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First-principles study of the dual doped graphene: Towards the promising anode materials for Li/Na-ion batteries

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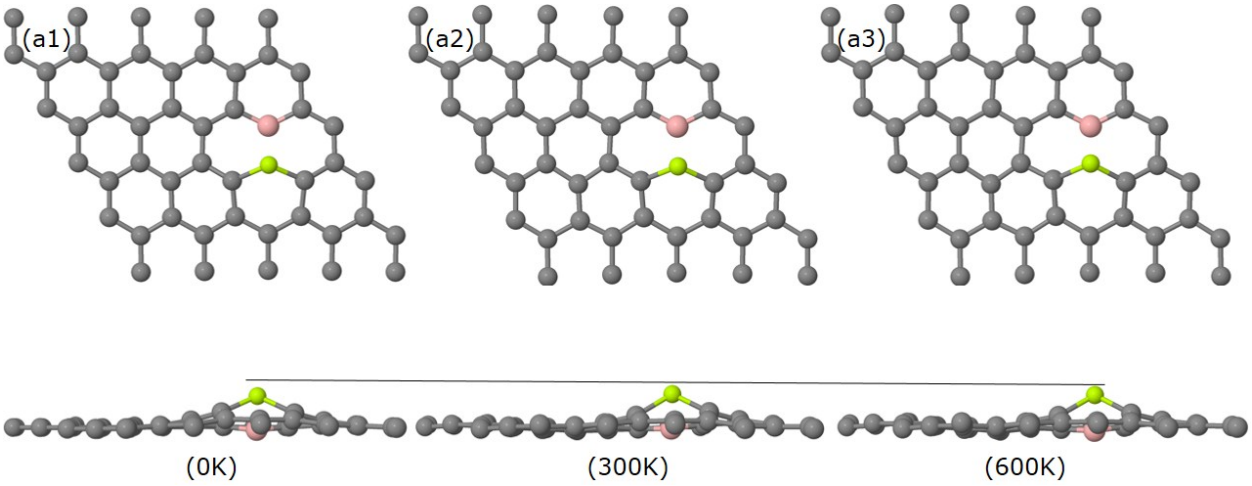


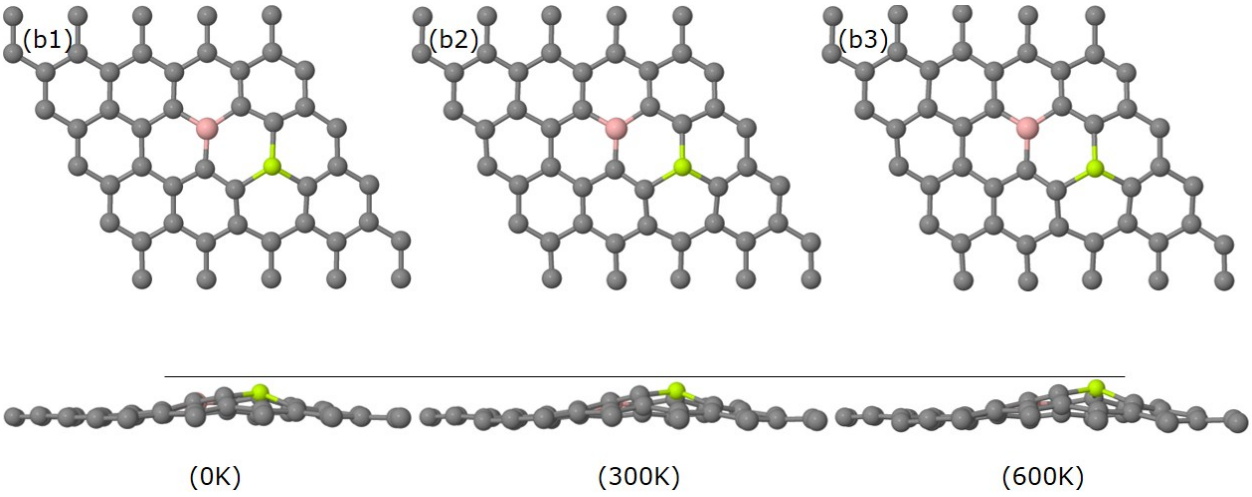


Figure S1: Top and side views of molecular dynamics geometries at various temperature are shown for (a1-a3) Be-B-ortho, and (b1-b3) Be-B-para dispositions. The results show that these structures are thermally stable and a just negligible change in the height of Be atom occurred even at 600K.

