Supporting Information

Tuning the electrochemical behavior of graphene oxide and reduced graphene oxide via doping hexagonal BN for high capacity negative electrode for Li and Na ion batteries

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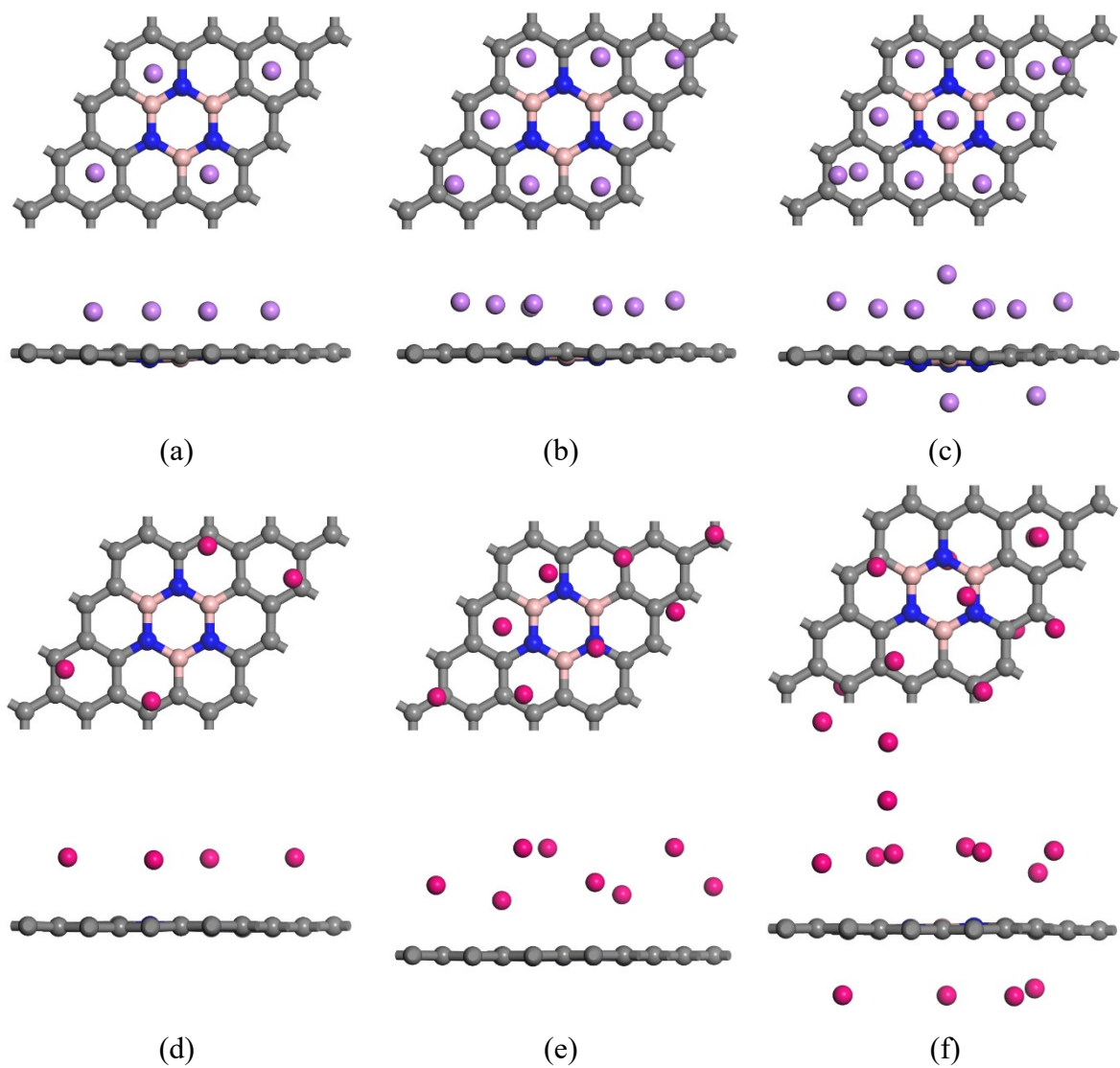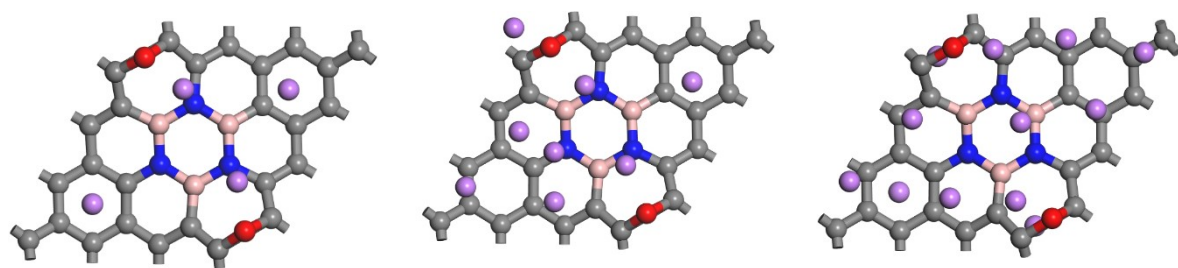*Corresponding author: Email: sdshamim@mbstu.ac.bd (Siraj Ud Daula Shamim)

