Supplementary Information

Optimal Balance: Alkali Metal-Doped Boron Carbide Nanosheets Achieve Superior Stability and Nonlinear Optical Responsiveness

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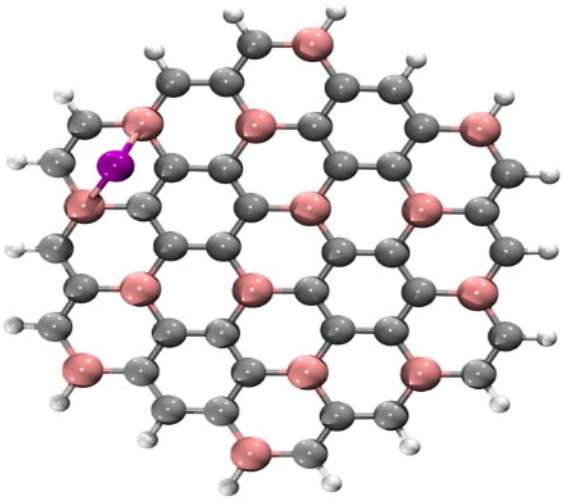
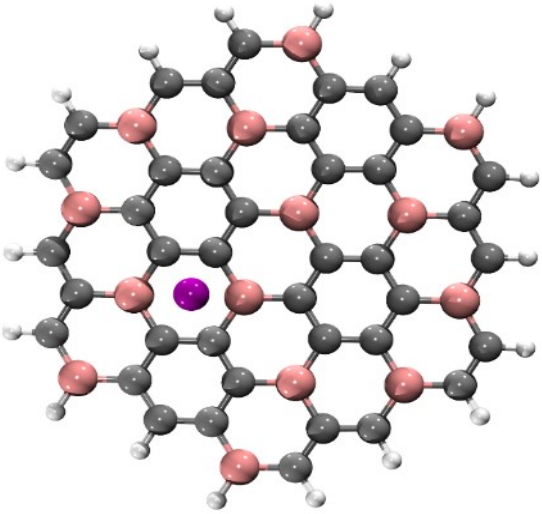
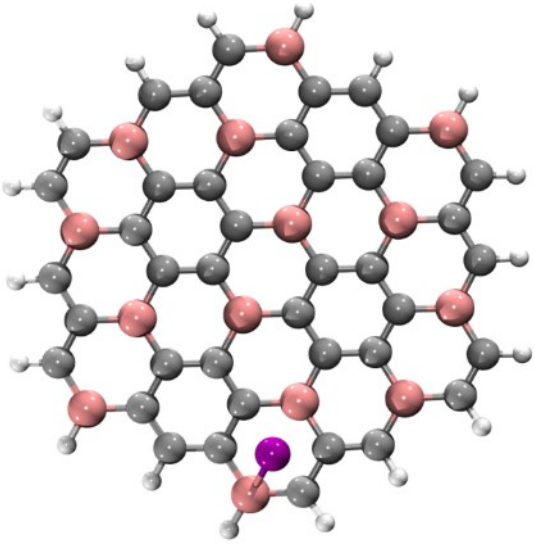
Li@BC nanosheet



Li@BC-B



Li@BC-C



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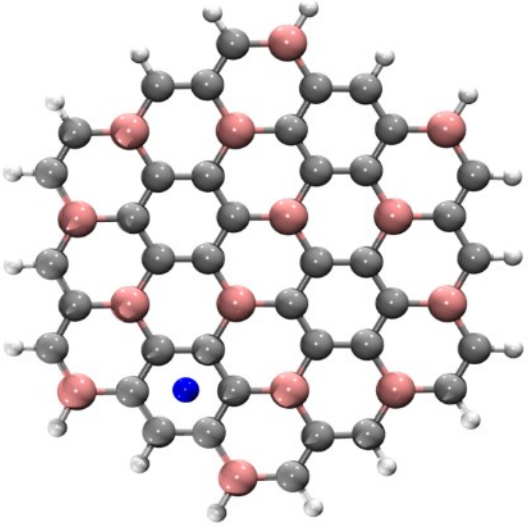
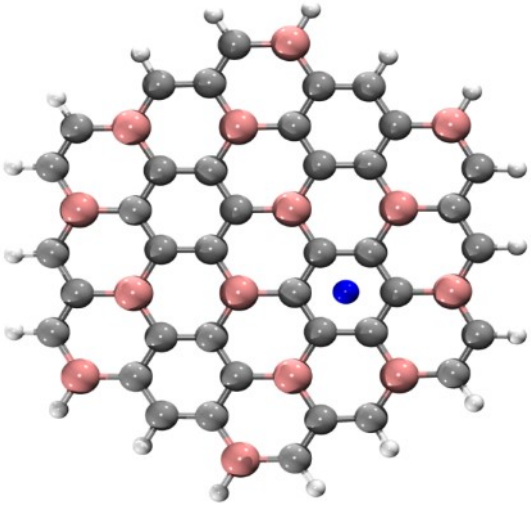
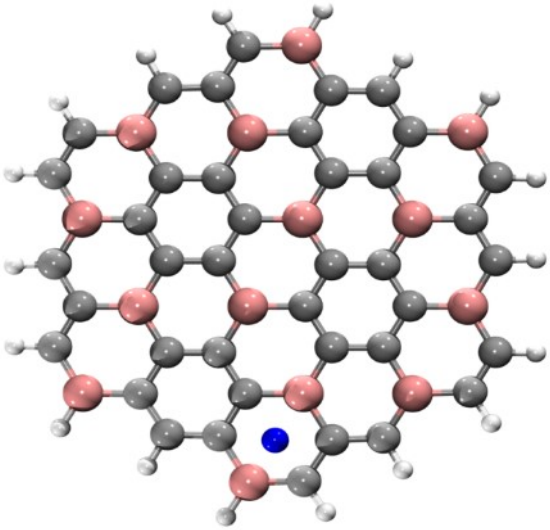


