

2D BN-Biphenylene: Structure Stability and Properties Tunability with DFT Perspective

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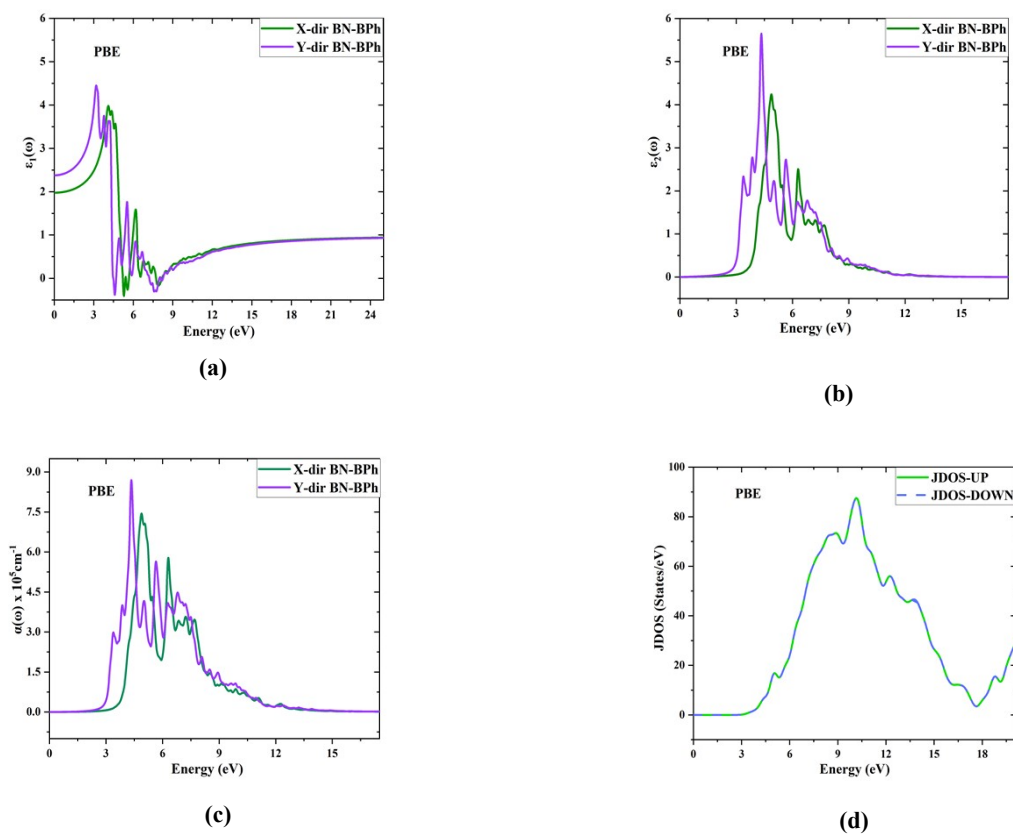
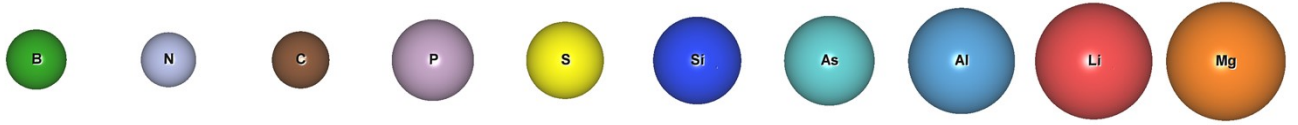
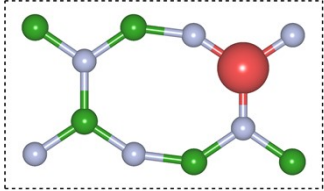


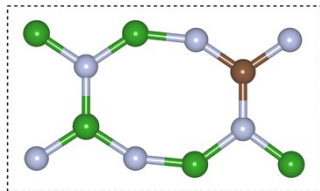
Fig. S1: Optical properties of BN-BPh sheet with PBE functional: (a) real part of dielectric constant, (b) imaginary part of dielectric constant, (c) absorption coefficient (d) Joint density of states.



