Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Surface Restructuring of Cu-based Single-atom Alloy Catalysts under Reaction Conditions: The Essential Role of Adsorbates

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Table S1. Adsorption energies (in eV) and C-C bond lengths ($d_{C\text{-}C}$, in Å) of acetylene on different alloy surfaces.

	M_1Cu_3		M_2Cu_2		M_3Cu_1		M_4Cu_0	
	E_{ad}	$d_{C\text{-}C}$	E_{ad}	$d_{C\text{-}C}$	E_{ad}	$d_{C\text{-}C}$	E_{ad}	$d_{C\text{-}C}$
Pd	-1.23	1.370	-1.12	1.366	-1.25	1.342	-1.23	1.360
Pt	-1.34	1.370	-1.33	1.359	-1.50	1.380	-1.39	1.363
Rh	-1.61	1.382	-2.30	1.387	-2.51	1.384	-2.46	1.410
Ni	-1.70	1.374	-2.24	1.375	-2.55	1.385	-2.85	1.399

Table S2. Adsorption energies (in eV) and C-C bond lengths ($d_{C\text{-}C}$, in Å) of ethylene on different alloy surfaces.

	M_1Cu_3		M_2Cu_2		M_3Cu_1		M_4Cu_0	
	E_{ad}	$d_{C\text{-}C}$	E_{ad}	$d_{C\text{-}C}$	E_{ad}	$d_{C\text{-}C}$	E_{ad}	$d_{C\text{-}C}$
Pd	-0.53	1.389	-0.50	1.388	-0.49	1.389	-0.47	1.388
Pt	-0.60	1.411	-0.60	1.473	-0.52	1.475	-0.51	1.471
Rh	-0.97	1.411	-0.91	1.413	-0.95	1.441	-0.92	1.411
Ni	-0.71	1.407	-0.77	1.434	-0.96	1.446	-0.95	1.447

Table S3. Energies of different alloy surfaces with an adsorbed hydrogen atom, where the energies of corresponding single atom alloy surfaces were set to zero.

$E_{x\text{-}H}$/eV	Pd	Pt	Rh	Ni
M_1Cu_3	0.00	0.00	0.00	0.00
M_2Cu_2	0.08	0.12	0.08	-0.11
M_3Cu_1	0.21	0.49	0.17	-0.21

Table S4. Adsorption energies of hydrogen atom over different alloy surfaces.

$E_{ad\text{-}H}$/eV	Pd	Pt	Rh	Ni
M_1Cu_3	-0.23	-0.27	-0.46	-0.39
M_2Cu_2	-0.28	-0.34	-0.52	-0.53
M_3Cu_1	-0.36	-0.25	-0.57	-0.67