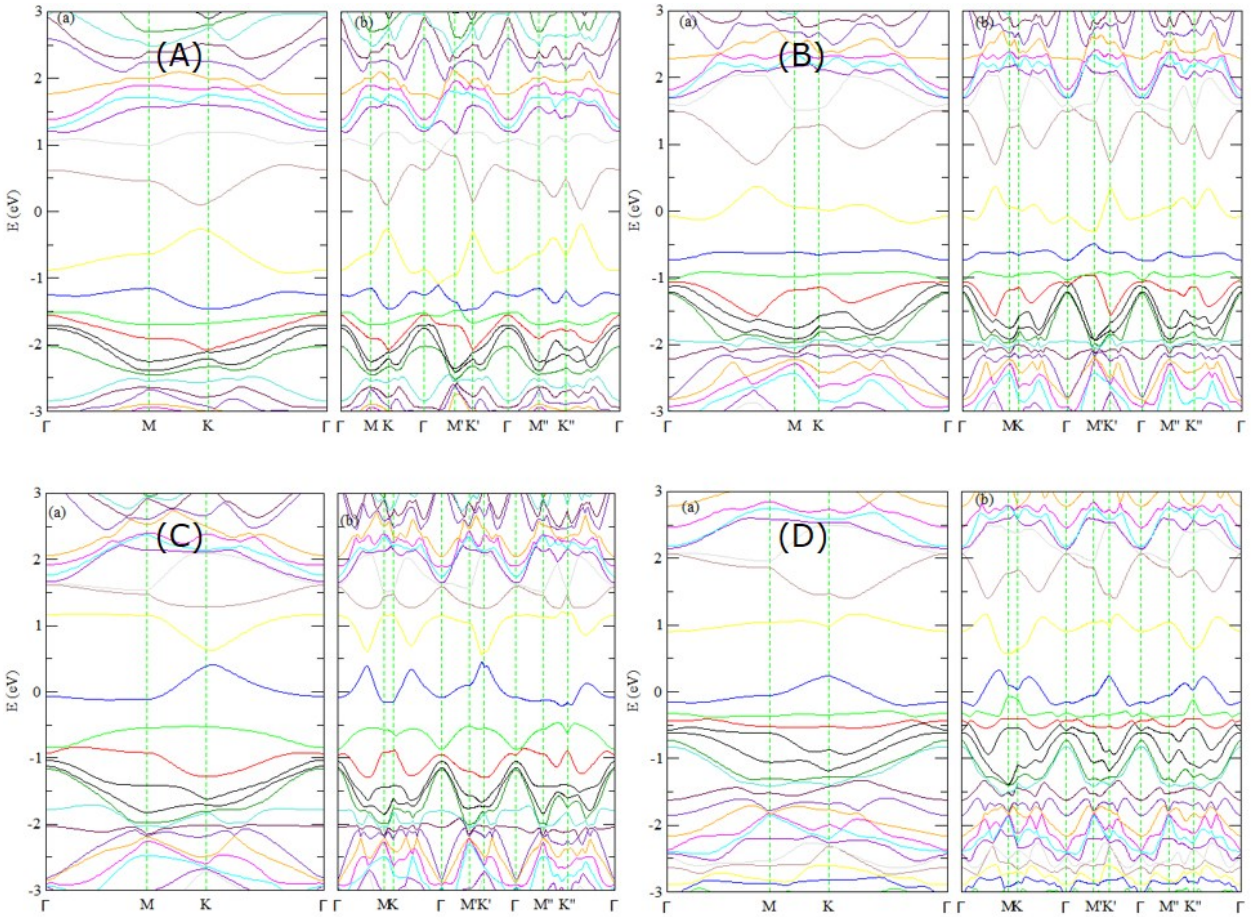
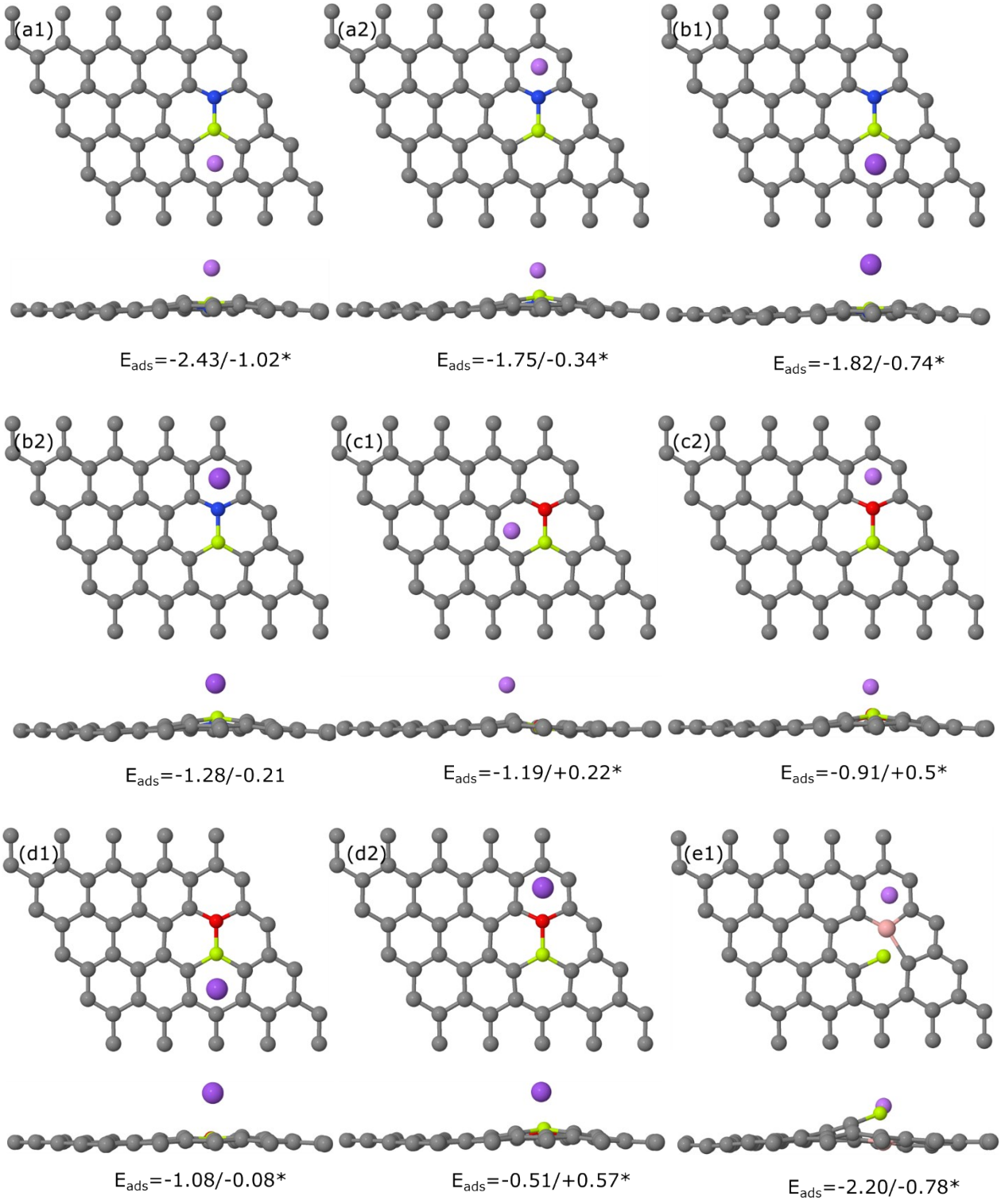
