Supplementary materials

Two-Dimensional Boron-Nitrogen-Carbon Monolayers with Tunable Direct Band Gaps

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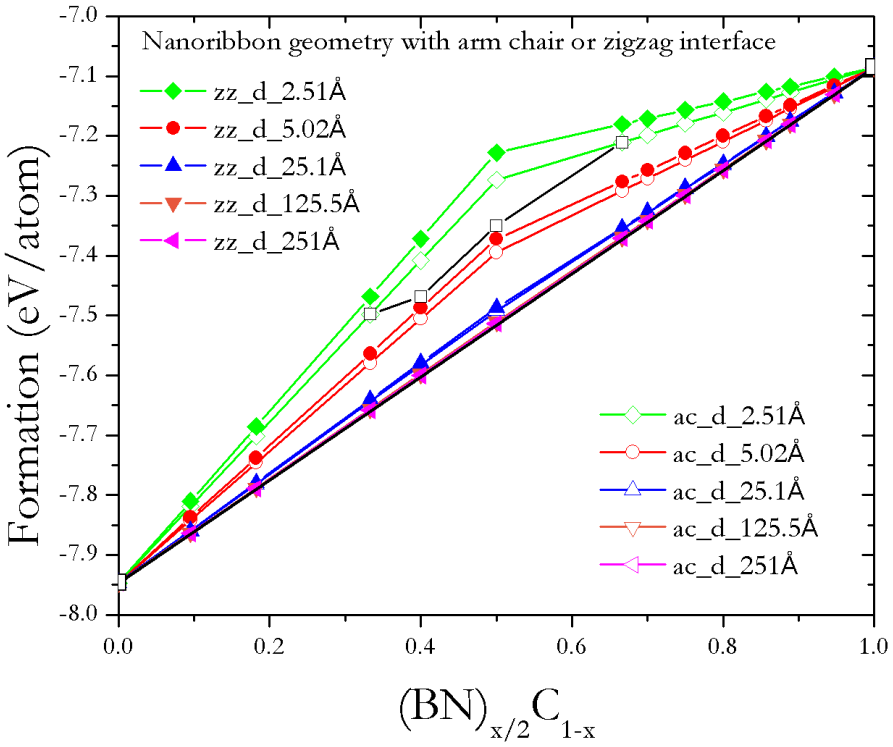

Figure S1. The formation energy for $(BN)_{x/2}C_{1-x}$. The hollow square symbols are the analytical results for the predicted four structures in Figure 1. The other hollow diamond, circle, up, down and left triangle symbols are the analytical results for the assumed nanoribbon geometry with armchair interface, while the solids ones are with zigzag interface. The black line is the formation energy for $(BN)_{x/2}C_{1-x}$ separated completely to pure graphene and BN. *d* is the width of graphene or BN nanoribbon.

In general, the formation energy for the assumed nanoribbon geometry with zigzag interface is higher than that with armchair one, which can be attributed to the higher interface energy in zigzag case. Moreover, the formation energy will decrease as the width of the carbon or BN ribbon increases, which reflects that $(BN)_{x/2}C_{1-x}$ is closer to full separation into graphene and *h*-BN when in a larger scale. The formation energy for the two predicted structures with zigzag interface (the second and third black points) is between the two with widths of 2.51 and 5.02Å using the assumed

nanoribbon geometry with zigzag interface. This is due to that the two predicted structures have the same nanoribbon geometry and its width is 4.35Å, located between 2.51 and 5.02Å. The formation energies using the assumed nanoribbon geometry with armchair interface are the same as those for the two predicted structures with armchair interface (the first and fourth black points), which is due to the same nanoribbon geometry and the same width used.

