Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information for

Electronic properties of *α*-Graphyne on hexagonal boron nitride and *α*-BNyne substrates

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Table S1. Structural properties of six emblematic configurations for *α*-GY/*h*-BN.

structure	lattice constant (Å)		interlayer distance (Å)	binding energy (meV/atom)
	a	b		
1	20.910	12.072	1.694	−121.636
2	21.067	12.163	1.996	−104.888
3	21.224	12.253	2.833	−89.363
4	21.380	12.344	3.335	−85.913
5	21.537	12.434	3.377	−84.520
6	21.694	12.525	3.392	−84.272

Table S2. Structural properties of six emblematic configurations for *α*-GY/*α*-BNy.

structure	lattice constant (Å) a = b	interlayer distance (Å)	binding energy (meV/atom)
1	6.970	3.354	−66.372
2	6.998	3.413	−65.121
3	7.026	3.485	−64.506
4	7.054	3.572	−64.082
5	7.082	3.569	−63.622
6	7.110	3.592	−63.187

Table S3. Bader charge and Net charge analysis of *α*-GY/*h*-BN. Here the positive denotes charge depletion, while the negative denotes excess charge accumulation.

Atom number	Atom species	Bader charge (e)	Net charge (e)
1	C	3.6326	0.3674
2	C	3.6038	0.3962
3	C	3.7317	0.2683

4	C	3.6309	0.3691
5	C	3.7032	0.2968
6	C	3.7397	0.2603
7	C	3.7201	0.2799
8	C	3.6967	0.3033
9	C	3.7155	0.2845
10	C	3.6932	0.3068
11	C	3.7216	0.2784
12	C	3.6265	0.3735
13	C	4.1768	-0.1768
14	C	3.8078	0.1922
15	C	3.9755	0.0245
16	C	3.9809	0.0191
17	C	4.1618	-0.1618
18	C	4.1872	-0.1872
19	C	4.3862	-0.3862
20	C	3.6505	0.3495
21	C	4.4659	-0.4659
22	C	3.9869	0.0131
23	C	3.9654	0.0346
24	C	3.8571	0.1429
25	C	4.1163	-0.1163
26	C	4.0348	-0.0348
27	C	3.9124	0.0876
28	C	3.9895	0.0105

29	C	3.9599	0.0401
30	C	4.3867	-0.3867
31	C	3.8061	0.1939
32	C	4.5498	-0.5498
33	C	3.7738	0.2262
34	C	4.2814	-0.2814
35	C	4.2218	-0.2218
36	C	4.3111	-0.3111
37	C	4.0202	-0.0202
38	C	4.4009	-0.4009
39	C	4.2144	-0.2144
40	C	4.2384	-0.2384
41	C	4.024	-0.024
42	C	4.1277	-0.1277
43	C	4.1078	-0.1078
44	C	4.2138	-0.2138
45	C	4.2508	-0.2508
46	C	4.2063	-0.2063
47	C	4.2505	-0.2505
48	C	3.7958	0.2042
49	N	7.1746	-2.1746
50	N	7.1918	-2.1918
51	N	7.2035	-2.2035
52	N	7.1945	-2.1945
53	N	7.1945	-2.1945

54	N	7.1977	-2.1977
55	N	7.2014	-2.2014
56	N	7.2	-2.2
57	N	7.2049	-2.2049
58	N	7.1998	-2.1998
59	N	7.2033	-2.2033
60	N	7.1897	-2.1897
61	N	7.1847	-2.1847
62	N	7.1859	-2.1859
63	N	7.2035	-2.2035
64	N	7.2009	-2.2009
65	N	7.2074	-2.2074
66	N	7.1933	-2.1933
67	N	7.1846	-2.1846
68	N	7.1983	-2.1983
69	N	7.196	-2.196
70	N	7.1937	-2.1937
71	N	7.2027	-2.2027
72	N	7.2048	-2.2048
73	N	7.2007	-2.2007
74	N	7.1859	-2.1859
75	N	7.2032	-2.2032
76	N	7.2154	-2.2154
77	N	7.2025	-2.2025
78	N	7.1806	-2.1806