Figure S1: Front and side views of optimized BN-G with diverse number of (a) 4Li, (b) 8Li, (c) 10Li, (d) 4Na, (e) 8Na and (f) 10Na atoms respectively.
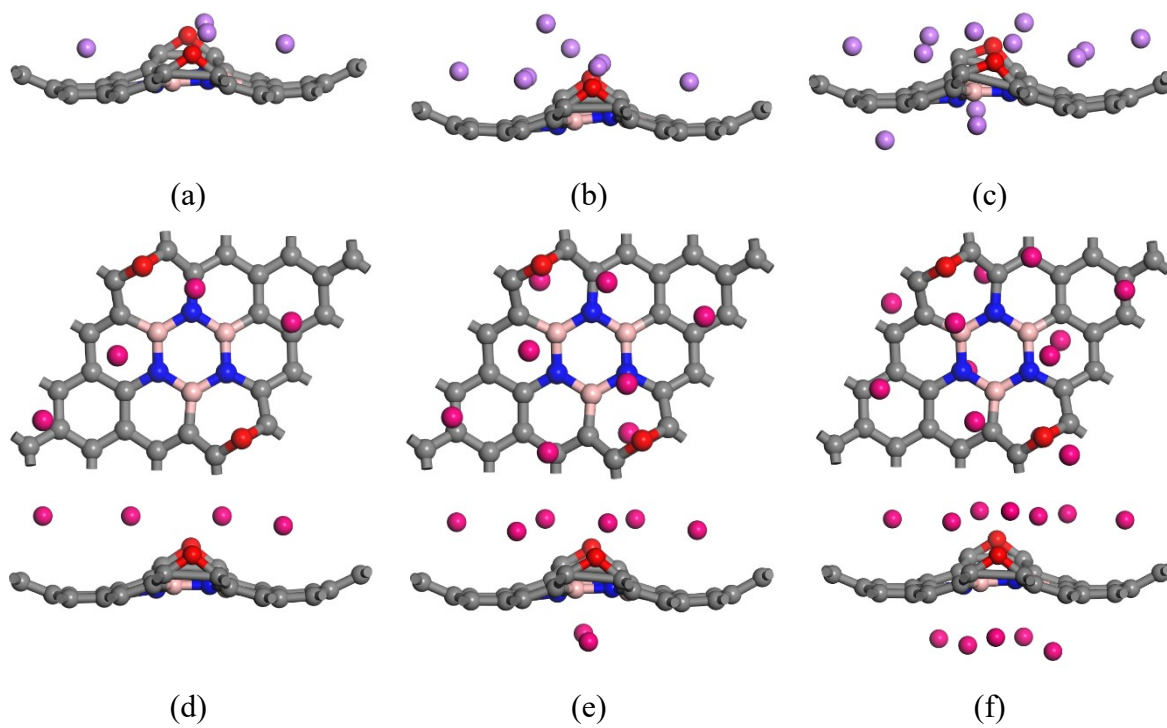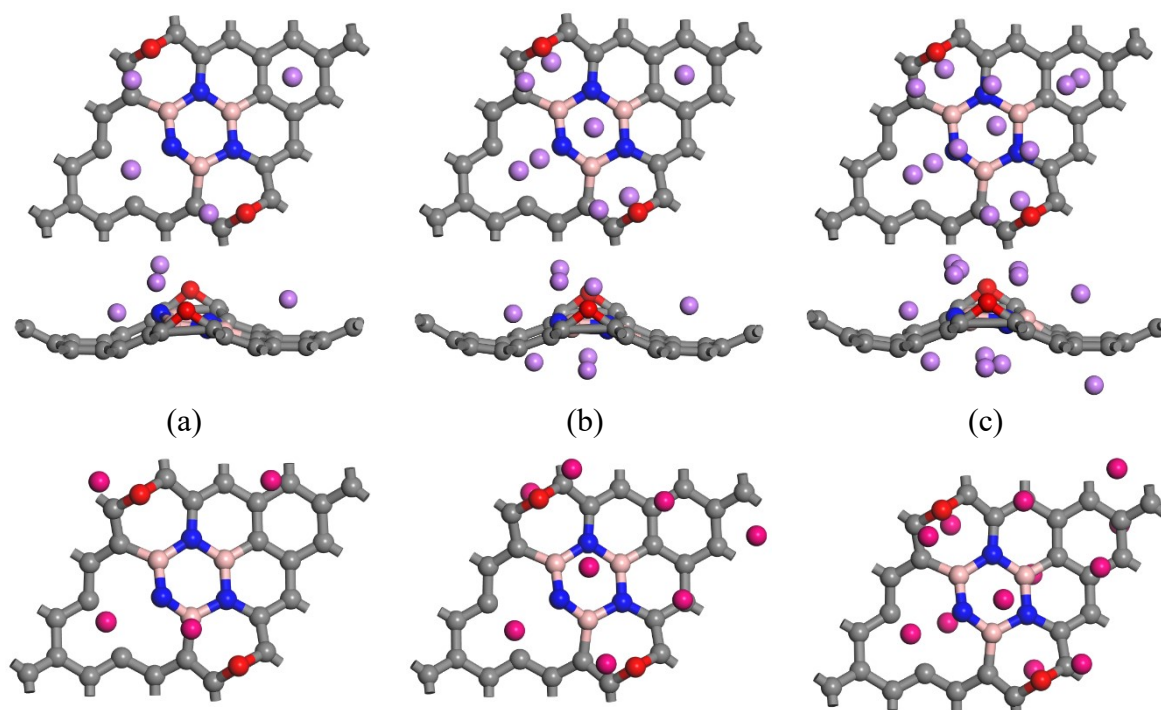
Figure S2: Front and side views of optimized BN-GO with diverse number of (a) 4Li, (b) 8Li, (c) 10Li, (d) 4Na, (e) 8Na and (f) 10Na atoms respectively.