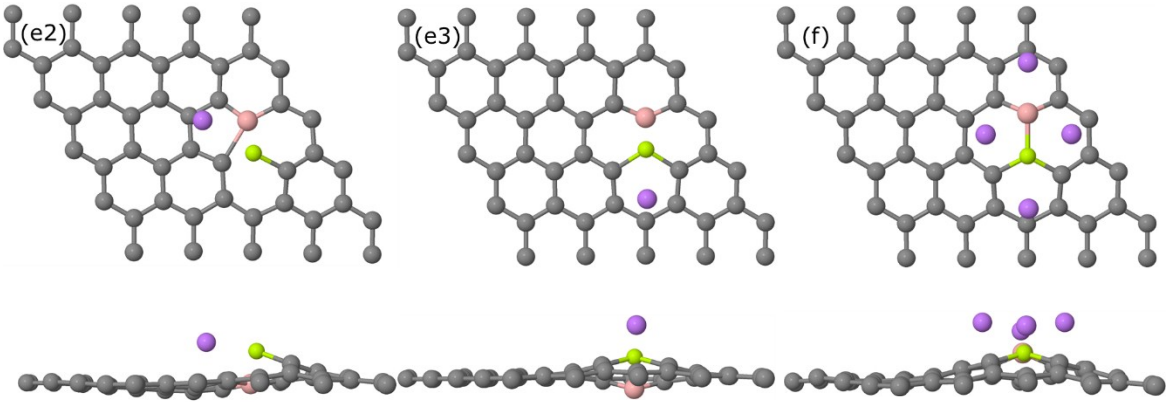