79	N	7.198	-2.198
80	N	7.1856	-2.1856
81	N	7.1835	-2.1835
82	N	7.2022	-2.2022
83	N	7.209	-2.209
84	N	7.1984	-2.1984
85	N	7.1899	-2.1899
86	N	7.1809	-2.1809
87	N	7.1884	-2.1884
88	N	7.1919	-2.1919
89	N	7.2084	-2.2084
90	N	7.2023	-2.2023
91	N	7.2013	-2.2013
92	N	7.1998	-2.1998
93	N	7.2062	-2.2062
94	N	7.1827	-2.1827
95	N	7.1879	-2.1879
96	N	7.2064	-2.2064
97	N	7.1984	-2.1984
98	N	7.1829	-2.1829
99	B	0.8165	2.1835
100	B	0.8096	2.1904
101	B	0.7949	2.2051
102	B	0.7974	2.2026
103	B	0.8179	2.1821

104	B	0.8136	2.1864
105	B	0.8019	2.1981
106	B	0.7893	2.2107
107	B	0.8008	2.1992
108	B	0.8182	2.1818
109	B	0.797	2.203
110	B	0.8072	2.1928
111	B	0.8135	2.1865
112	B	0.7933	2.2067
113	B	0.7885	2.2115
114	B	0.7971	2.2029
115	B	0.8034	2.1966
116	B	0.82	2.18
117	B	0.8139	2.1861
118	B	0.8082	2.1918
119	B	0.7928	2.2072
120	B	0.7997	2.2003
121	B	0.8025	2.1975
122	B	0.7943	2.2057
123	B	0.7996	2.2004
124	B	0.8235	2.1765
125	B	0.8035	2.1965
126	B	0.7993	2.2007
127	B	0.8064	2.1936
128	B	0.8052	2.1948

129	B	0.8008	2.1992
130	B	0.7961	2.2039
131	B	0.8019	2.1981
132	B	0.7964	2.2036
133	B	0.8009	2.1991
134	B	0.804	2.196
135	B	0.8117	2.1883
136	B	0.8131	2.1869
137	B	0.8152	2.1848
138	B	0.7959	2.2041
139	B	0.8011	2.1989
140	B	0.7982	2.2018
141	B	0.8027	2.1973
142	B	0.8137	2.1863
143	B	0.8025	2.1975
144	B	0.8042	2.1958
145	B	0.8078	2.1922
146	B	0.792	2.208
147	B	0.7953	2.2047
148	B	0.8018	2.1982