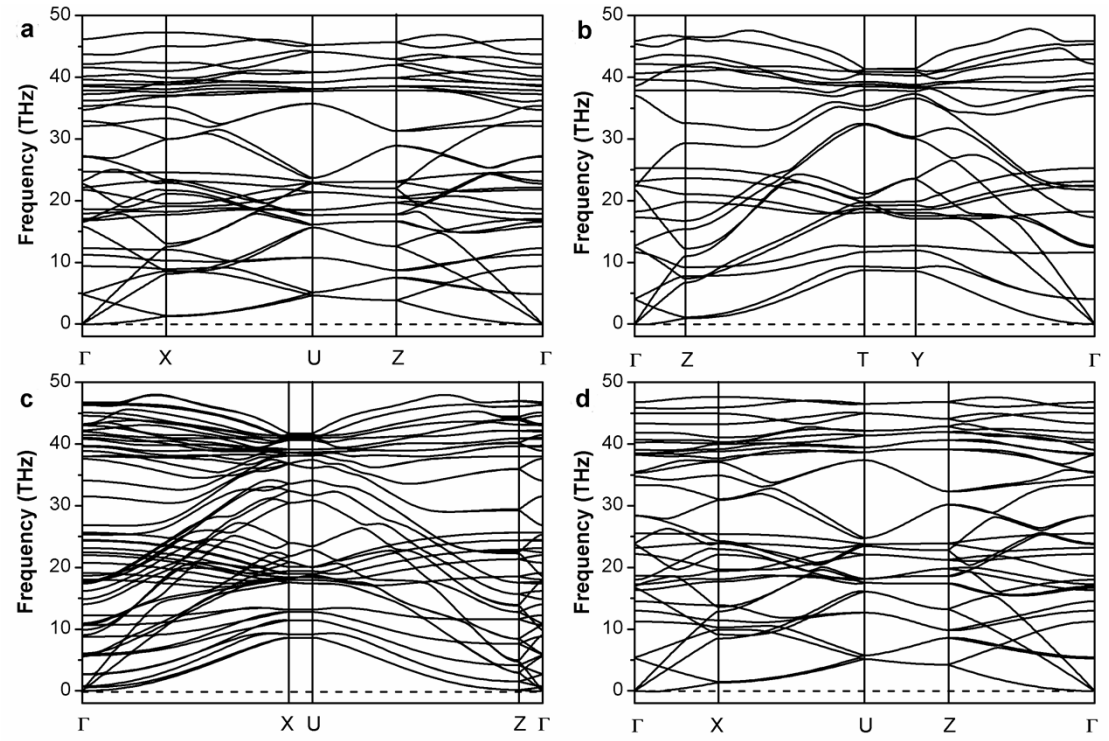

Figure S2. Phonon dispersion curves of predicted $B_{x/2}N_{x/2}C_{1-x}$ structures. Phonon dispersion curves of (**a**) BNC, (**b**) BNC_2, (**c**) BNC_3, and (**d**) BNC_4. The results reveal that all predicted structures are dynamically stable.

Table S1

	Lattice constants	Atomic positions			
BNC	a = 7.519	B1	0.08520	0.98784	0.50000
	b = 4.331	B2	0.91480	0.48784	0.50000
	c = 10.630	B3	0.75012	0.99395	0.50000
		B4	0.24988	0.49395	0.50000
		C1	0.42180	0.67752	0.50000
		C2	0.57820	0.17752	0.50000
		C3	0.41817	0.00742	0.50000
		C4	0.58183	0.50742	0.50000
		N1	0.91903	0.15573	0.50000
		N2	0.08097	0.65573	0.50000
		N3	0.74662	0.65759	0.50000
		N4	0.25338	0.15759	0.50000
BNC_2	a = 8.689	B1	0.57603	0.00000	0.50000
	b = 2.484	B2	0.32525	0.50000	0.50000
	c = 10.954	C1	0.90214	0.00000	0.50000
		C2	0.06842	0.00000	0.50000
		C3	0.14914	0.50000	0.50000
		C4	0.82183	0.50000	0.50000
		N1	0.41156	0.00000	0.50000
		N2	0.66189	0.50000	0.50000
BNC_3	a = 2.479	B1	0.50000	0.40136	0.50000
	b = 21.664	B2	0.00000	0.90136	0.50000
	c = 9.241	B3	0.50000	0.00196	0.50000
		B4	0.00000	0.50196	0.50000
		C1	0.50000	0.13295	0.50000
		C2	0.00000	0.63295	0.50000
		C3	0.50000	0.33079	0.50000
		C4	0.00000	0.83079	0.50000
		C5	0.50000	0.19935	0.50000
		C6	0.00000	0.69935	0.50000
		C7	0.00000	0.23182	0.50000
		C8	0.50000	0.73182	0.50000
		C9	0.00000	0.29834	0.50000
		C10	0.50000	0.79834	0.50000
		C11	0.00000	0.10061	0.50000
		C12	0.50000	0.60061	0.50000
		N1	0.00000	0.43613	0.50000
		N2	0.50000	0.93613	0.50000

		N3	0.00000	0.03656	0.50000
		N4	0.50000	0.53656	0.50000
BNC_4	a = 7.480	B1	0.08152	0.96658	0.50000
	b = 4.300	B2	0.91848	0.46658	0.50000
	c = 11.385	C1	0.58374	0.15059	0.50000
		C2	0.41626	0.65059	0.50000
		C3	0.58110	0.48458	0.50000
		C4	0.41890	0.98458	0.50000
		C5	0.74675	0.97787	0.50000
		C6	0.25325	0.47787	0.50000
		C7	0.25454	0.15097	0.50000
		C8	0.74546	0.65097	0.50000
		N1	0.91163	0.13061	0.50000
		N2	0.08837	0.63061	0.50000