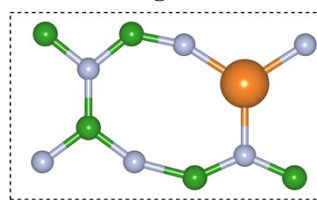
1. LiB_5N_6



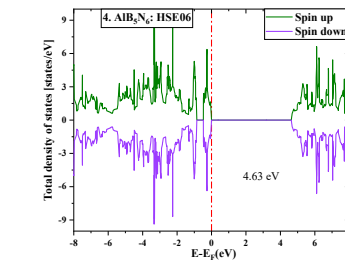
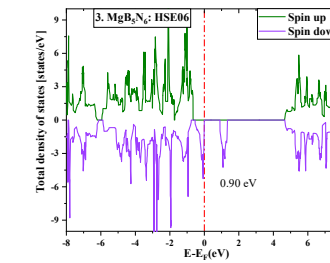
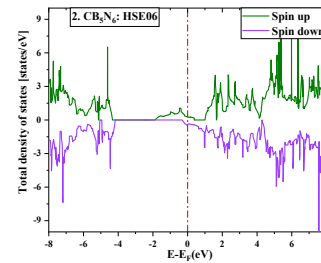
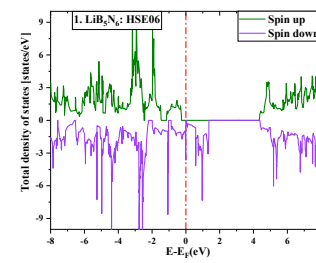
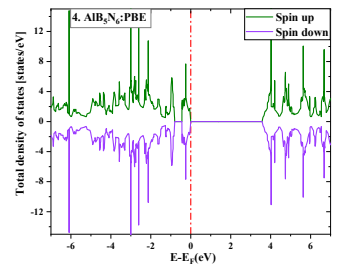
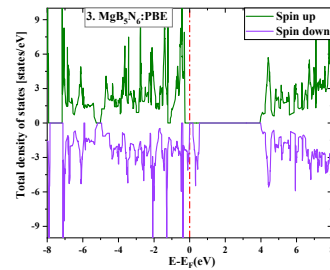
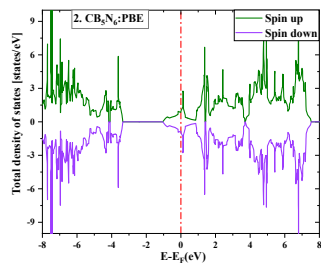
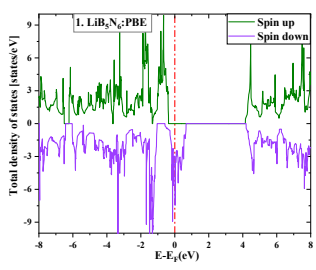
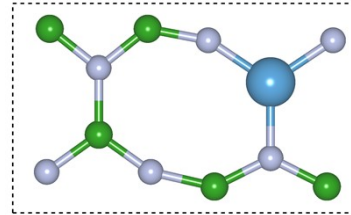
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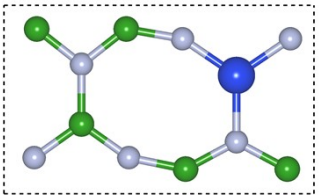
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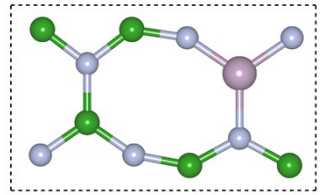