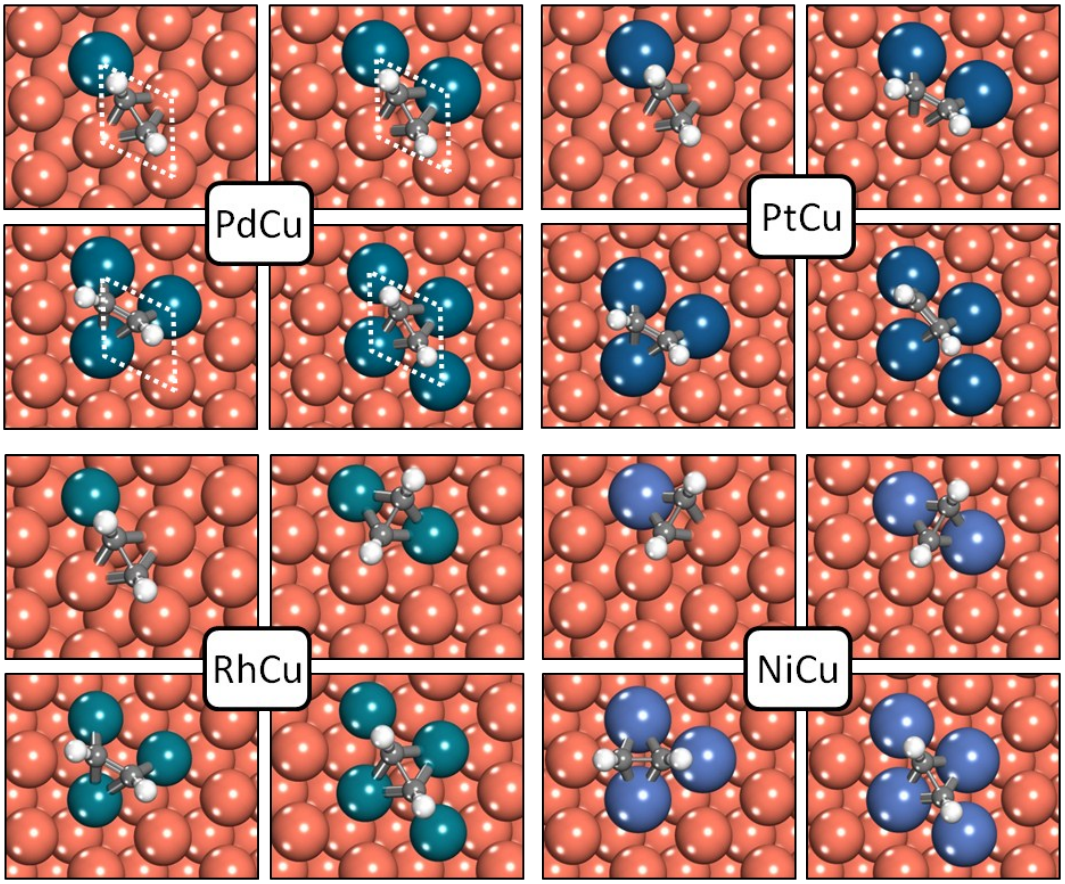

Figure S1. The most stable structures of SAA and aggregated-SAA surfaces of PdCu, PtCu, RhCu and NiCu alloys with adsorbed acetylene.

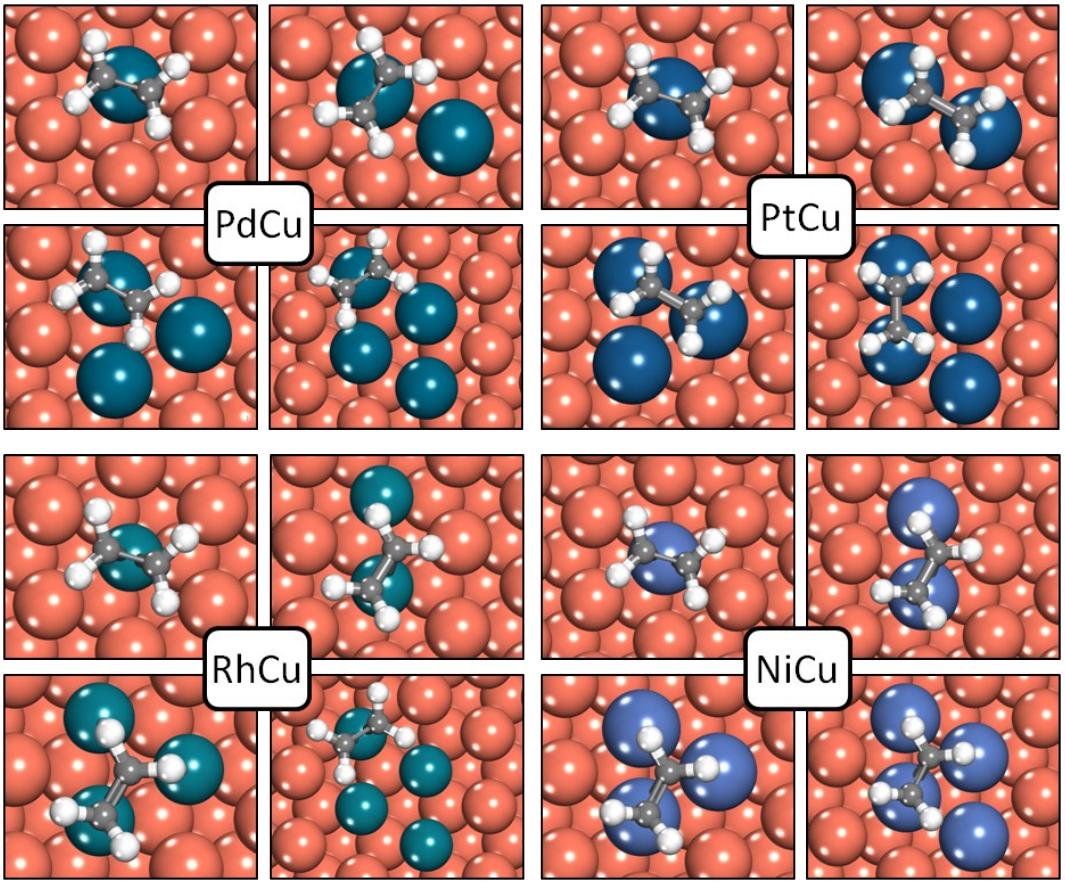

Figure S2. The most stable structures of SAA and aggregated-SAA surfaces of PdCu, PtCu, RhCu and NiCu alloys with adsorbed ethylene.