Figure S2: Electronic bands structures calculated at (a) classic G-M-K-G, and (b) special G-M-K-G-M'-K'-G-M''-K''-G paths for (A) BeO doped, (B) BeN doped, (C) ortho Be-B doped, and (D) para Be-B doped graphene are shown.

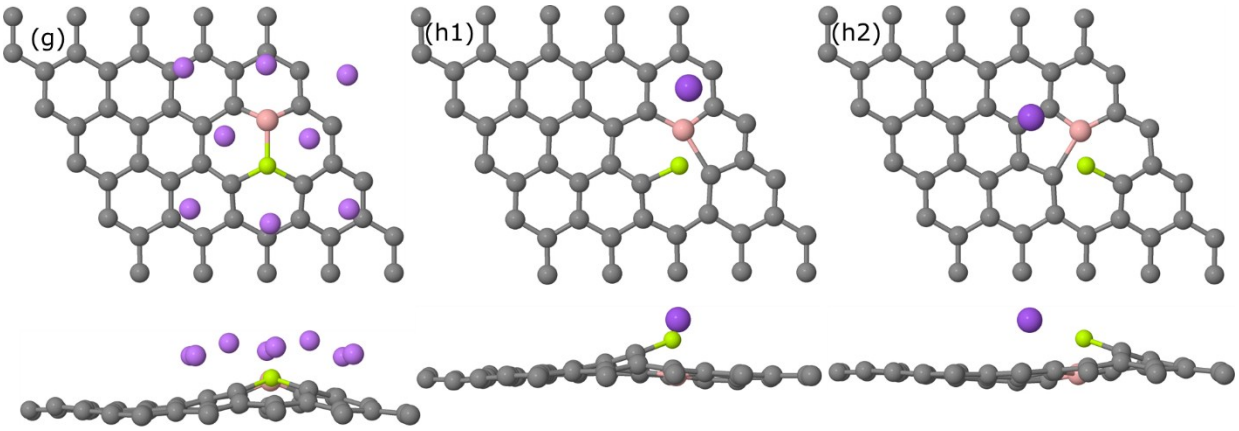




E_{ads}=-2.14/-0.73*

E_{ads}=-1.93/-0.52*

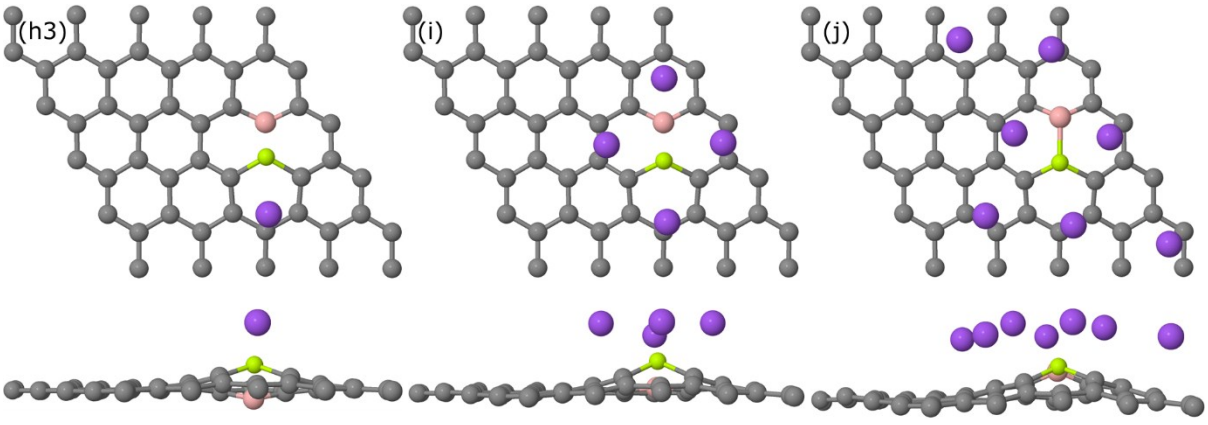
E_{ads}=-1.74/-0.33*



E_{ads}=-1.41/-0.001*

E_{ads}=-1.67/-0.60*

E_{ads}=-1.62/-0.54*



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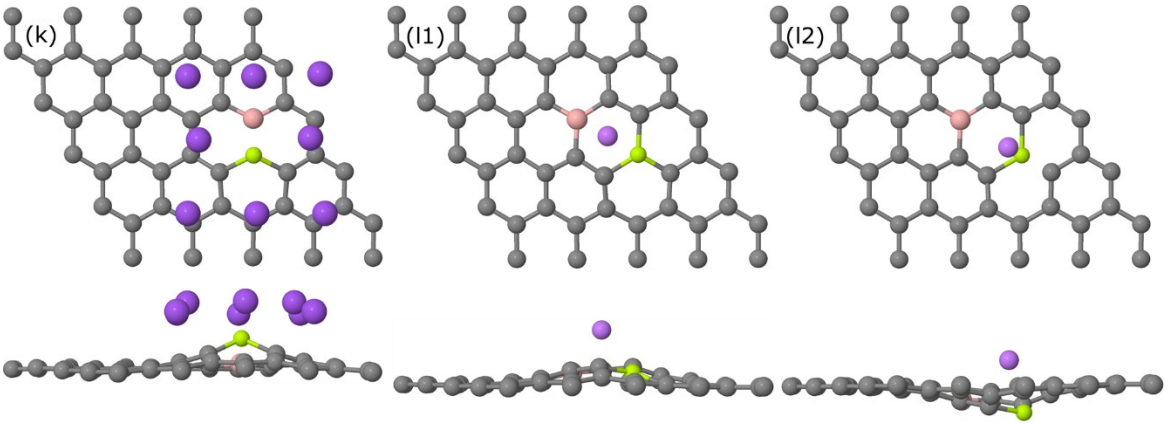

