Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information

Atomistic understanding of lateral growth of graphene from edge of h-BN domain: towards sharp in-plane junction

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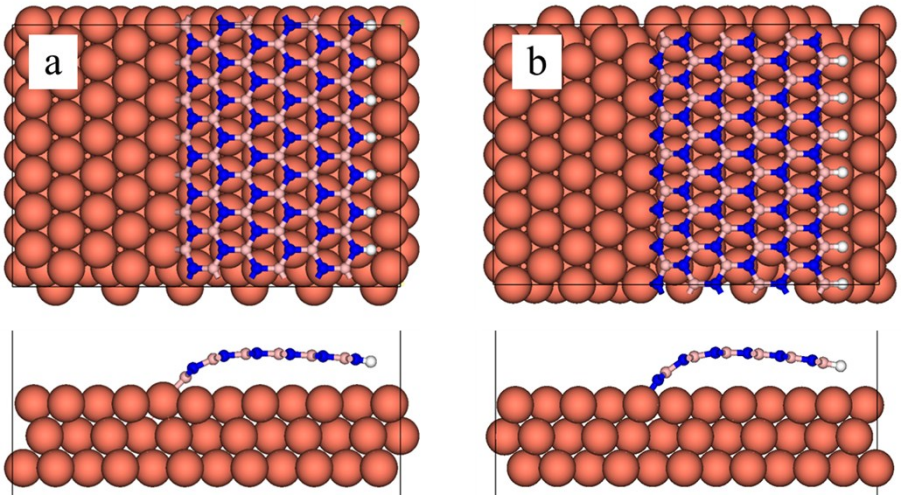

Fig. S1 Atomic models of the BN nanoribbon on Cu(111) substrate for all calculations: (a) B-edge and (b) N-edge as the nucleation sites of graphene.

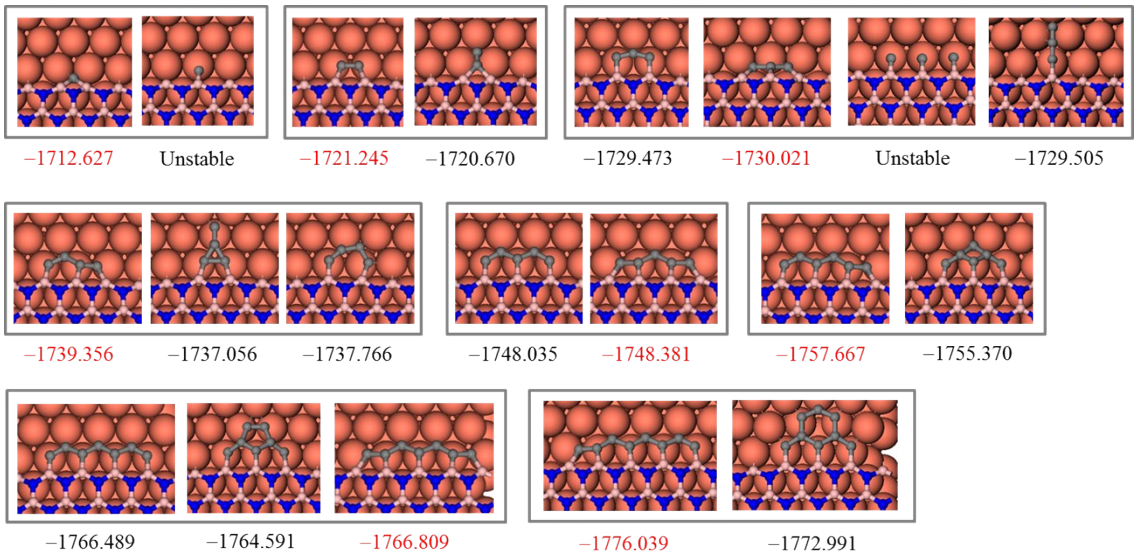

Fig. S2 Several considered configurations of C_i clusters at B-edge with i=1~8. The corresponding DFT total energies (in unit of eV) are listed below. For each C_i, the red number represents the most stable structure. For clarity, only part of the structure within the supercell is shown.