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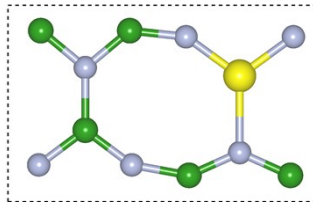
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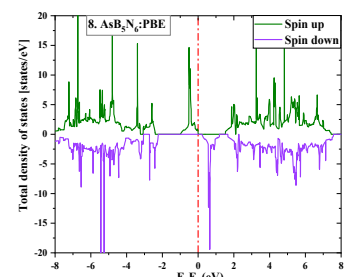
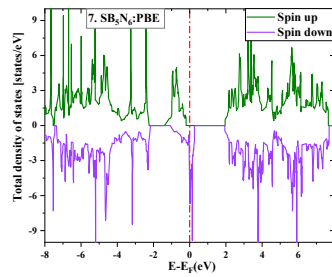
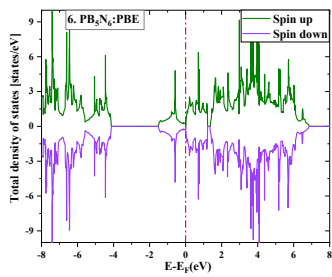
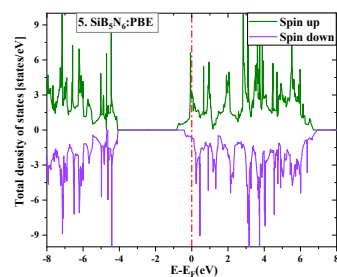
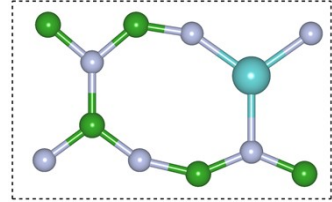
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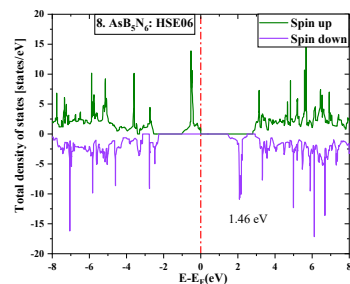
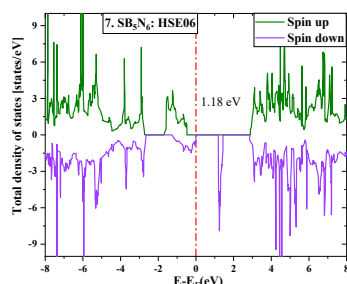
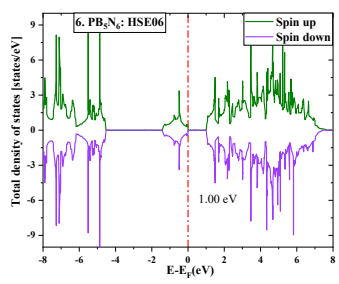
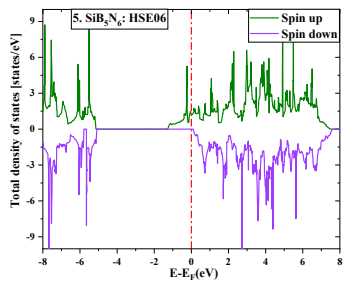