Na@BC-F

Na@BC nanosheet



Na@BC-G



Na@BC-H

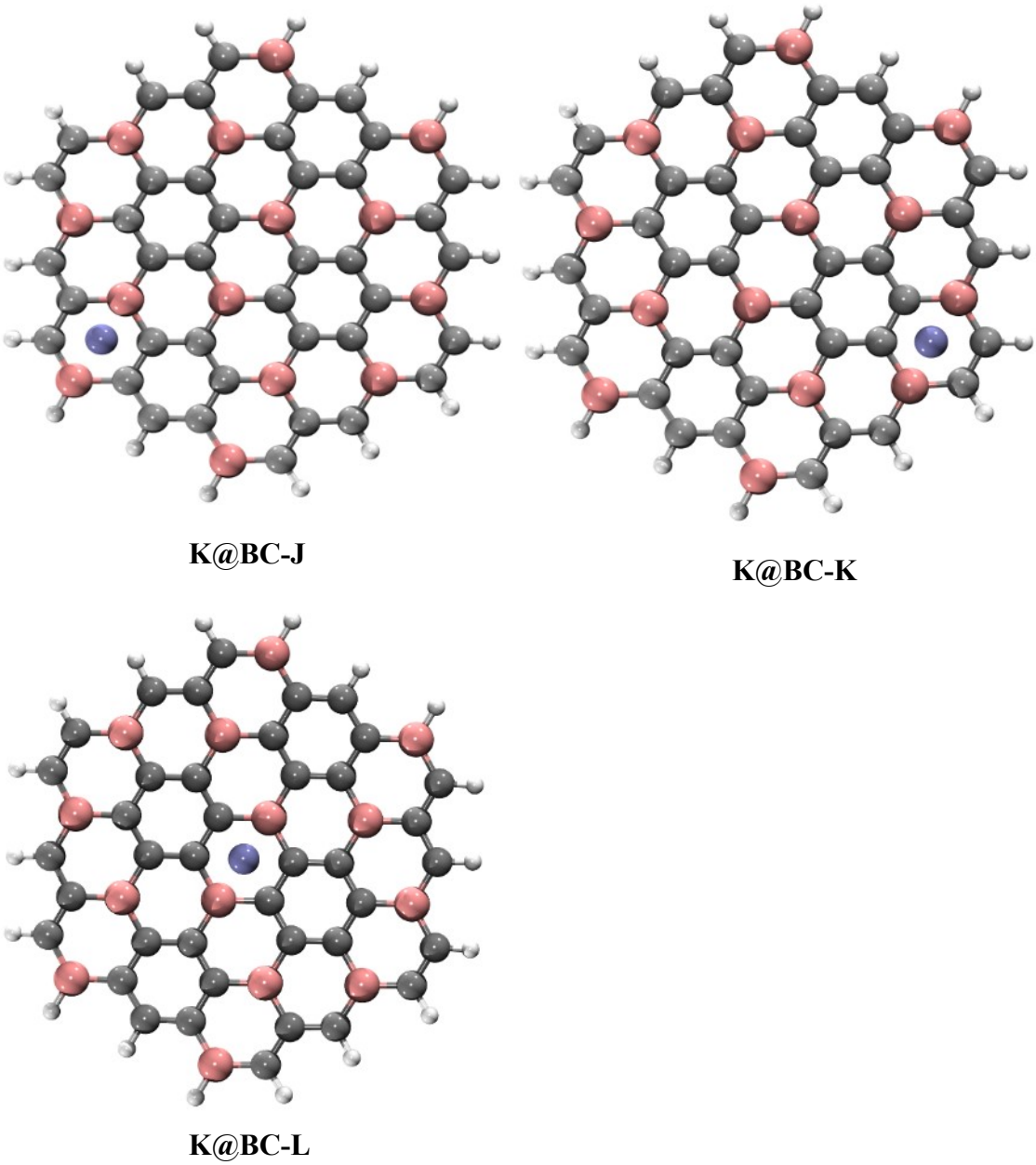
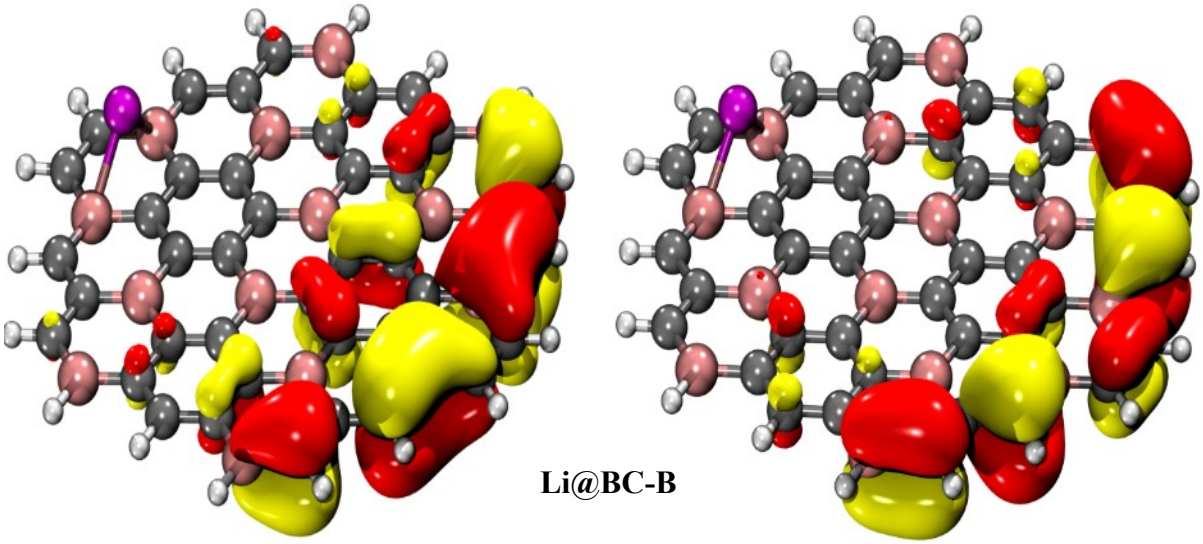


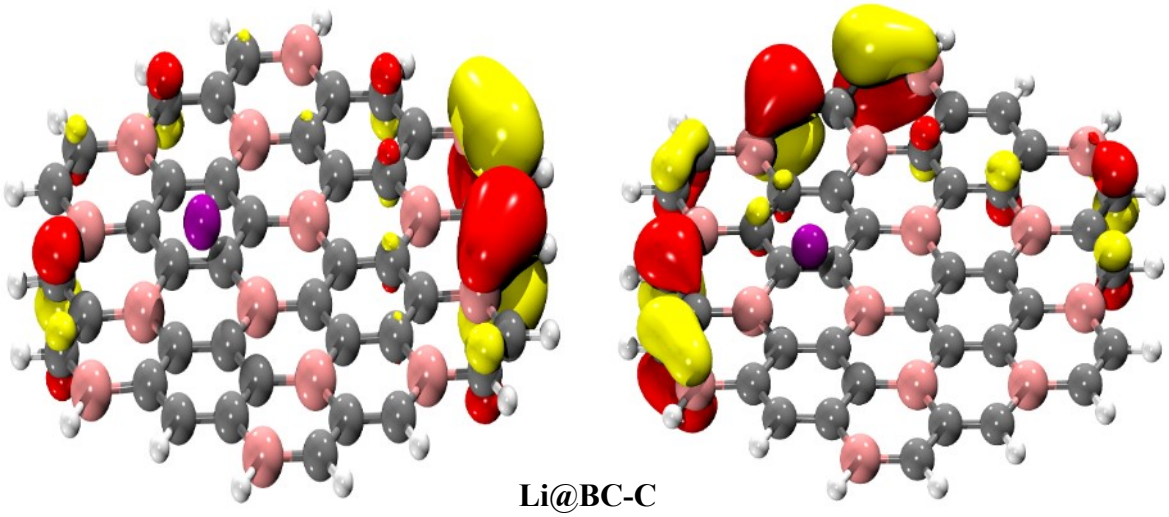
Fig.S1. Optimized structures of BC nanosheet doped with alkali metals Li@BC (B-D), Na@BC (F-H) and K@BC (J-L)