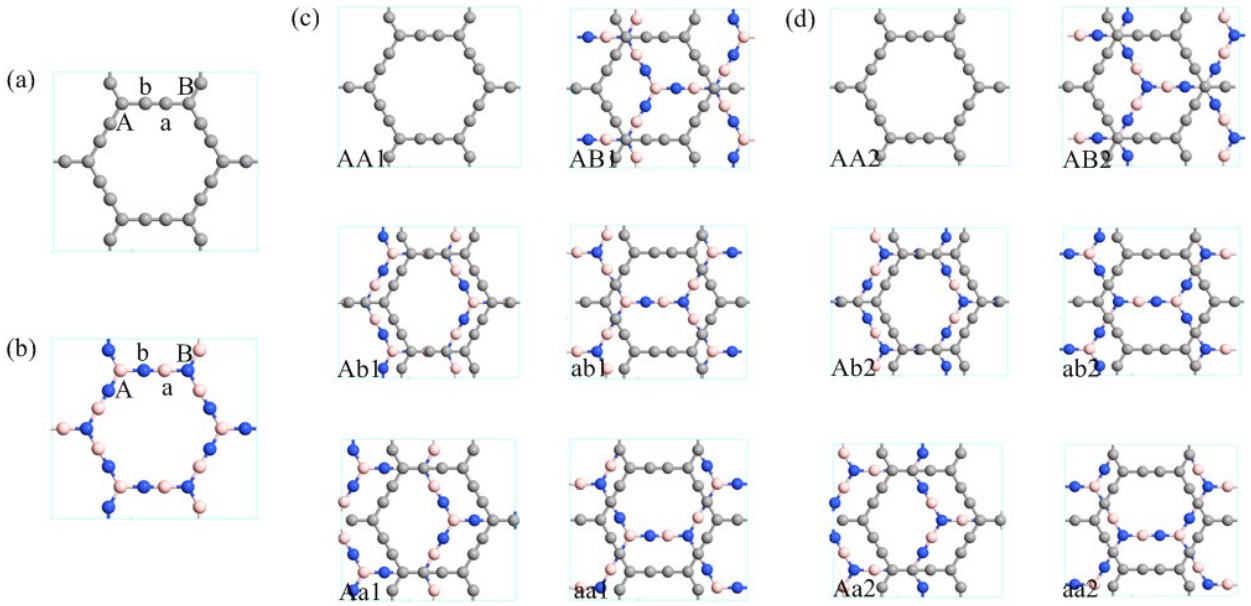

Figure S1. The crystal structure of (a) α-GY and (b) α-BNy. The names of the inequivalent C, B and N atoms are indicated. Different stacking modes of (c) C-B case and (d) C-N case for α-GY/α-BNy.

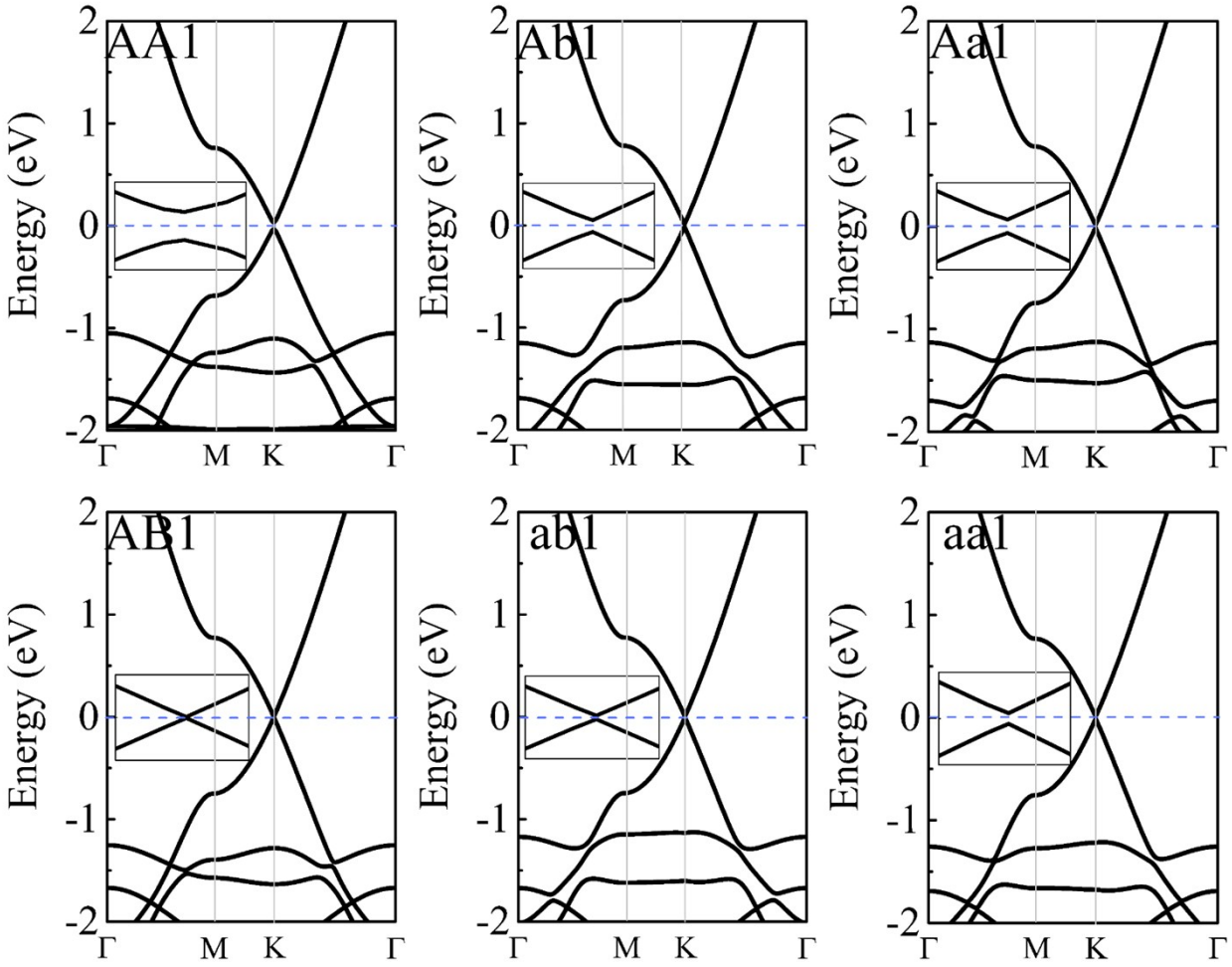

Figure S2. Band structures of different stacking modes for *α*-GY/*α*-BNy in C-B case.

