

Supplementary Materials:

Effects of Cu ratio on the C₁-C₆ growth mechanism on copper-nickel bimetallic surface

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Table S1 Adsorption energy E_{ads}(eV) and Muliken Charge of C_n on the surfaces

n	Configuration	Ni		Ni ₂ Cu ₁		Ni ₁ Cu ₂		Cu	
		E _{ads} /eV	Muliken charge/e	E _{ads} /eV	Muliken charge/e	E _{ads} /eV	Muliken charge/e	E _{ads} /eV	Muliken charge/e
1	-	-2.745	-0.448	-2.554	-0.405	-2.388	-0.373	-2.225	-0.343
2	-	-3.248	-0.538	-3.047	-0.481	-2.782	-0.394	-2.625	-0.354
3	-	-3.364	-0.638	-3.101	-0.551	-2.892	-0.493	-2.643	-0.423
4	-	-3.461	-0.711	-3.163	-0.610	-2.912	-0.544	-2.662	-0.477
	chain	-3.808	-0.760	-3.512	-0.619	-3.275	-0.610	-2.986	-0.529
5	ring ^a	-3.958	-0.882	-3.583	-0.773	-3.276	-0.675	-	-
	ring ^b	-	-	-3.593	-0.780	3.298	-0.680	-3.007	-0.594
	chain	-4.075	-0.763	-3.772	-0.662	-3.441	-0.587	-3.174	-0.511
6	ring ^a	-3.861	-0.851	-3.443	-0.759	-2.722	-0.640	-	-
	ring ^b	-	-	-3.535	-0.755	-3.193	-0.678	-2.565	-0.591

a: The center of the carbon ring is placed above the Ni atom

b: The center of the carbon ring is placed above the Cu atom

Table S2 Shortest distance between chains of C_n and surface L_{min}(Å)

L _{min} /Å	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆
Ni	1.107	1.301	1.395	1.376	1.375	1.362
Ni ₂ Cu ₁	1.128	1.328	1.422	1.405	1.405	1.391

Ni ₁ Cu ₂	1.144	1.356	1.455	1.413	1.403	1.397
Cu	1.159	1.377	1.466	1.432	1.442	1.416