Li@BC nanosheet

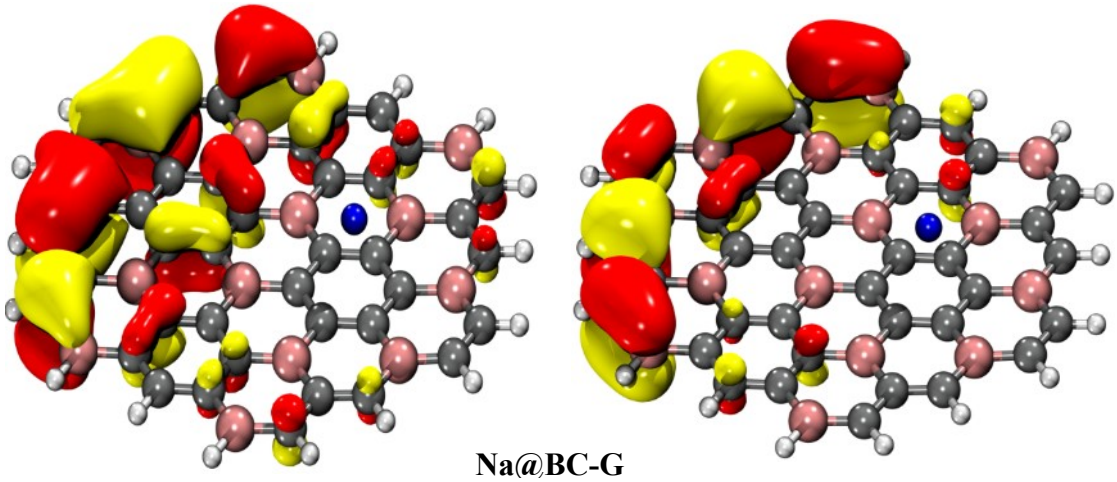
HOMO **LUMO**



Li@BC-B

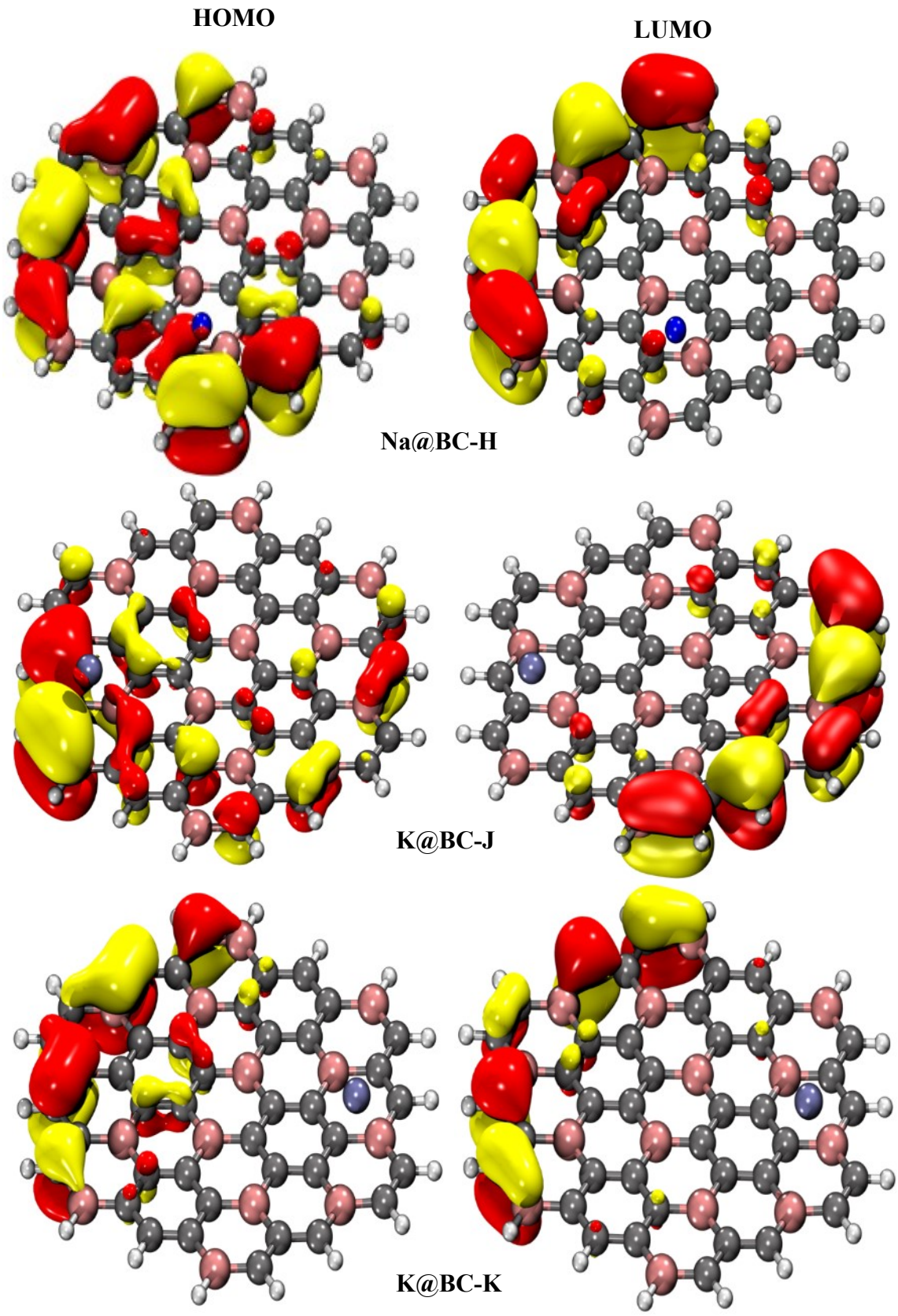


Li@BC-C



Na@BC-G

Na@BC nanosheet



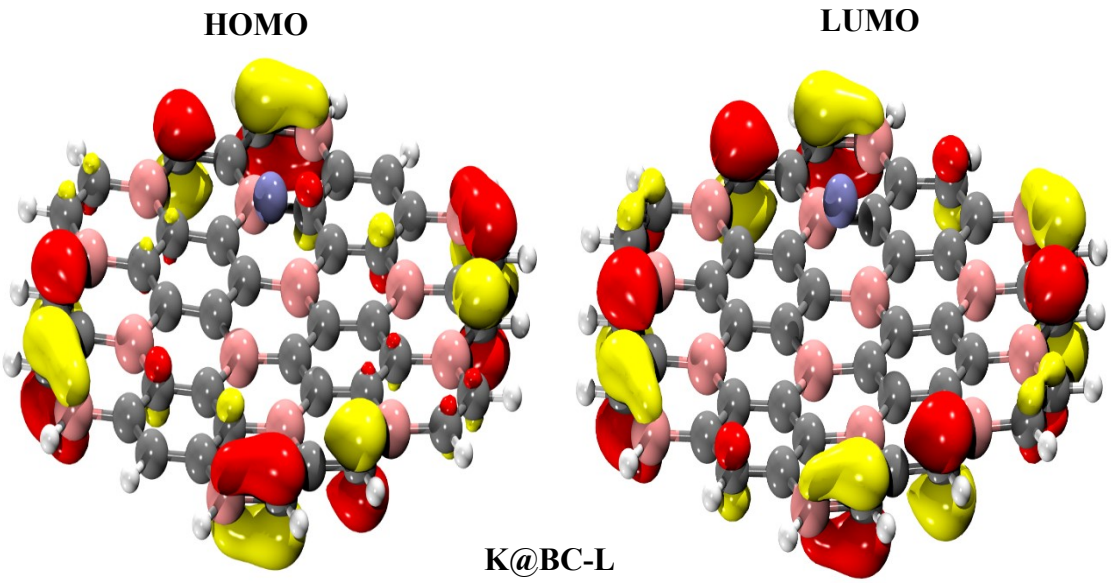
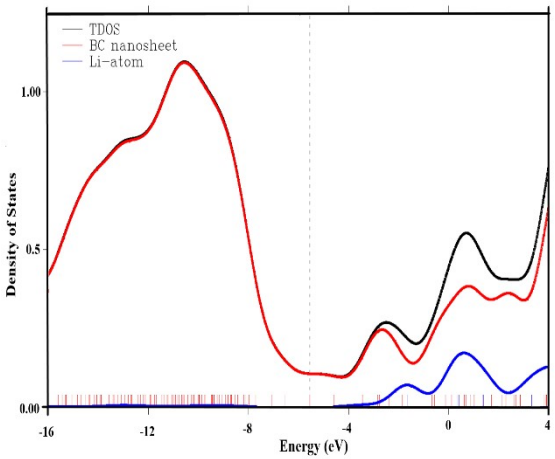
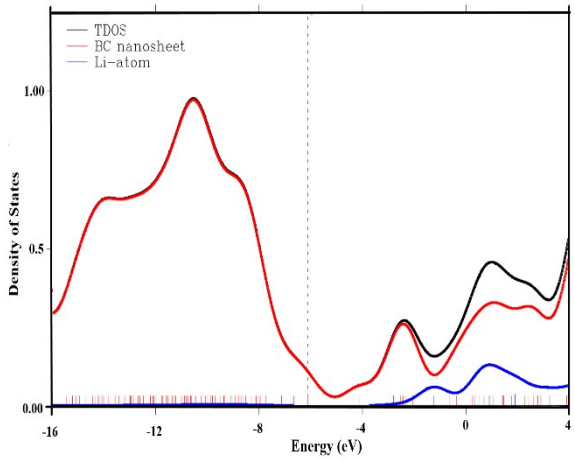
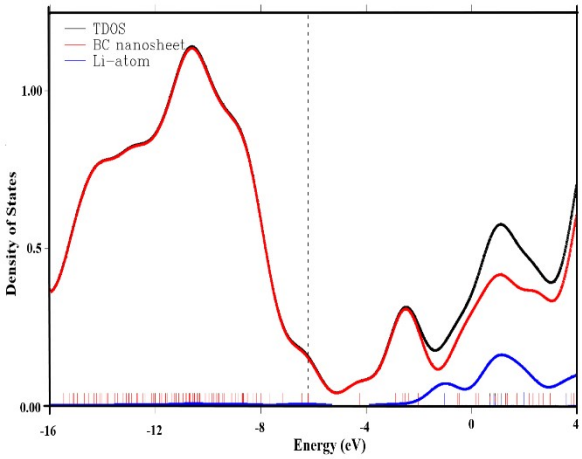


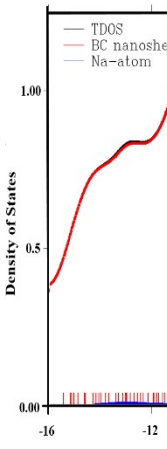
