Supplementary Material

Graphene layers on bimetallic Ni/Cu(111) surface and near surface alloys in controlled growth of graphene

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Table S1 Bader charges (e/atom) of Ni(111), Cu(111) and Ni/Cu(111) SAs and NASs

	*L_1	L_2	L_3	L_4	L_5	L_6
Ni(111)	-0.03	+0.03	0.00	0.00	+0.03	-0.03
Ni(111)-Ni-Cu	0.00	-0.01	+0.01	0.00	+0.03	-0.03
Ni(111)-Cu-Ni	-0.04	+0.06	-0.02	0.00	+0.03	-0.03
Cu(111)-Ni-Cu	0.01	-0.04	+0.03	+0.01	+0.02	-0.03
Cu(111)-Cu-Ni	-0.06	+0.06	0.00	+0.01	+0.02	-0.03
Cu(111)	-0.02	+0.02	0.00	0.00	+0.02	-0.02

*The L_n is the number of the substrate layer.

Table S2 Bader charges (e/atom) of the graphene bottom layer and metal substrates. C_A and C_B correspond to the illustration in Fig. 4, which are indicated C atoms sitting on top of the Ni atoms (labeled as the C_A) and sitting on hollow sites (labeled as the C_B). The Ni_n and Cu_n represent the Ni and Cu atom at the n layer of the Ni/Cu SAs and NSAs.

Stacking		**Monolayer**		Bilayer			
				AB		AA	
Location		FCC	HCP	FCC	HCP	FCC	HCP
Ni(111)	C_{A1}	- 0.24	- 0.24	- 0.22	- 0.24	- 0.22	- 0.24
	C_{B1}	+0.12	+0.11	+0.10	+0.12	+0.10	+0.12
	Ni_1	+0.11	+0.11	+0.11	+0.12	+0.12	+0.12
	Ni_2	+0.01	+0.01	+0.01	+0.01	+0.02	+0.01
	Ni_3	0.00	0.00	0.00	0.00	0.00	0.00
Ni(111)-Cu-Ni	C_{A1}	- 0.21	- 0.21	- 0.25	- 0.21	- 0.24	- 0.21
	C_{B1}	+0.12	+0.12	+0.13	+0.12	+0.11	+0.11
	Ni1	+0.06	+0.06	+0.11	+0.07	+0.11	+0.07
	Cu_2	+0.05	+0.05	+0.04	+0.04	+0.04	+0.04
	Ni_3	- 0.02	- 0.02	- 0.02	- 0.02	- 0.02	- 0.02
Cu(111)-Cu-Ni	C_{A1}	- 0.22	- 0.22	- 0.22	- 0.22	- 0.22	- 0.22
	C_{B1}	+0.06	+0.06	+0.07	+0.07	+0.07	+0.07
	Ni_1	+0.14	+0.14	+0.14	+0.14	+0.14	+0.14
	Cu_2	+0.02	+0.03	+0.02	+0.03	+0.02	+0.02
	Cu_3	- 0.01	0.00	0.00	0.00	0.00	0.00
Ni(111)-Ni-Cu	C_{A1}	- 0.17	- 0.16	- 0.17	- 0.17	- 0.18	- 0.18
	C_{B1}	+0.16	+0.15	+0.16	+0.16	+0.16	+0.17
	Cu_1	+0.02	+0.01	+0.01	+0.02	+0.02	+0.01
	Ni_2	- 0.01	- 0.01	0.00	- 0.01	- 0.01	0.00
	Ni_3	+0.01	+0.01	0.00	+0.01	+0.01	0.00
Cu(111)-Ni-Cu	C_{A1}	- 0.11	- 0.11	- 0.12	- 0.12	- 0.13	- 0.12
	C_{B1}	+0.09	+0.09	+0.10	+0.10	+0.10	+0.10
	Cu_1	+0.02	+0.02	+0.02	+0.03	+0.04	+0.03
	Ni_2	- 0.03	- 0.03	- 0.03	- 0.03	- 0.03	- 0.03

	Cu_3	+0.02	+0.03	+0.02	+0.02	+0.02	+0.02
Cu(111)	C_{A1}	-0.13	-0.11	-0.12	-0.12	-0.12	-0.11
	C_{B1}	+0.10	+0.10	+0.10	+0.10	+0.10	+0.10
	Cu_1	0.00	-0.01	0.00	0.00	0.00	0.00
	Cu_2	+0.02	+0.02	+0.02	+0.02	+0.02	+0.02
	Cu_3	+0.01	+0.01	+0.01	+0.01	+0.01	+0.01