 |
| 0.4672113650511491 | 0.467211285712862  | 0.5000000000000000 |
| 0.5327836106014843 | 0.5327839635983835 | 0.5000000000000000 |
| 0.592963764429919  | 0.59296459585735   | 0.5000000000000000 |
| 0.6666641611622097 | 0.6666642439564683 | 0.5000000000000000 |
| 0.8140640368300751 | 0.8140642439564683 | 0.5000000000000000 |
2. Most stable adsorption sites for Li, Na, Mg and Ca atoms over B-graphdiyne.

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 \( \Delta Q \) 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 | -1.75 eV | 0.65 eV | -1.22 eV |
| \( L_{B-Li} \)             | 2.453 Å, Z=0.0 Å | 2.9 Å, Z=0.0 Å | 2.5 Å, Z=1.38 Å | 2.627 Å, Z=1 Å |
| \( \Delta Q \)             | 0.994 | 0.993 | 1.467 | 1.469 |
| Second                      | 1C top | B top | B top | C3-C3 bridge |
| \( E_{ad} \)               | -1.22 eV | -1.34 eV | 0.73 eV | -0.94 eV |
| \( L_{C3-C3} \)            | 2.054 Å | 2.431 Å | 2.388 Å | 2.33 Å |
| \( \Delta Q \)             | 0.988 | 0.992 | 1.252 | 1.4 |
| Third                       | B top | 1C top | B top |
| \( E_{ad} \)               | -1.19 eV | -1.32 eV | -0.85 eV |
| \( L_{B-Li} \)             | 2.106 Å | 2.45 Å | 2.343 Å |
| \( \Delta Q \)             | 0.989 | 0.992 | 1.44 |