Fig.S2. HOMO and LUMO of BC nanosheet doped with alkali metals Li@BC (B-D), Na@BC (F-H) and K@BC (J-L)


TDOS
BC nanosheet
Li-atom
Density of States
Energy (eV)

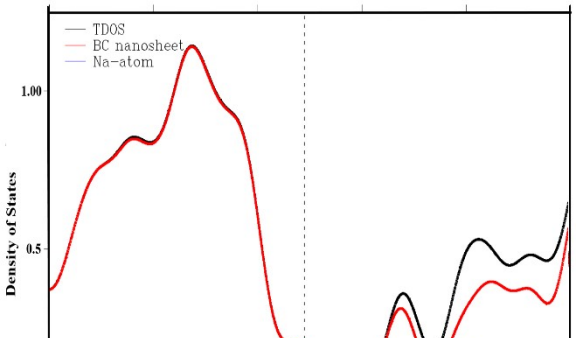

TDOS
BC nanosheet
Li-atom
Density of States
Energy (eV)

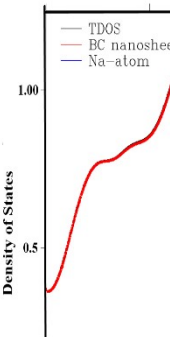

TDOS
BC nanosheet
Li-atom
Density of States
Energy (eV)