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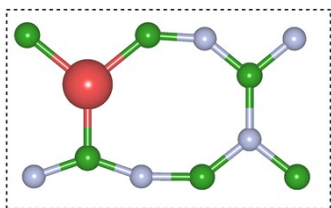


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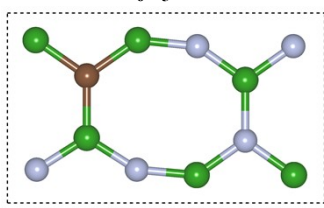




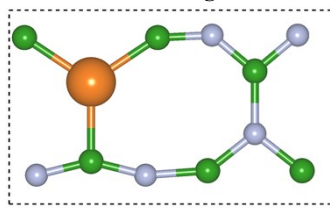
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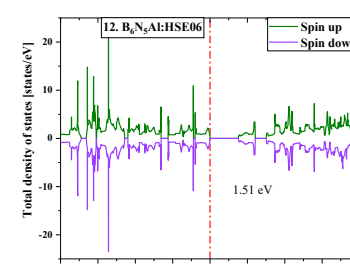
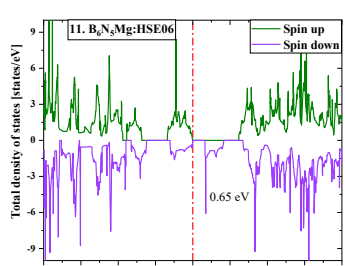
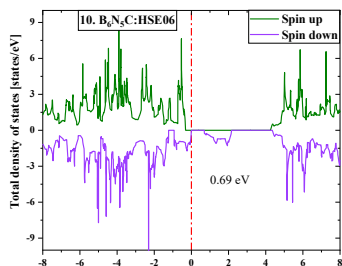
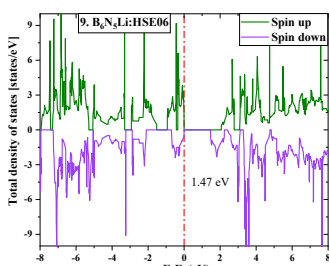
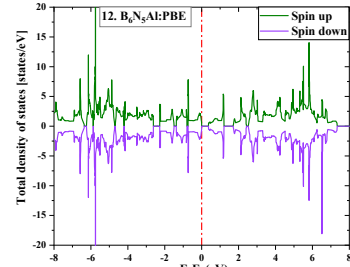
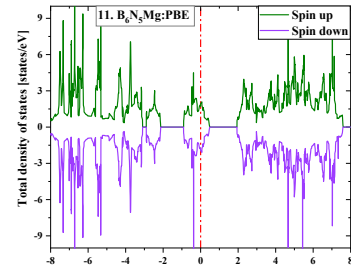
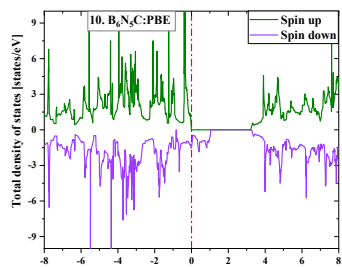
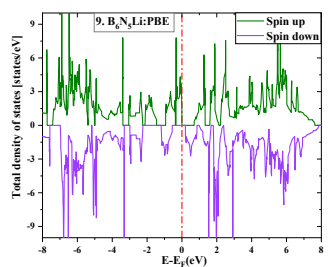
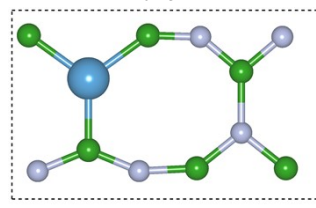
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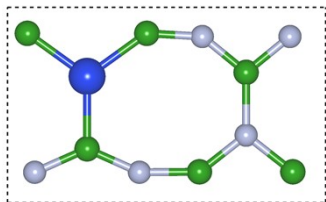
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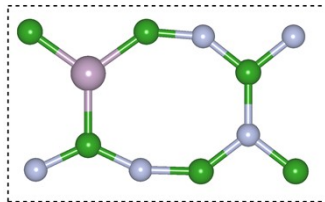
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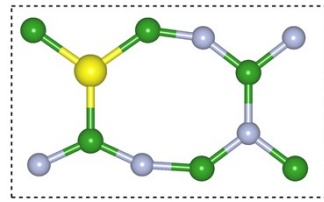
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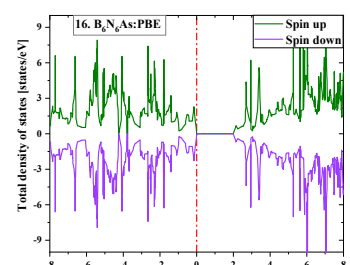
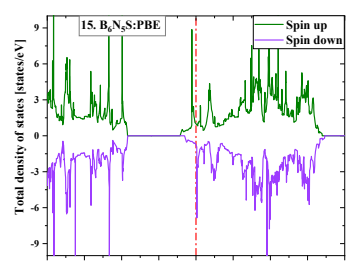
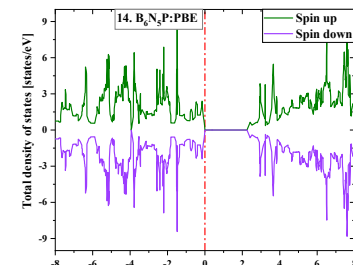
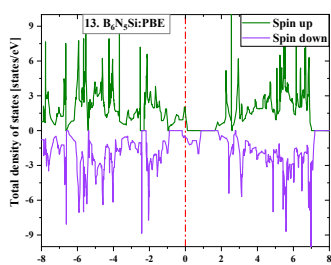
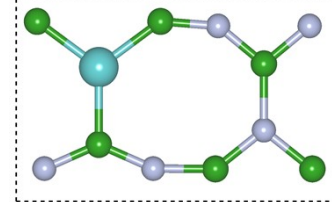
14. B_6N_5P



