

Supporting Information

Designing Two Dimensional Dodecagonal Boron Nitride

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Table S- 1: Bader charge analysis on hexagonal boron nitride

No.	Atoms	X	Y	Z	Charge transfer
1	B	0.00	0.00	11.34	2.28
2	N	0.00	2.74	11.34	-2.28
3	B	4.75	0.00	11.34	2.28
4	N	4.75	2.74	11.34	-2.28
5	B	-2.37	4.11	11.34	2.28
6	N	-2.37	6.85	11.34	-2.28
7	B	2.37	4.11	11.34	2.28
8	N	2.37	6.85	11.34	-2.28

Table S- 2: Bader charge analysis on octagonal boron nitride

No.	Atoms	X	Y	Z	Charge transfer
1	B	2.79	0.92	11.34	-2.32
2	N	5.45	0.91	11.34	2.32
3	N	9.59	0.92	11.34	2.33
4	B	12.24	0.92	11.34	-2.33
5	N	0.92	2.98	11.34	2.33
6	B	0.92	5.64	11.34	-2.33
7	B	7.52	2.79	11.34	-2.33
8	N	7.52	5.44	11.34	2.32
9	N	2.99	7.52	11.34	2.33
10	B	5.64	7.51	11.34	-2.33
11	B	9.40	7.51	11.34	-2.32
12	N	12.05	7.51	11.34	2.32
13	N	7.52	9.58	11.34	2.33
14	B	7.52	12.24	11.34	-2.33
15	B	0.92	9.39	11.34	-2.32
16	N	0.92	12.05	11.34	2.33

Table S- 3: Bader charge analysis on dodecagonal boron nitride

No.	Atoms	X	Y	Z	Charge transfer
1	B	3.72	3.79	11.34	2.32
2	N	5.22	6.21	11.34	-2.31
3	B	7.88	6.07	11.34	2.32
4	N	10.15	7.63	11.34	-2.32
5	B	11.60	9.86	11.34	2.32
6	N	14.45	9.76	11.34	-2.33
7	N	4.92	1.42	11.34	-2.33

8	B	7.77	1.32	11.34	2.33
9	N	9.22	3.56	11.34	-2.33
10	B	11.50	5.12	11.34	2.32
11	N	14.15	4.98	11.34	-2.31
12	B	15.66	7.40	11.34	2.32