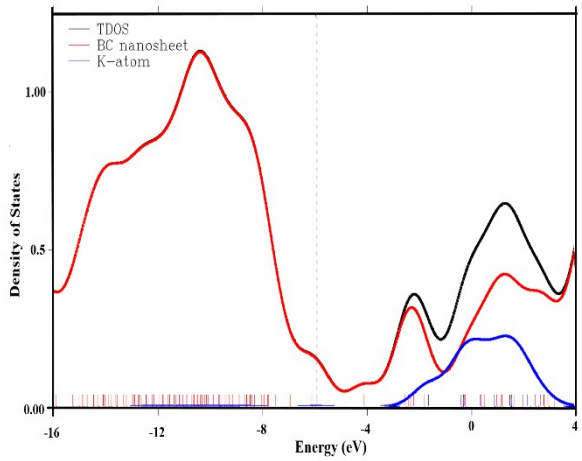
Li@BC-B


TDOS
Na-atom
Density of States

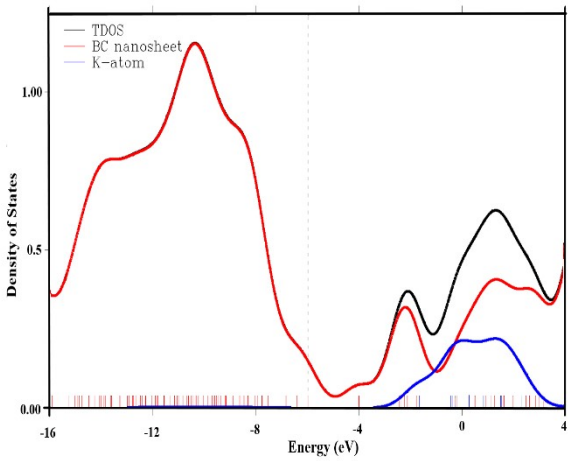
Li@BC-D


TDOS
BC nanosheet
Na-atom
Density of States

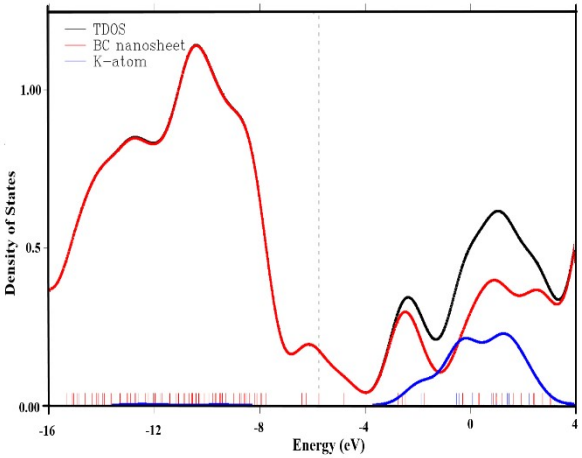

TDOS
Na-atom
Density of States



K@BC-J



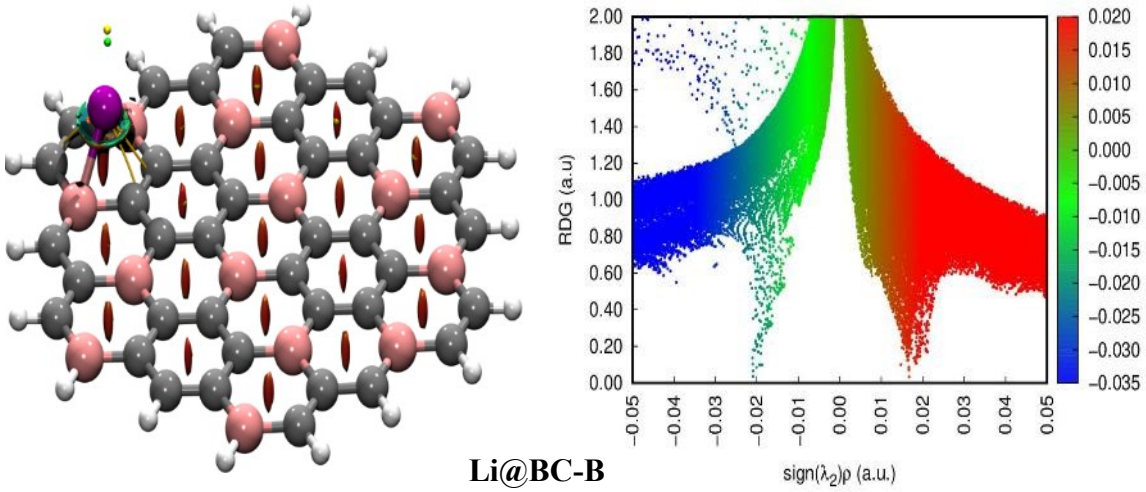
K@BC-K



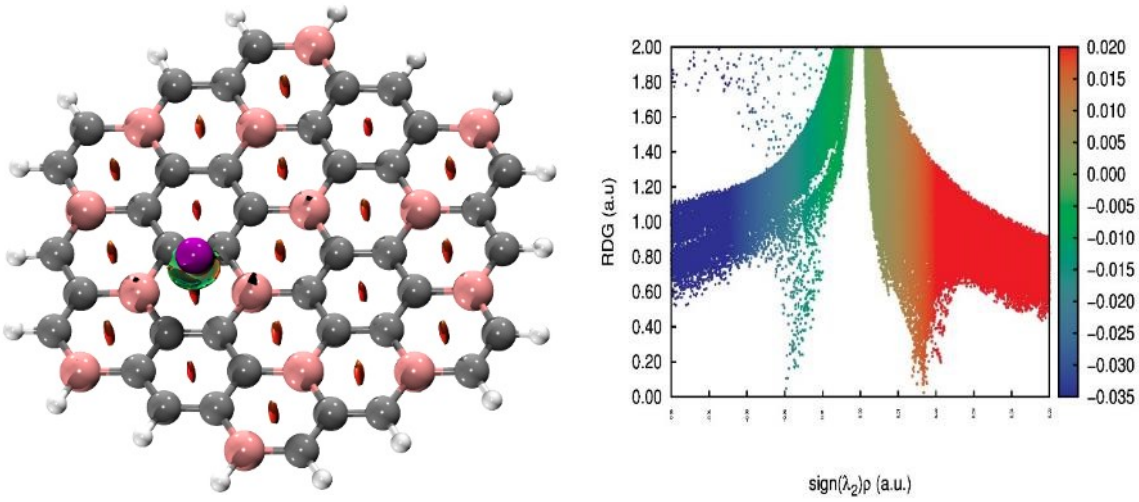
K@BC-L

Fig.S3. PDOS and TDOS of BC nanosheet doped with alkali metals Li@BC (B-D), Na@BC (F-H) and K@BC (J-L)