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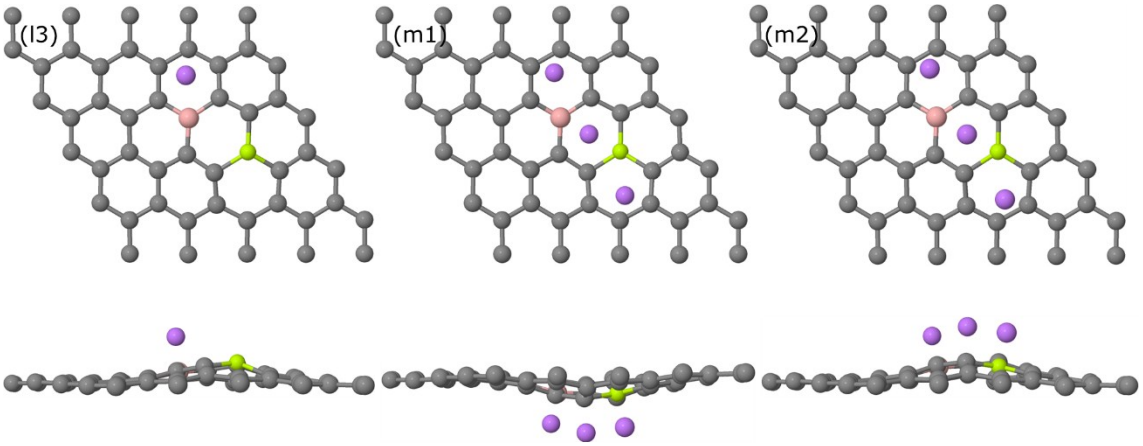
E_{ads}=-3.44/-2.03*

E_{ads}=-3.44/-2.03*



E_{ads}=-3.07/-1.66*

E_{ads}=-2.32/-0.91*

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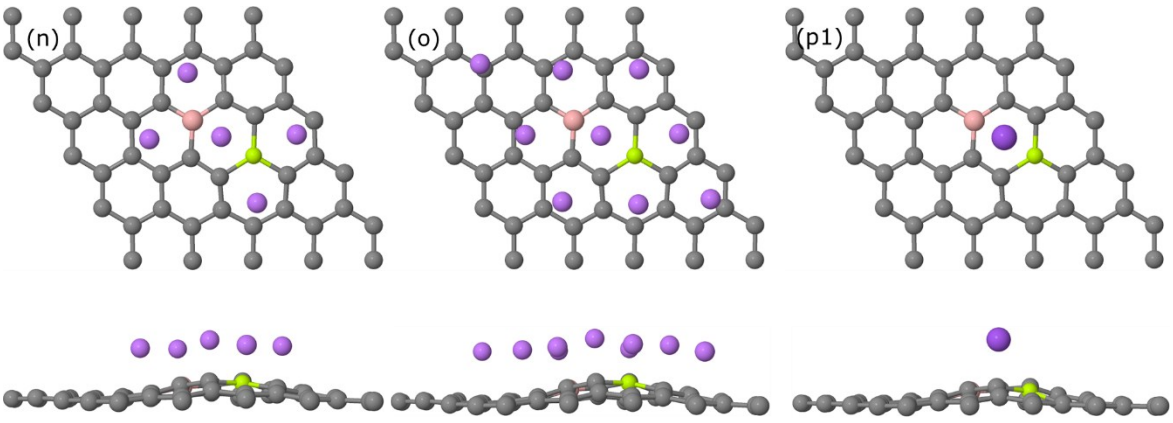

