ESI

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

Saif Ullah, a,* Pablo A. Denis, b and Fernando Sato a

a- Departamento de Física, Instituto de Ciências Exatas, Campus Universitário, Universidade Federal de Juiz de Fora, Juiz de Fora, MG 36036-900, Brazil

b- Computational Nanotechnology, DETEMA, Facultad de Química, UDELAR, CC 1157, 11800 Montevideo, Uruguay

*email: sullah@fisica.ufjf.br
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.
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$_8$BeBC$_6$, and (b) Na$_8$BeBC$_{16}$ are shown.