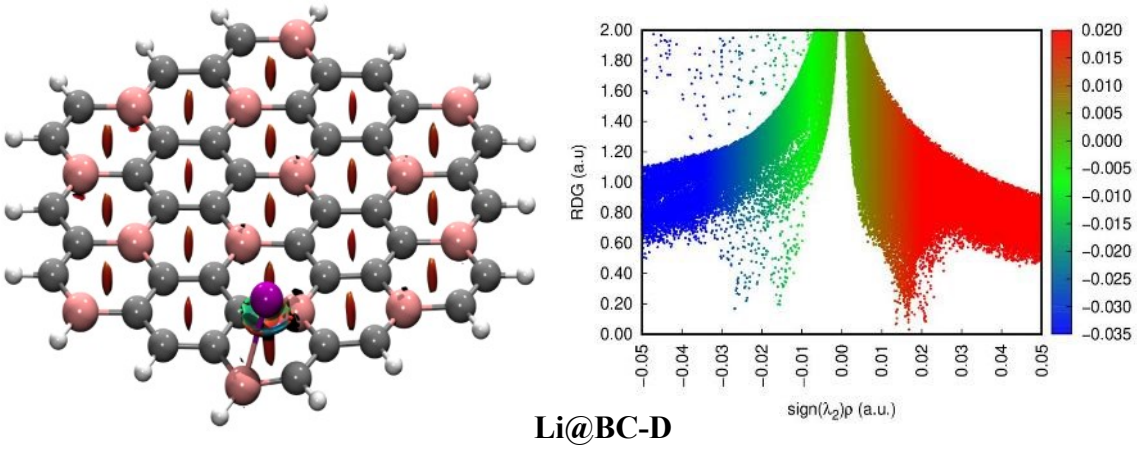
3D-isosurface **2D-RDG**



Li@BC-B

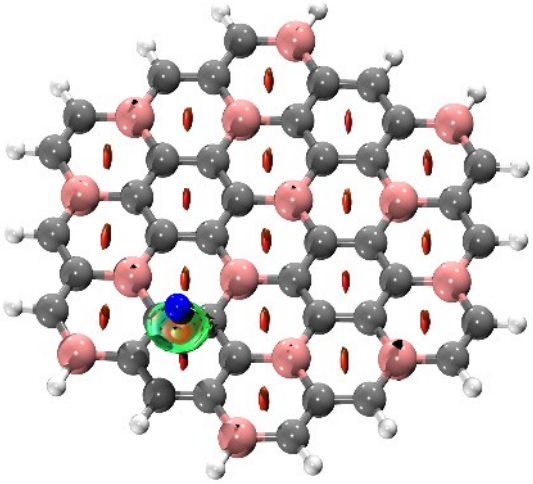


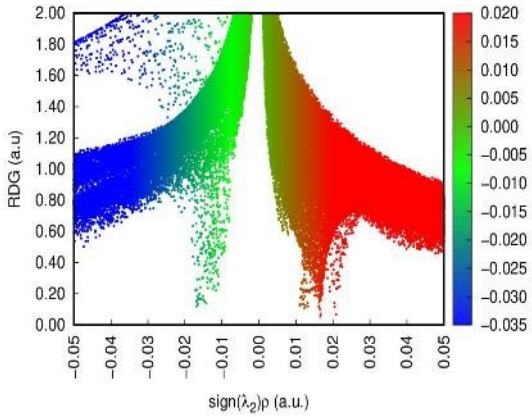
Li@BC-C



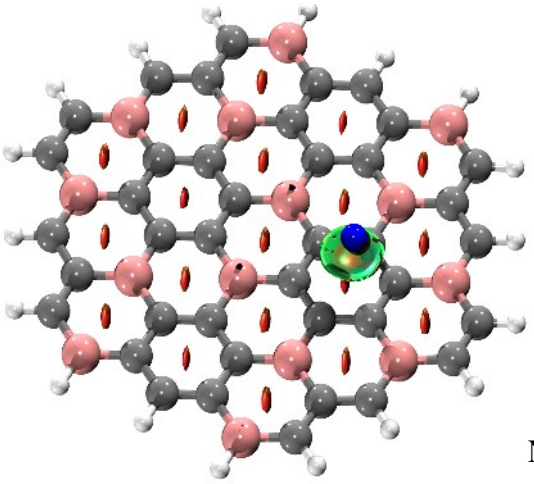
Li@BC-D

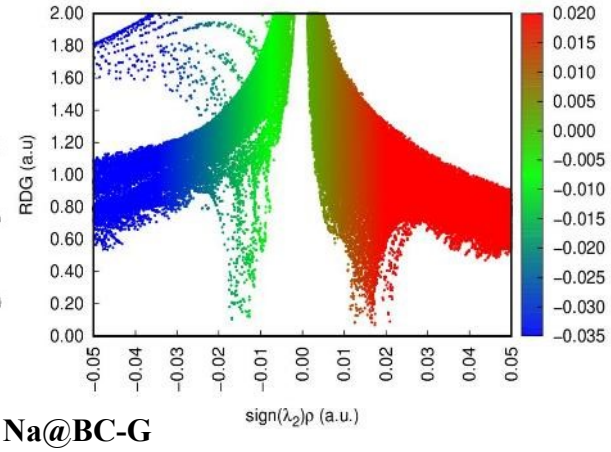
3D-isosurface **2D-RDG**



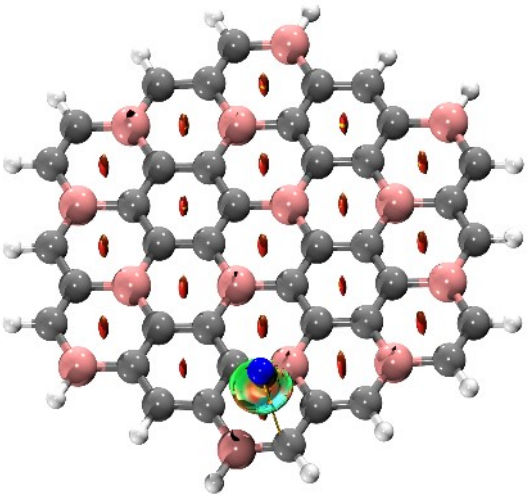