E_{ads}=-2.02/-0.60*

E_{ads}=-1.60/-0.18*

E_{ads}=-2.82/-1.75*

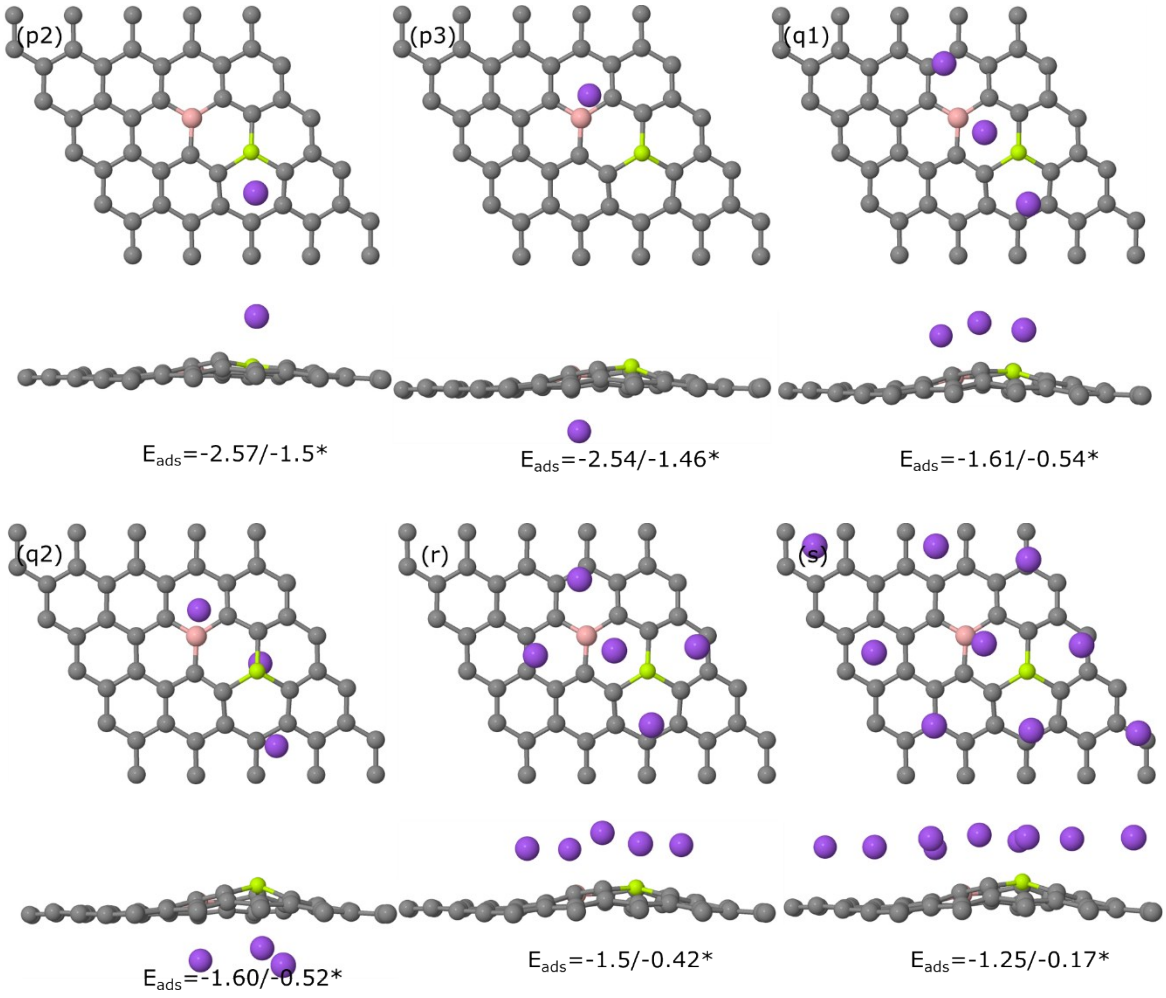

Figure S3: Top and side view of (a1-a2) Li adsorbed BeN DDG, (b1-b2) Na adsorbed BeN DDG, (c1-c2) Li adsorbed BeO DDG, (d1-d2) Na adsorbed BeO DDG, (e1-g) Li adsorption on Be-B ortho, (h1-k) Na adsorption on Be-B ortho, (l1-o) Li adsorption on Be-B para, (p1-s) Na adsorption on Be-B para DDG are shown. The * values are calculated by using the energies of Li/Na in their bulk bcc structures.