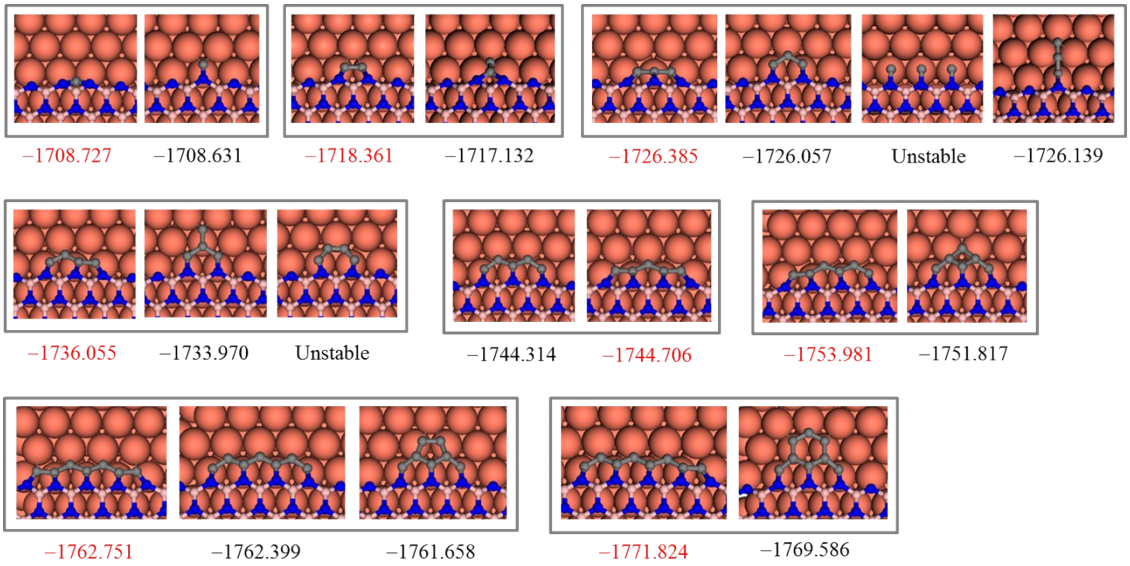

Fig. S3 Several considered configurations of C_i clusters at N-edge with i=1~8. The corresponding DFT total energies (in unit of eV) are listed below. For each C_i, the red number represents the most stable structure.