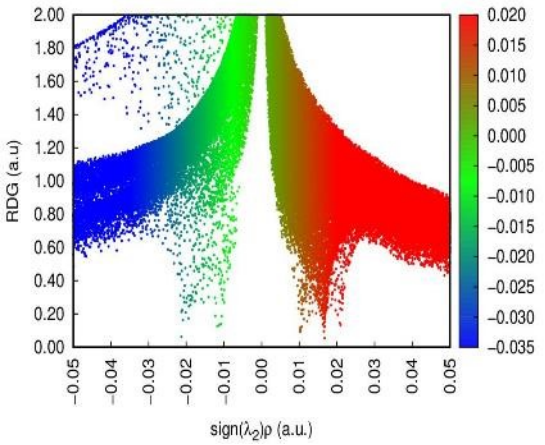
Na@BC-F





Na@BC-G





Na@BC-H

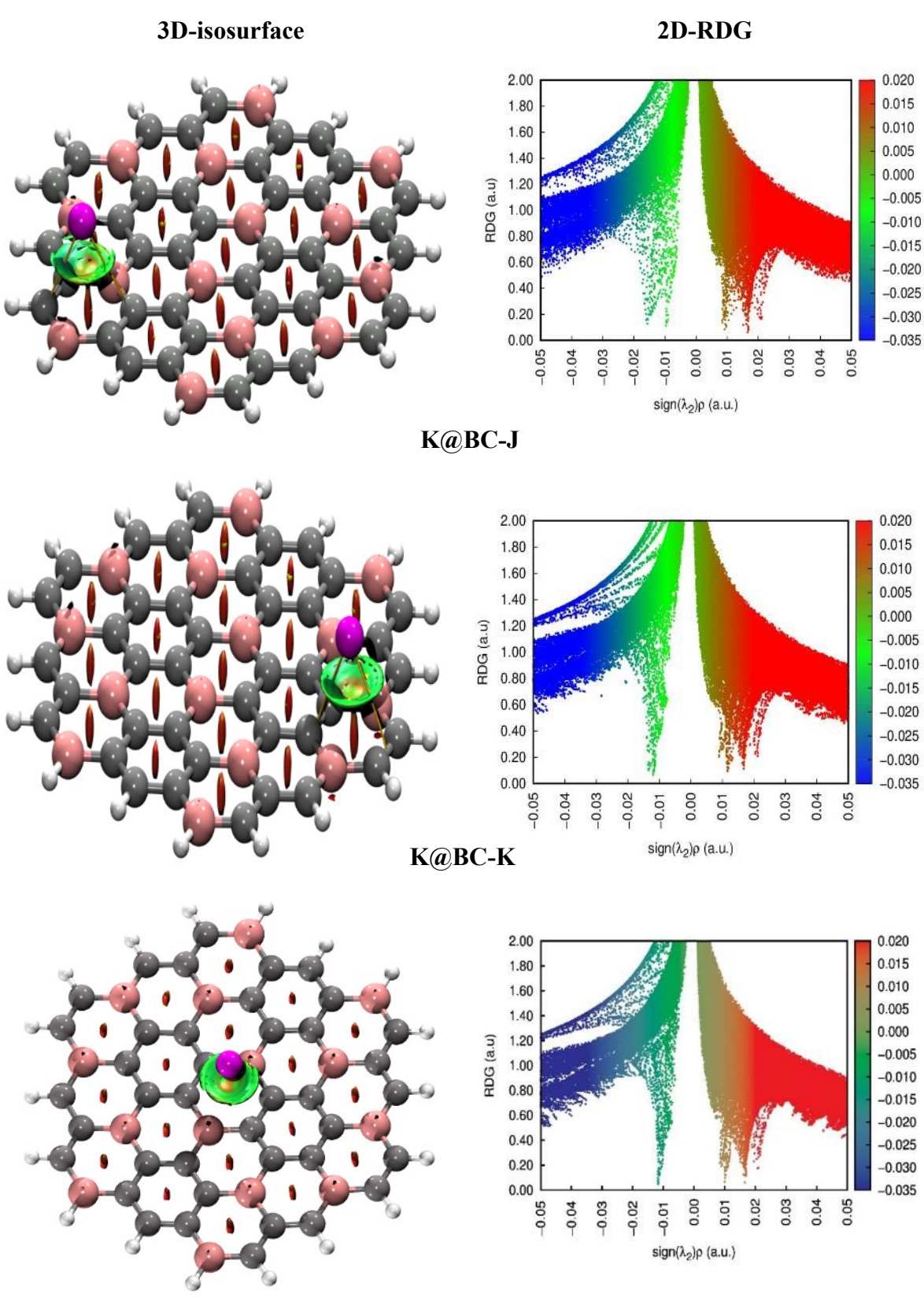
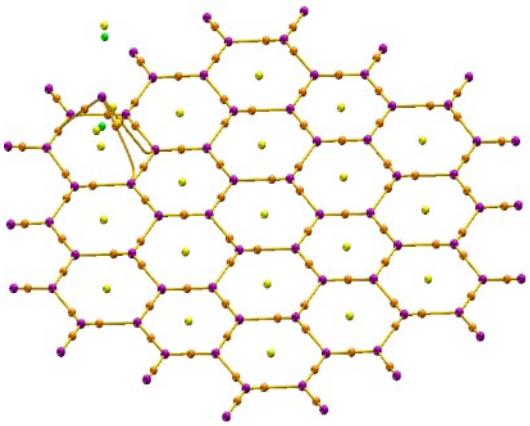
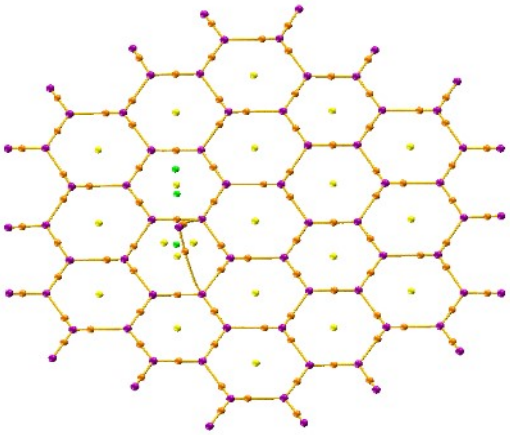


Fig.S4. NCI analysis (3D-isosurface and 2D-RDG graphs) of BC nanosheet doped with alkali metals Li@BC (B-D), Na@BC (F-H) and K@BC (J-L) isomers