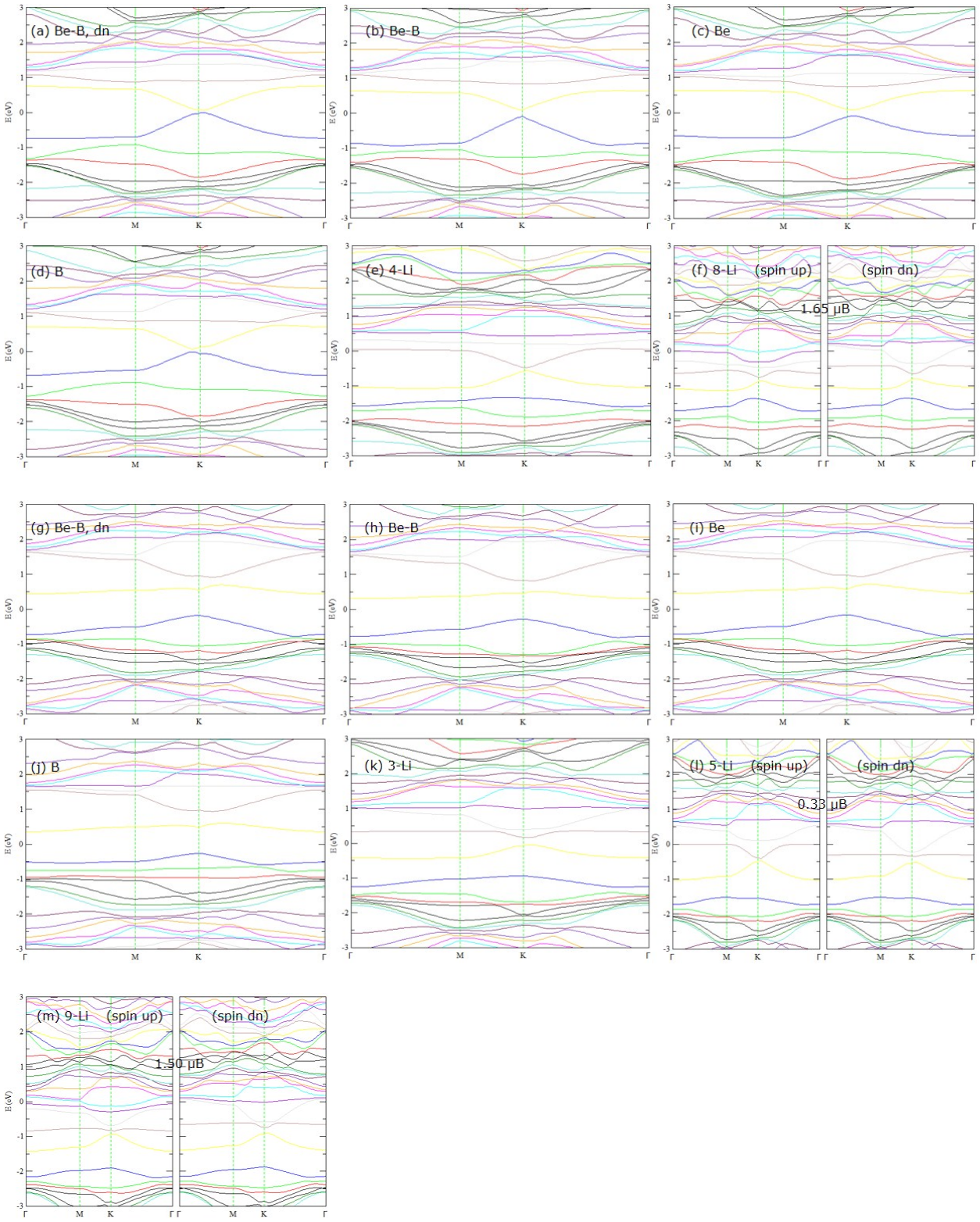

Figure S4: Electronic bands structures of Li adsorbed on (a-f) ortho Be-B doped, and (g-m) para Be-B doped graphene are plotted.