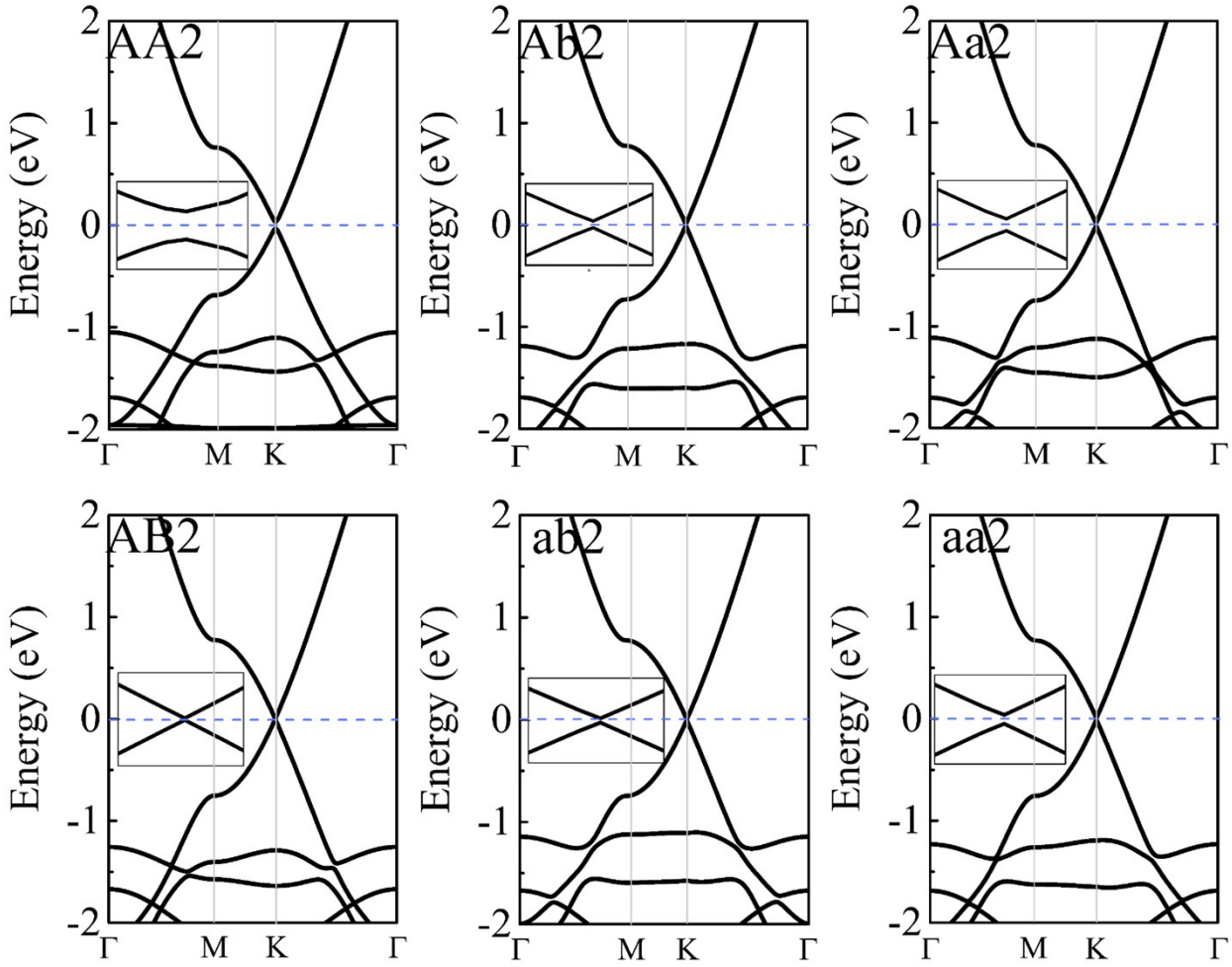

Figure S3. Band structures of different stacking modes for *α*-GY/*α*-BNy in C-N case.