15. B_6N_5S



16. B_6N_5As



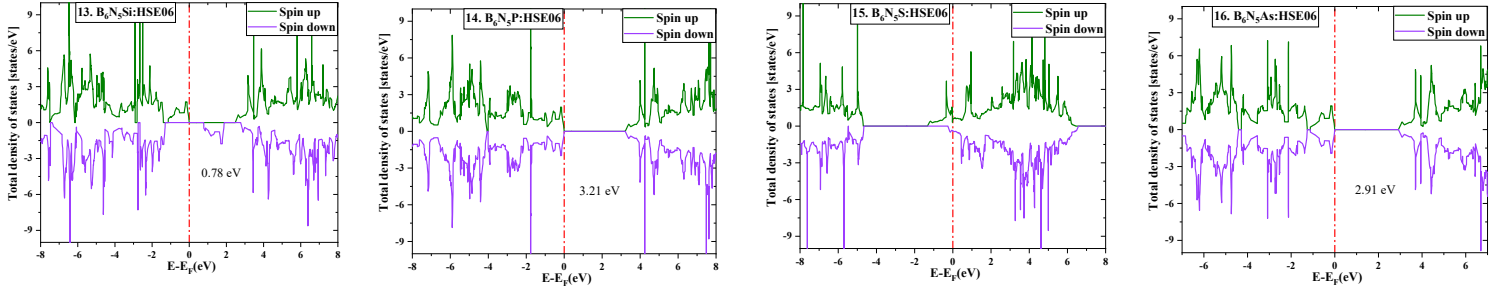
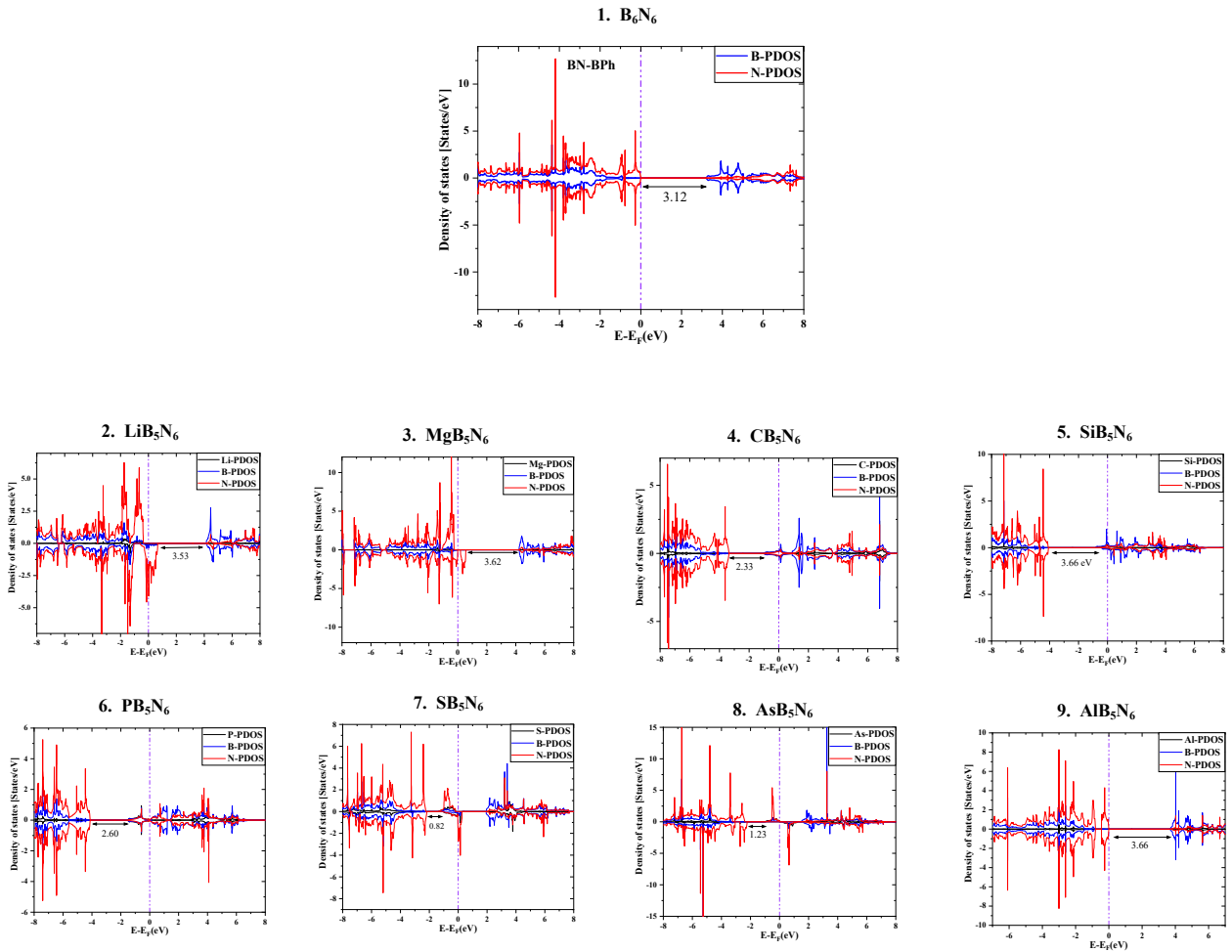