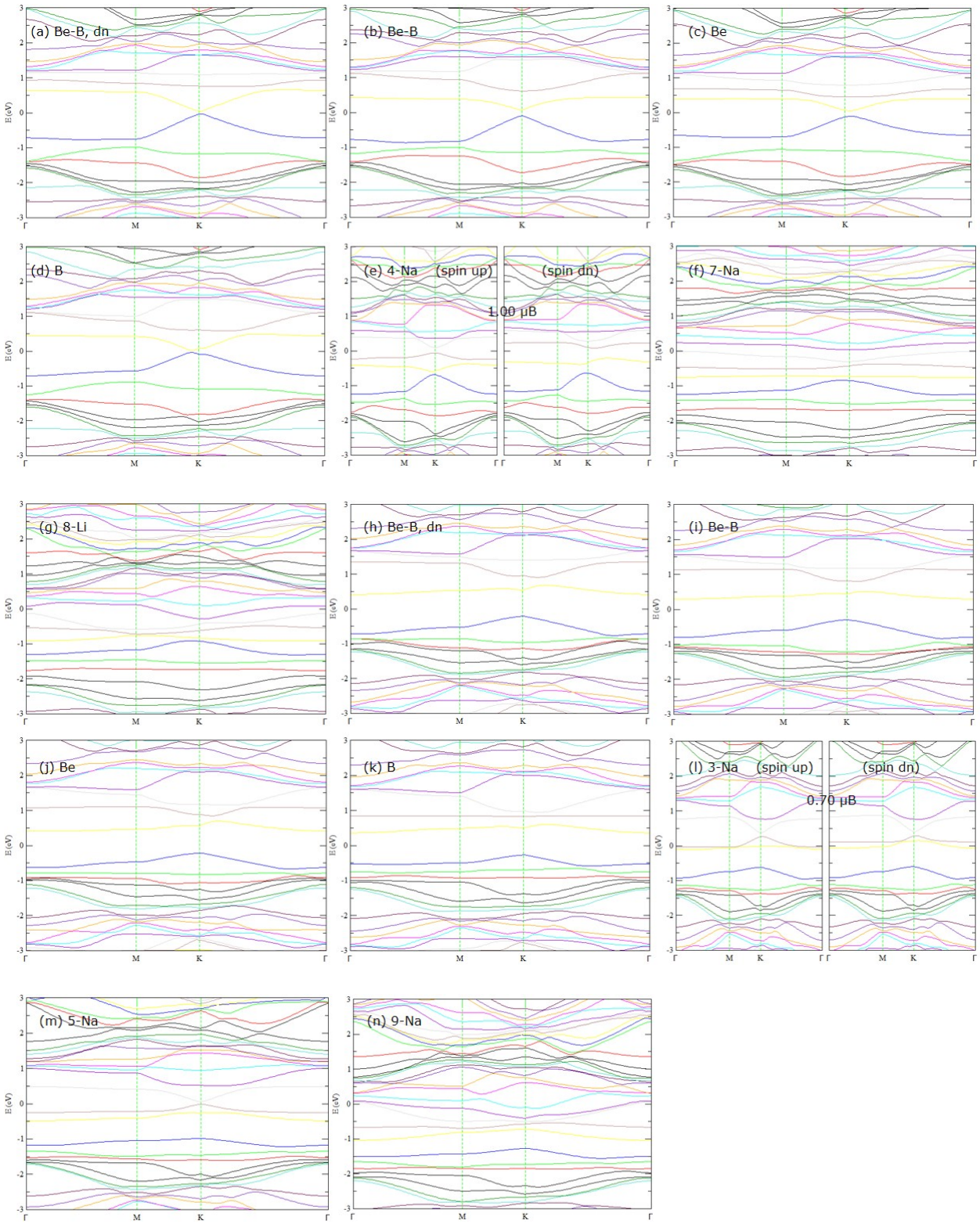

Figure S5: Electronic bands structures of Na adsorbed (a-g) ortho Be-B, and (h-n) para Be-B doped graphene are plotted.

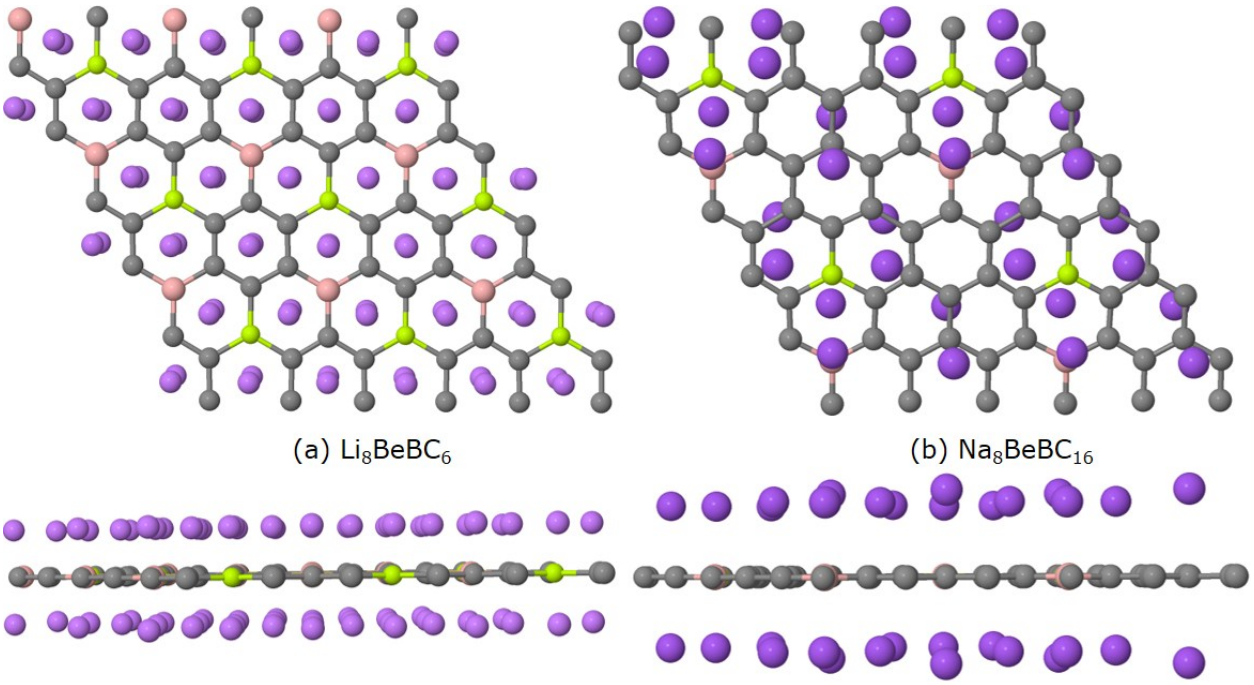

Figure S6: Top and side views of (a) Li_8BeBC_6, and (b) Na_8BeBC_{16} are shown.