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B-C-N hybrid porous sheet: An efficient metal-free visible-light absorption material

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In this work, the formation energy is defined as $E_f = \frac{E_{PG} - n_C\mu_C - n_H\mu_H - n_N\mu_N - n_B\mu_B}{n_C + n_H + n_N + n_B}$, where E_{PG} is the total energy of the porous graphene in unit cell, n_C, n_H, n_N, and n_B are the numbers of C, H, N, B atoms in PG, and the corresponding chemical potentials are $\mu_C = \frac{E_{graphene}}{n_C}$, $\mu_N = \frac{E_{N_2}}{2}$, $\mu_H = \frac{E_{H_2}}{2}$, $\mu_B = \frac{E_{rhombohedral\ \alpha-B_{12}\ crystal}}{n_B \text{ in rhombohedral } \alpha\text{-}B_{12} \text{ crystal}}$.

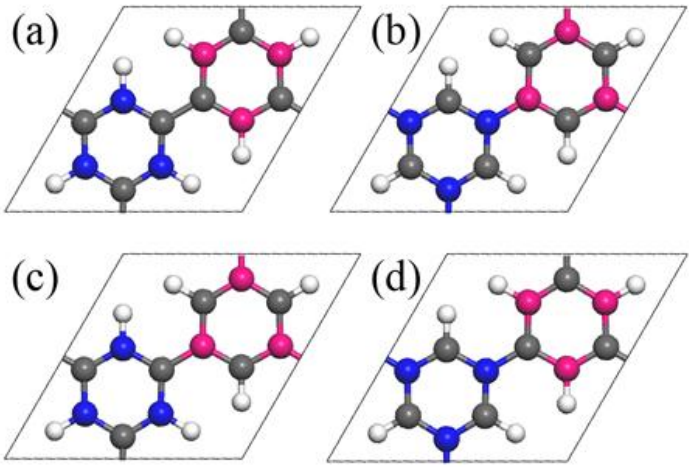

Figure S1. Four possible configurations of porous graphene doped by B and N atoms, with different hexagon-connecting bondings: (a) C-C bonding, (b) N-B bond, (c) C-B bond, (d) N-C bond. In which, (a) structure is the most favorable structure of the BN-PG, while the other three considered structures are less stable with higher energies by 1.66, 1.53, 3.95 eV, respectively.

Optimized fractional coordinates (in Å) of BN-PG (a)

a = 7.550 Å b = 7.550 Å c = 18 Å

α = 90° β = 90° γ = 120°

B	0.42633698	0.21552636	0.283333
B	0.77603073	0.21550146	0.283333
B	0.77600831	0.56521475	0.283333
C	0.5415145	0.09617049	0.283333
C	0.54148847	0.45005336	0.283333
C	0.89536443	0.45003128	0.283333

C	0.10945611	0.55711719	0.283333
C	0.43438402	0.55709047	0.283333
C	0.43437357	0.88203834	0.283333
H	0.14633701	0.30599573	0.283333
H	0.14635352	0.84515549	0.283333
H	0.68548546	0.8451545	0.283333
H	0.23882188	0.12180415	0.283333
H	0.86977763	0.12175383	0.283333
H	0.86972846	0.75271763	0.283333
N	0.22459086	0.46244501	0.283333
N	0.22457743	0.76692519	0.283333
N	0.52903363	0.7668958	0.283333

Optimized fractional coordinates (in Å) of BN-PG (b)

a = 7.676 Å b = 7.676 Å c = 18 Å

α = 90° β = 90° γ = 120°

B	0.54696588	0.10715922	0.283333
B	0.54696036	0.44455102	0.283333
B	0.88434951	0.44454678	0.283333
C	0.225251	0.4637427	0.283333
C	0.22524984	0.76626638	0.283333
C	0.52777661	0.76626515	0.283333
C	0.42927758	0.21701195	0.283333
C	0.77450145	0.21701251	0.283333
C	0.77449664	0.56223309	0.283333
H	0.14405783	0.30135068	0.283333
H	0.14405508	0.84746298	0.283333
H	0.69017054	0.84745598	0.283333
H	0.26425548	0.13450256	0.283333
H	0.85701129	0.13449985	0.283333
H	0.85700929	0.72725543	0.283333
N	0.11924964	0.56200527	0.283333
N	0.42951146	0.56200488	0.283333
N	0.42951352	0.87226457	0.283333

Optimized fractional coordinates (in Å) of BN-PG (c)

a = 7.752 Å b = 7.752 Å c = 18 Å

α = 90° β = 90° γ = 120°

B	0.54631073	0.10586459	0.283333
B	0.54631455	0.44519746	0.283333
B	0.88564588	0.445192	0.283333
C	0.11552732	0.56014151	0.283333

C	0.43137835	0.56013885	0.283333
C	0.43137913	0.87599153	0.283333
C	0.43293056	0.2188394	0.283333
C	0.77267268	0.21883939	0.283333
C	0.77267146	0.55857817	0.283333
H	0.15208979	0.31742501	0.283333
H	0.15209479	0.83942625	0.283333
H	0.6740944	0.83942287	0.283333
H	0.26793875	0.13634707	0.283333
H	0.85516511	0.13634067	0.283333
H	0.85516615	0.72357103	0.283333
N	0.2280144	0.46926328	0.283333
N	0.22801064	0.76350579	0.283333
N	0.52225831	0.76350613	0.283333

Optimized fractional coordinates (in Å) of BN-PG (d)

a = 7.524 Å b = 7.524 Å c = 18 Å

α = 90° β = 90° γ = 120°

B	0.42402616	0.21438892	0.283333
B	0.77712044	0.21437214	0.283333
B	0.77713886	0.56749891	0.283333
C	0.54219942	0.09763486	0.283333
C	0.54220753	0.44931631	0.283333
C	0.89387495	0.44930852	0.283333
C	0.22254474	0.45832521	0.283333
C	0.22254204	0.76897133	0.283333
C	0.53318845	0.7689697	0.283333
H	0.13992978	0.29310933	0.283333
H	0.13993573	0.8515825	0.283333
H	0.69840293	0.85157889	0.283333
H	0.23873029	0.12174587	0.283333
H	0.86977528	0.12173541	0.283333
H	0.86977121	0.75279136	0.283333
N	0.11433985	0.55954532	0.283333
N	0.43196971	0.55954556	0.283333
N	0.43196564	0.87717083	0.283333