Figure S-1: DOS of hexagonal boron nitride

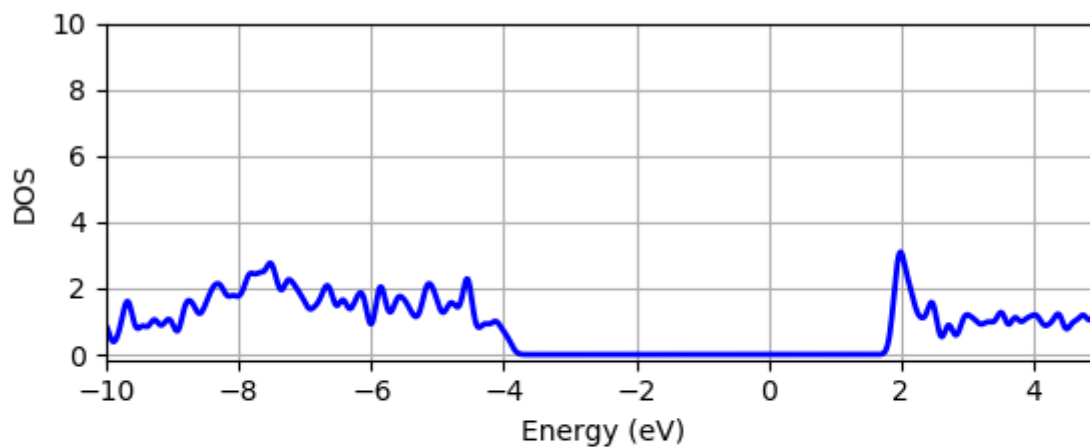


Figure S-2 : DOS of octagonal boron nitride

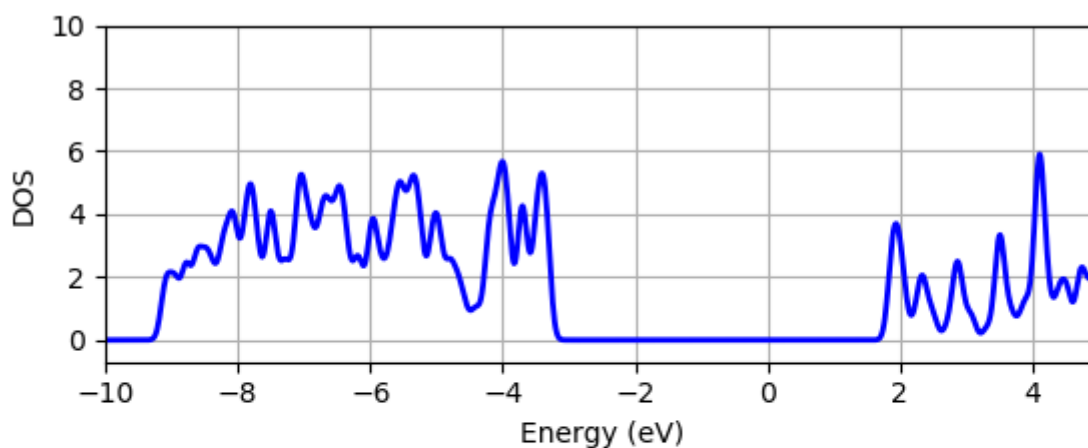


Figure S-3: DOS of dodecagonal boron nitride

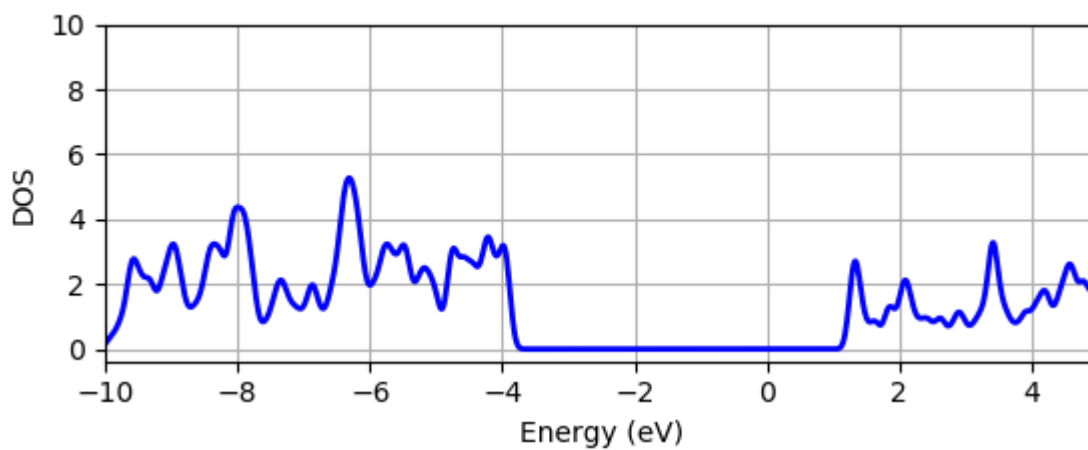


Figure S-4: PDOS of hexagonal boron nitride

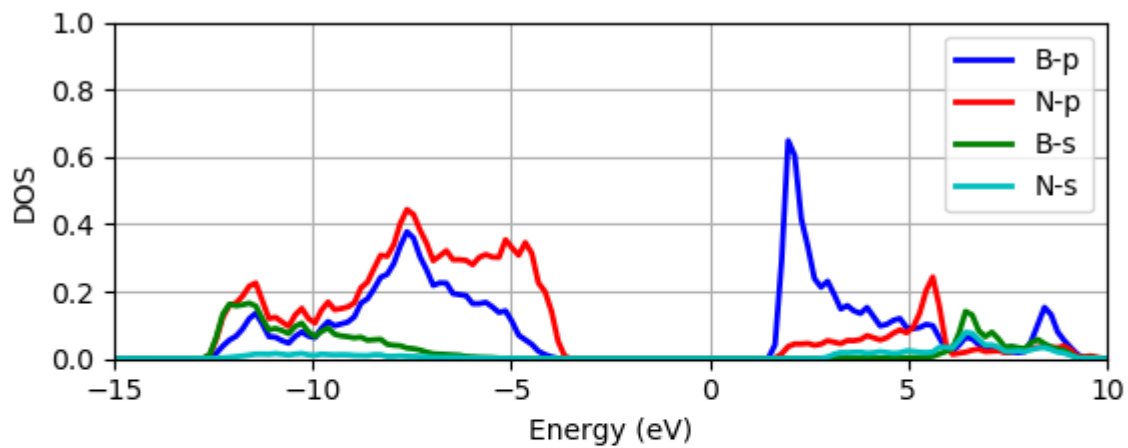


Figure S-5: PDOS of octagonal boron nitride

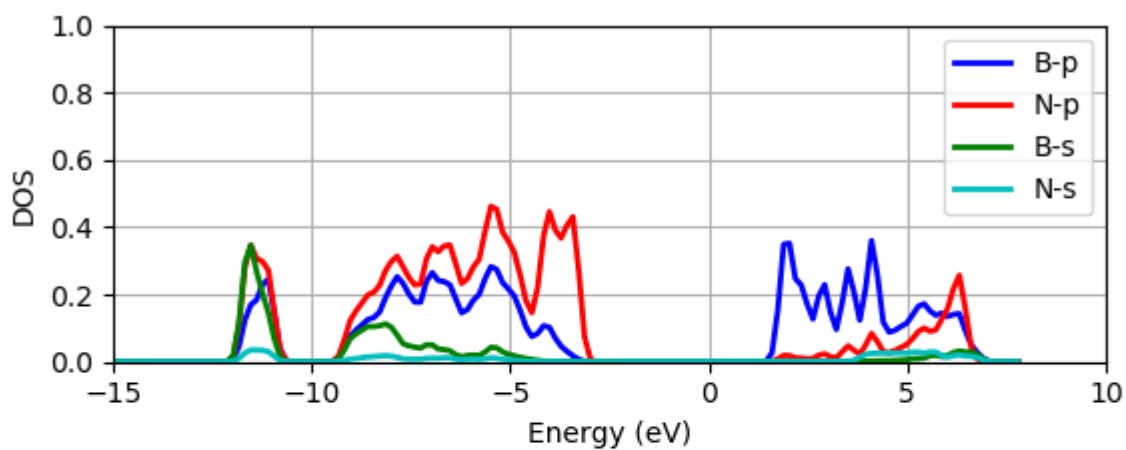


Figure S-6: PDOS of dodecagonal boron nitride