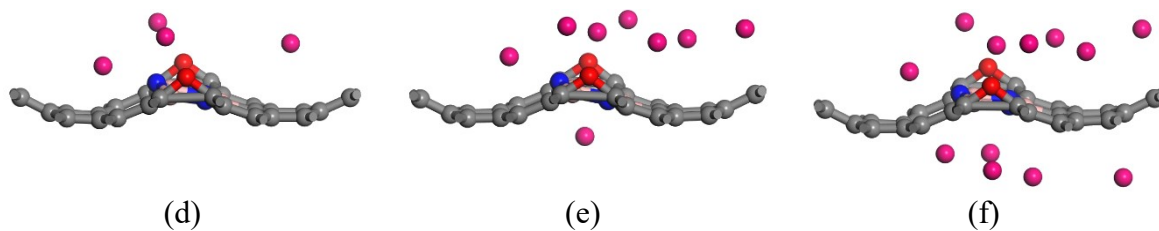(d)   (e)   (f)

Figure S3: Front and side views of optimized BN-rGO with diverse number of (a) 4Li, (b) 8Li, (c) 10Li, (d) 4Na, (e) 8Na and (f) 10Na atoms respectively.

(a)   (b)   (c)

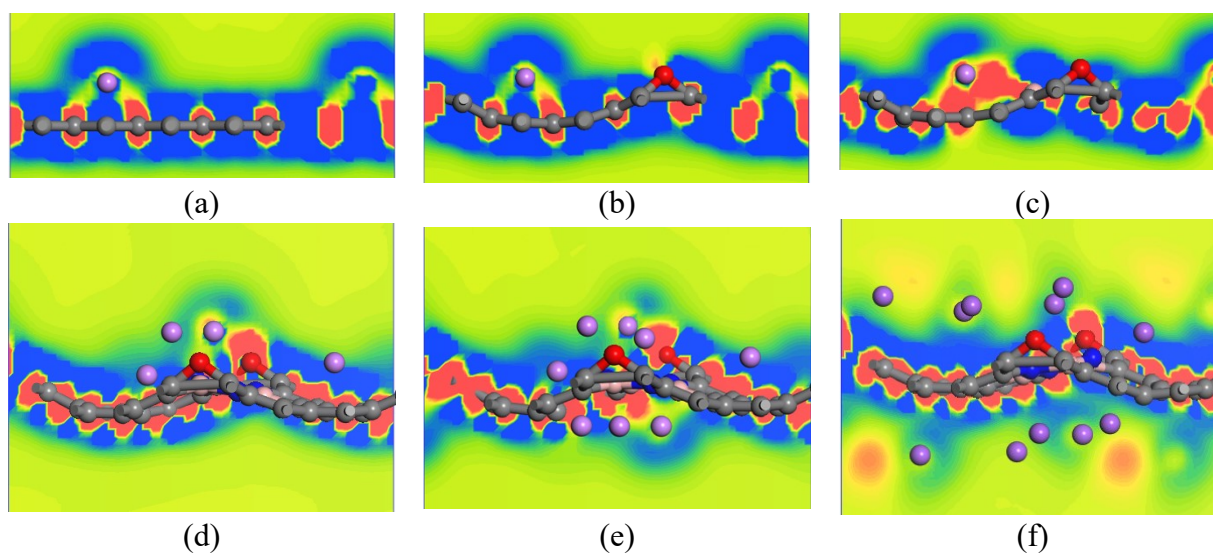(d)   (e)   (f)

Figure S4: Deformation density map for most stable adsorption