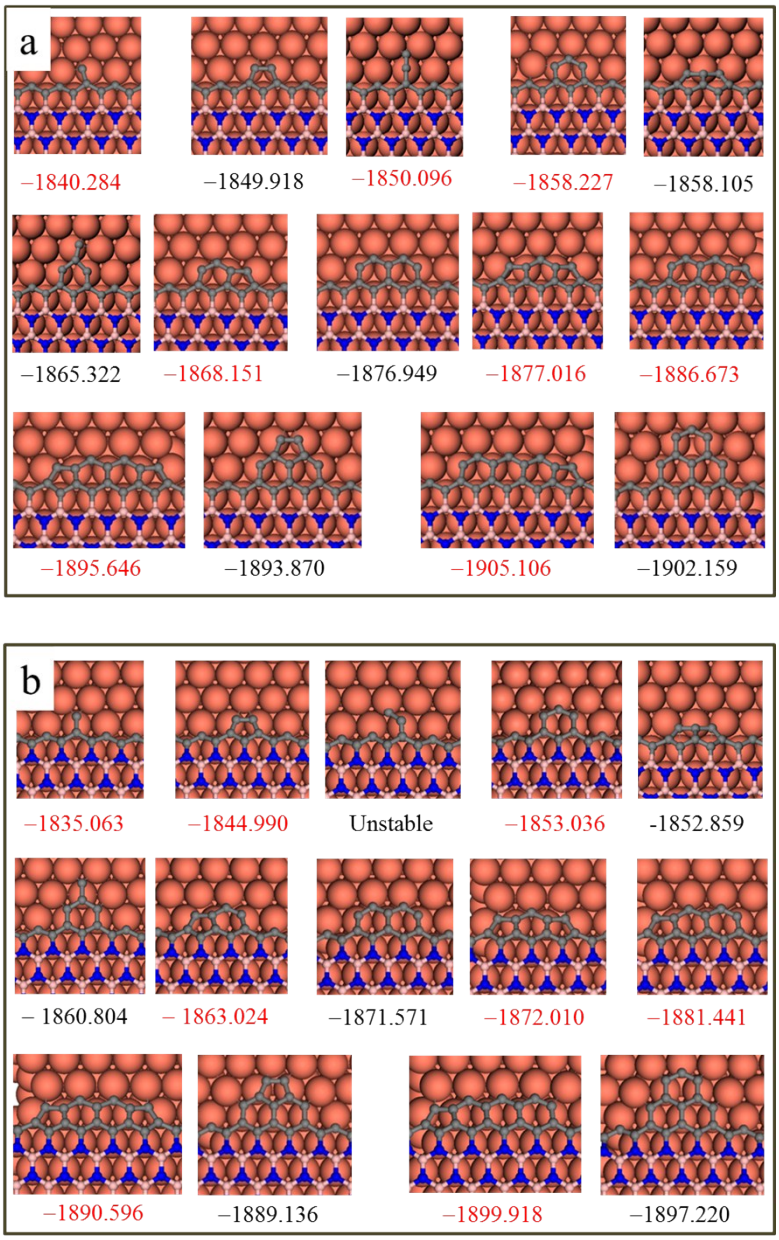

Fig. S4 Several considered configurations of C_i clusters at BC/NC-edges with i=1~8. The corresponding DFT total energies (in unit of eV) are listed below. For each C_i, the red number represents the most stable structure.

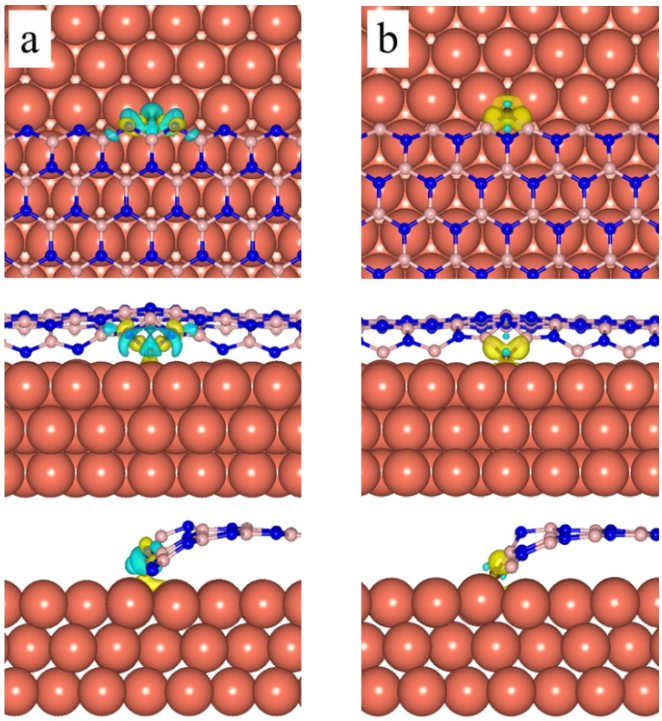

Fig. S5 Charge density differences between the carbon monomer at (a) N-edge and (b) B-edge on Cu(111) substrates, respectively. The blue (yellow) parts represent the deficiency (aggregation) of electrons. The isosurface is 0.01 |e|/Å^3.