Fig. S2: Geometrically optimized unit cell of Li, C, Mg, Al, Si, P, S, As atom substitute to B and N atom in BN-BPh unit cell along their electronic structure. Below the optimized structure of external atom substituted unit cell, its total density of states with PBE and HSE06 functional are plotted in first and second row. We have used notations: 1. legend for atoms with elements name on their spheres are shown 2. N.name-of-unit-cell, N.name-of-unit-cell:PBE and N.name-of-unit-cell:HSE06 represents the structure-name, DOS with PBE and DOS with HSE06, where N serial number of a structure.



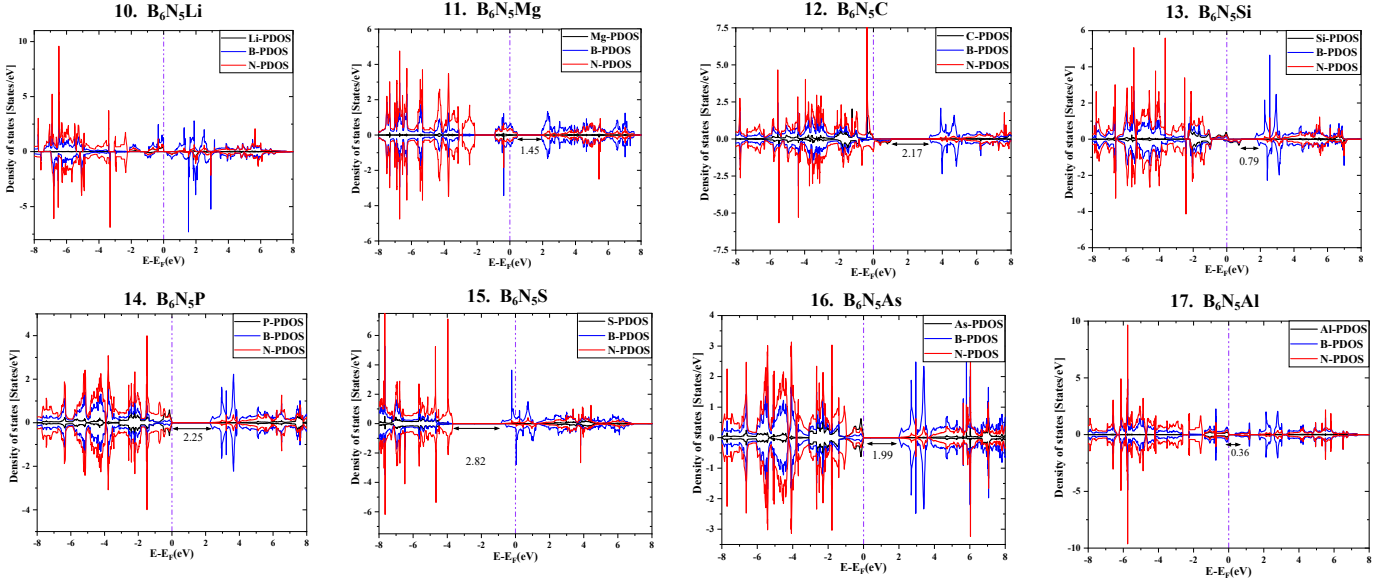


Fig. S3: Partial density of states (PDOS) of atoms, B, N and X in X-doped BN-BPh. Where X are Li, Mg, C, Si, P, S, As and Al substituted to B and N atom of BN-BPh sheet. The X substituted to B and N atom of BN-BPh are plotted in first and second column.