site for Li adsorption on (a) BN-G, (b) BN-GO and (c) BN-rGO and diverse number of (d) 4 Li, (e) 8 Li and (f) 12 Li on BN-rGO; where red color indicates the electron enrichment area and blue color indicates the electron deficient area. The iso-surface is set at ± 0.02 e/$\overset{\circ}{A}^3$.

(a)
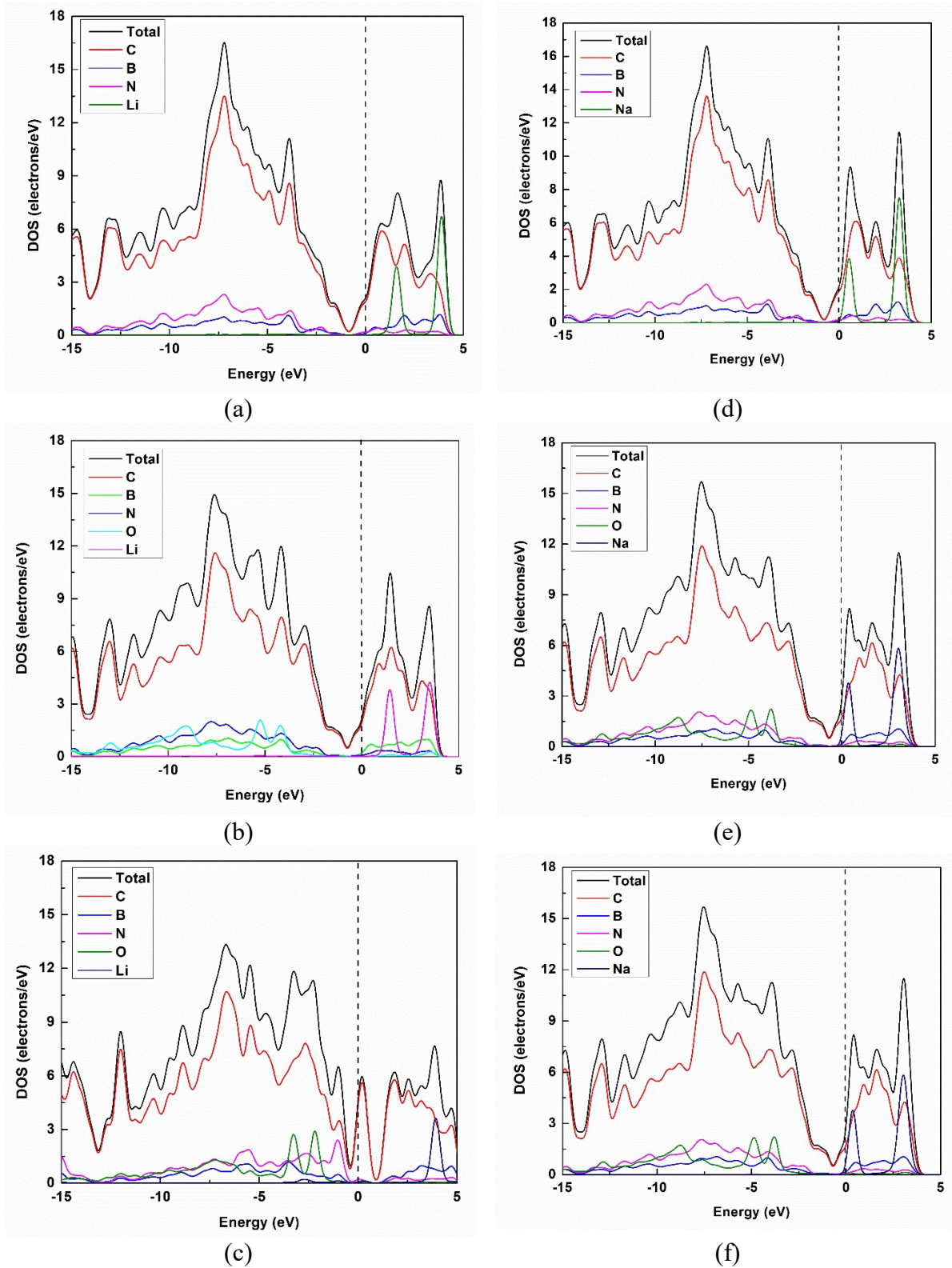
(d)