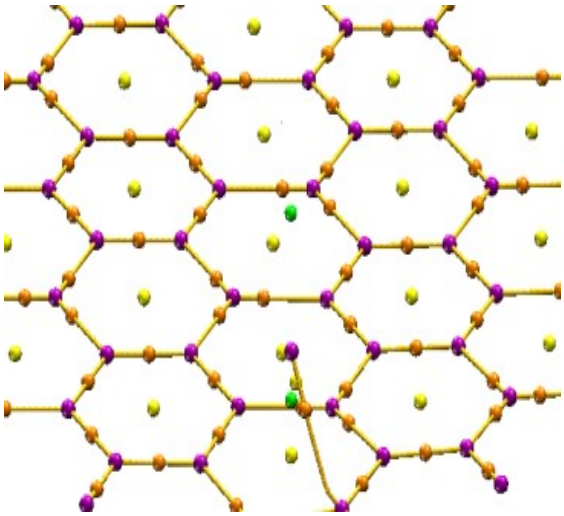
Li@BC nanosheet



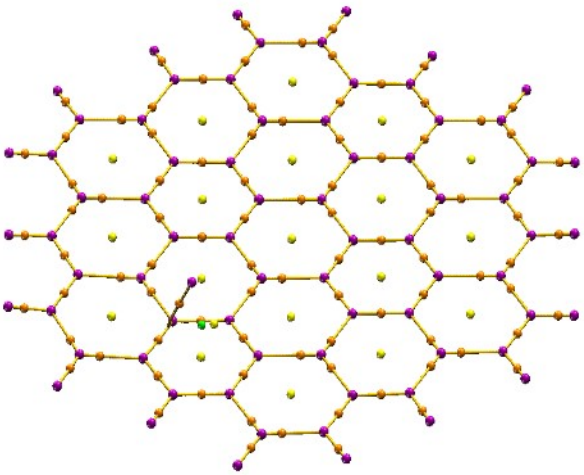
Li@BC-B



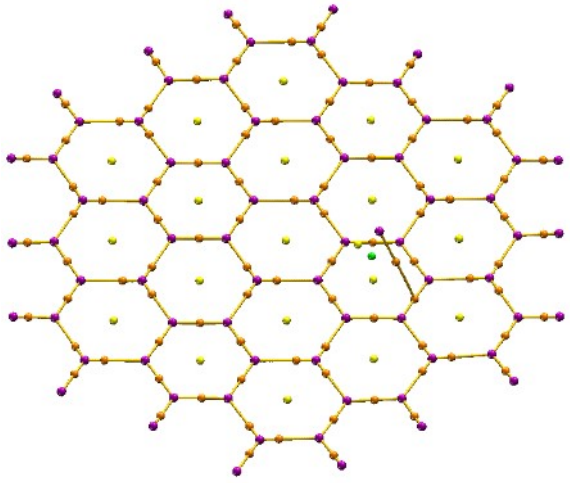
Li@BC-C



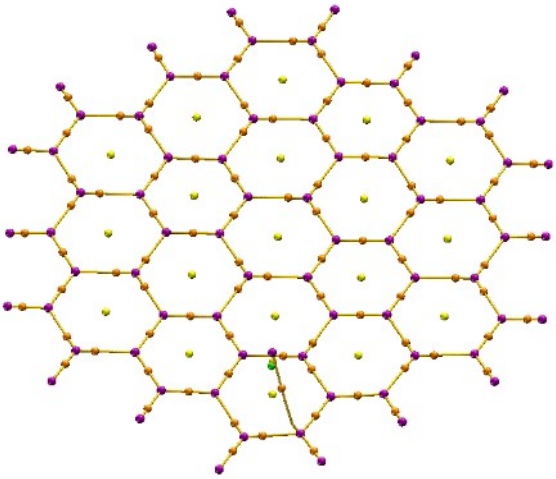
Li@BC-D



Na@BC-F

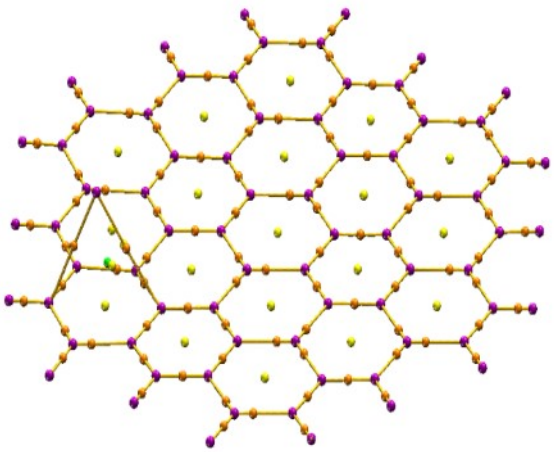


Na@BC-G

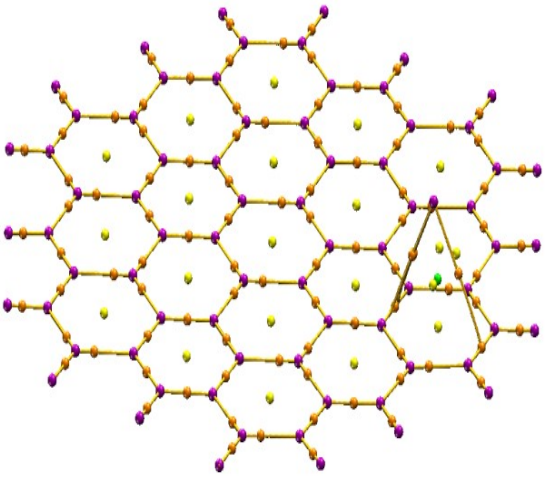


Na@BC-H

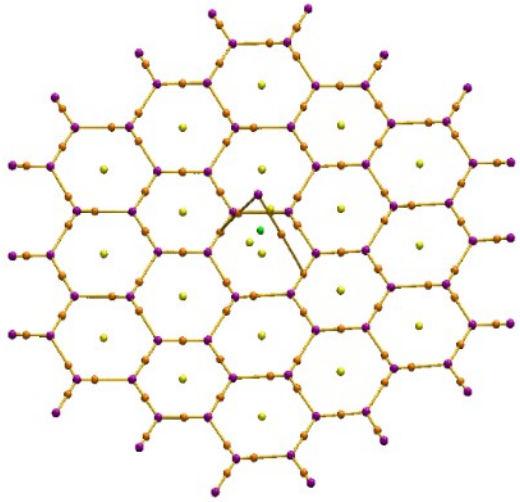
Na@BC nanosheet



K@BC-J



K@BC-K



K@BC-L

Fig.S5. QTAIM topological structures of BC nanosheet doped with alkali metals Li@BC (B-D), Na@BC (F-H) and K@BC (J-L) isomers

Table S1: Comparison table of previously reported β_o values to the current study

Sr No.	Complex	Level of Theory	Maximum β_o values (au)	References
1	Li@BC-C	M062X/6-31G(d,p)	3.11×10^5	Current study
2	Para-nitroaniline (*p*-NA)	M062X/6-31G(d,p)	1.0×10^3	[1]
3	Alkali metal doped Al-BN/P-BN nanosheets	M062X/6-31+G(d)	6.1×10^4	[2]
4	M@SiCNs	B3LYP/6-31g(d)	7.7×10^4	[3]
5	M@GeC nanoflakes	M062X/6-31G(d,p)	3.4×10^4	[4]
6	K-exo-R6	M062X/6-311++G(d,p)	4.2×10^3	[5]
7	K@C_2N	B3LYP/6-31G(d,p)	8.02×10^4	[6]

References:

[1] S. Muhammad, R.A. Shehzad, J. Iqbal, A.G. Al-Sehemi, M. Saravanabhavan, M. Khalid, Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of para-nitroaniline, Journal of Theoretical and Computational Chemistry 18(06) (2019) 1950030.

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[5] S. Abdolahi Joneghani, Z. Biglari, A. Gholipour, Alkali Metal Doping for Enhancement of Nonlinear Optical Properties of Dicyclopenta[4,3,2,1-ghi:4′,3′,2′,1′-pqr]perylene: A New Bowl-Shaped Fragment of Fullerene C70, Journal of Inorganic and Organometallic Polymers and Materials 31(2) (2021) 648-658.

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