Table S1: Optimized structure of BN-BPh:

```

Unit_cell:B6N6
1.0000000000000000
 7.6580370324993998  -0.0000000000000000  0.0000000000000000
-0.0000000000000000  4.5530028432465341  0.0000000000000000
 0.0000000000000000  0.0000000000000000  15.0000000000000000
  B      N
  6      6
Direct
0.7500000000000000  0.6421894712788402  0.5000000000000000
0.2500000000000000  0.3578105287211599  0.5000000000000000
0.4051488445350434  0.8580607942538511  0.5000000000000000
0.9051488445350425  0.1419392057461483  0.5000000000000000
0.0948511554649570  0.8580607942538511  0.5000000000000000
0.5948511554649575  0.1419392057461483  0.5000000000000000
0.2500000000000000  0.6792660726147466  0.5000000000000000
0.7500000000000000  0.3207339273852544  0.5000000000000000
0.9060261380288906  0.8169439333960340  0.5000000000000000
0.4060261380288901  0.1830560666039664  0.5000000000000000
0.5939738619711094  0.8169439333960340  0.5000000000000000
0.0939738619711095  0.1830560666039665  0.5000000000000000

```

Table S2: Irreducible representation (ir-label) of modes of BN-BPh system

S.N.	Frequency (cm ⁻¹)	ir-label
1	87.962	Au
2	135.099	B3g
3	237.882	B1g
4	252.617	B3g
5	279.402	B2u
6	440.635	Ag
7	477.803	B2g
8	515.993	B3u
9	535.478	B1g
10	574.160	B3g
11	617.088	B2u
12	693.082	B3g
13	695.575	Au
14	738.721	B2g
15	750.018	B1u
16	757.821	B2u
17	823.519	Ag
18	827.790	B2g
19	892.812	B3u
20	935.706	B2g
21	956.189	B1u
22	968.554	Ag
23	1,097.046	B3u
24	1,186.030	Ag
25	1,194.250	B3u
26	1,210.190	B1u
27	1,281.595	B1u
28	1,300.575	Ag
29	1,310.804	B3u
30	1,409.426	B2g
31	1,451.775	Ag
32	1,474.385	B2g
33	1,495.340	B1u

Table S3: Intensity peak table of Infrared and Raman spectrum for BN-BPh.

S.N.	Frequency (cm ⁻¹)	IR-intensity	Raman-intensity
1	87.962	0.000	0.000
2	135.099	0.000	0.348
3	237.882	0.000	0.058
4	252.617	0.000	0.488
5	279.402	0.000	0.000
6	440.635	0.000	8.225
7	477.803	0.000	0.358
8	515.993	0.012	0.000
9	535.478	0.000	0.060
10	574.160	0.000	0.526
11	617.088	0.002	0.000
12	693.082	0.000	0.999
13	695.575	0.000	0.000
14	738.721	0.000	1.555
15	750.018	0.052	0.000
16	757.821	0.112	0.000
17	823.519	0.000	8.569
18	827.790	0.000	1.079
19	892.812	0.015	0.000
20	935.706	0.000	35.439
21	956.189	0.435	0.000
22	968.554	0.000	356.219
23	1,097.046	0.013	0.000
24	1,186.030	0.000	240.933
25	1,194.250	0.085	0.000
26	1,210.190	0.001	0.000
27	1,281.595	6.352	0.000
28	1,300.575	0.000	34.108
29	1,310.804	11.091	0.000
30	1,409.426	0.000	18.395
31	1,451.775	0.000	352.911
32	1,474.385	0.000	72.122
33	1,495.340	0.303	0.000

Table S4: Comparison of Bandtunning with doping of 8.33% and 4.16% by replacing B/N with external atoms (X) where X are C, Li, Mg, P, S, Si, Al and As.

S.N.	X	System [B-->X in BN-BPh]		System [N-->X in BN-BPh]	
		Bandgap (PBE) with 8.33 % doping	Bandgap (PBE) with 4.16 % doping	Bandgap (PBE) with 8.33 % doping	Bandgap (PBE) with 4.16 % doping
1.	Li	semi-metal	semi-metal	0.19	0.16
2.	C	metal	0.78	semimetal	Defect at 0.5 eV
3.	Mg	semi-metal	semi-metal	metal	0.39
4.	Al	3.57	3.24	0.37	0.37
5.	Si	metal	metal	metal	Defect at 0.45 eV
6.	P	metal	1.03	2.25	2.10
7.	S	semi-metal	semi-metal	metal	metal
8.	As	0.21	0.58	1.99	2.45