(b)

(e)

(c)

(f)

Figure S5: PDOS of Li atom adsorption on (a) BN-G, (b) BN-GO and (c) BN-rGO nanosheets and Na atom adsorption on (d) BN-G, (e) BN-GO and (f) BN-rGO at most stable adsorption sites.
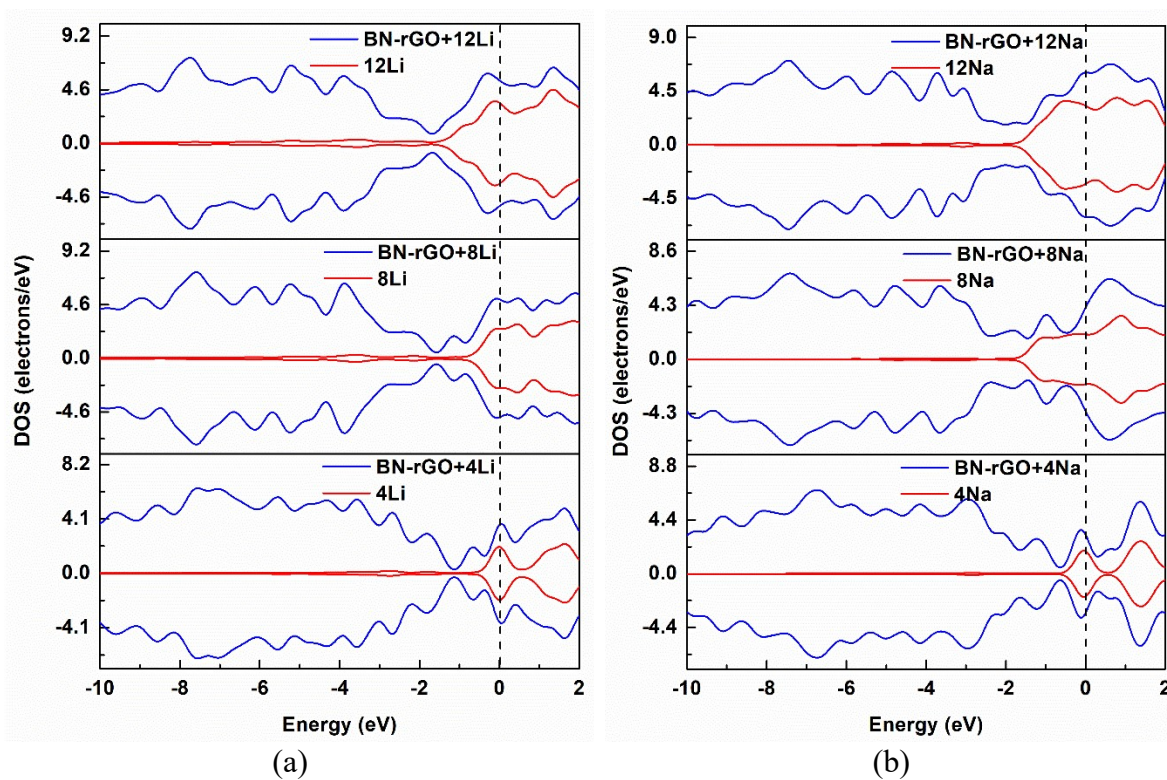
Figure S6: Spin polarized PDOS of BN-rGO nanosheet with diverse number of a) Li and b) Na atoms.