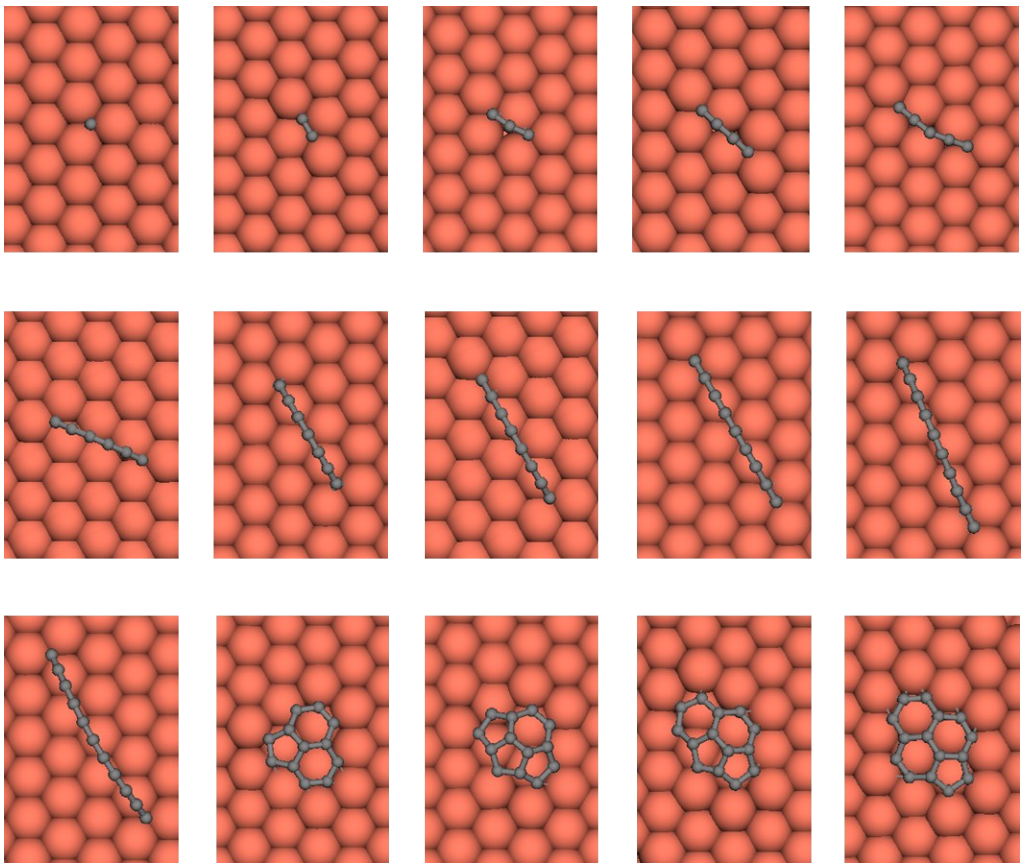

Fig. S6 Atomic configurations of C_i clusters with i = 1~15 on Cu(111) terrace. The critical size of transition from 1D chains to 2D islands is at i = 12.

(a)

$$\sigma = \frac{A_D}{A_T} = \frac{\sqrt{3}}{4}\frac{L^2}{A_T}$$

A_D is the area of *h*-BN domain and L is the edge length.

$$L = \sqrt{\frac{4\sigma A_T}{\sqrt{3}}}$$

$$A_N = 3La = 3\sqrt{\frac{4\sigma A_T}{\sqrt{3}}} \times a = 9.7\sqrt{\sigma A_T}$$

a = 2.13 Å, is the distance between two adjacent BN zigzag rows.

$$\frac{A_N}{A_{Cu}} = \frac{A_N}{(1-\sigma)A_T} = \frac{9.7}{1-\sigma}\sqrt{\frac{\sigma}{A_T}}$$

(b)

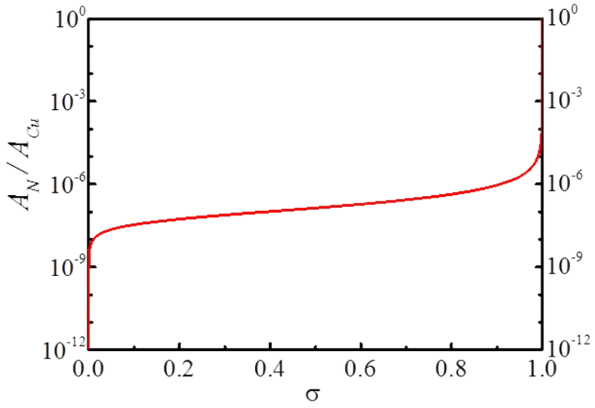

Fig. S7 (a) Derivation of the formula of effective nucleation area ratio (A_N/A_{Cu}), i.e., Eq.(8) of the main text. (b) Effective nucleation area ratio as a function of coverage of BN domains (σ).

Table S1. The populating and formation energies of C_i clusters with i = 0~8 at different edges of *h*-BN domain and on Cu terrace.

	i	1	2	3	4	5	6	7	8
ΔE_i (eV)	B-edge	0.922	0.638	0.480	–0.079	0.231	–0.03	0.114	0.026
	BC-edge	2.252	–0.378	0.947	–0.668	0.391	–0.401	0.283	–0.204
	N-edge	2.501	–0.474	1.232	–0.414	0.605	–0.019	0.486	0.183
	NC-edge	2.332	–0.671	1.210	–0.732	0.270	–0.175	0.101	–0.066
ε_i (eV)	B-edge	0.922	1.560	2.041	1.962	2.193	2.163	2.277	2.303
	BC-edge	2.252	1.874	2.821	2.154	2.545	2.144	2.427	2.223
	N-edge	2.401	1.923	3.056	2.542	3.047	2.928	3.314	3.397
	NC-edge	2.332	1.661	2.871	2.140	2.410	2.235	2.336	2.270
	Cu-terrace	2.683	2.407	3.854	4.176	5.107	5.804	6.574	7.238