Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Support information for

Natural arrangement of AgCu bimetallic nanostructures through Oleylamine reduction

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Table S1. Cristalographic data obtained from the Rietveld Refinement.

Compound	AgCu10-90	AgCu50-50	AgCu90-10
	Phase 1		
Space group	Fm-3m	Fm-3m	Fm-3m
	Ag *4a (0 0 0)*	Ag *4a(0 0 0)*	Ag *4a(0 0 0)*
B_{iso}(Å²)	5.46(8)	1.33(2)	2.05(13)
a_o(Å)	4.094(4)	4.093()	4.094(1)
V(Å³)	68.61(12)	68.57(3)	68.61(2)
	Phase 2		
Space group	Fm-3m	Fm-3m	Fm-3m
	Cu *4a (0 0 0)*	Cu *4a(0 0 0)*	Cu *4a(0 0 0)*
Biso(Å²)	4.942(6)	2.91(6)	8.963(18)
ao(Å)	3.628(3)	3.625(1)	3.631(2)
V(Å³)	47.74(7)	47.63(3)	47.87(4)
Reliability factors	**AgCu10-90**	**AgCu50-50**	**AgCu90-10**
χ2	2.59	10.6	4.97
Rp(%)	4.11	7.44	6.76
Rwp(%)	5.66	10.6	9.47
Rbragg Phase 1(%)	8.21	6.48	5.33
Rbragg Phase 2(%)	2.42	5.12	3.39

Table S2. Cu-Ag energies relative to lowest energy configuration.

Energy Difference (meV/atom)				
Label	**Number of atoms**	**Cu@Ag**	**Ag@Cu**	**Ag-Cu***
AgCu9010	4213 (5 nm)	0.00	4.07	7.74
AgCu5050		0.00	12.67	9.13
AgCu1090		0.39	25.00	0.00
AgCu9010	10000 (6.5 nm)	0.00	8.84	1.94
AgCu5050		0.00	17.35	3.08
AgCu1090		0.62	25.67	0.00

* Ag-Cu denotes the janus configuration.

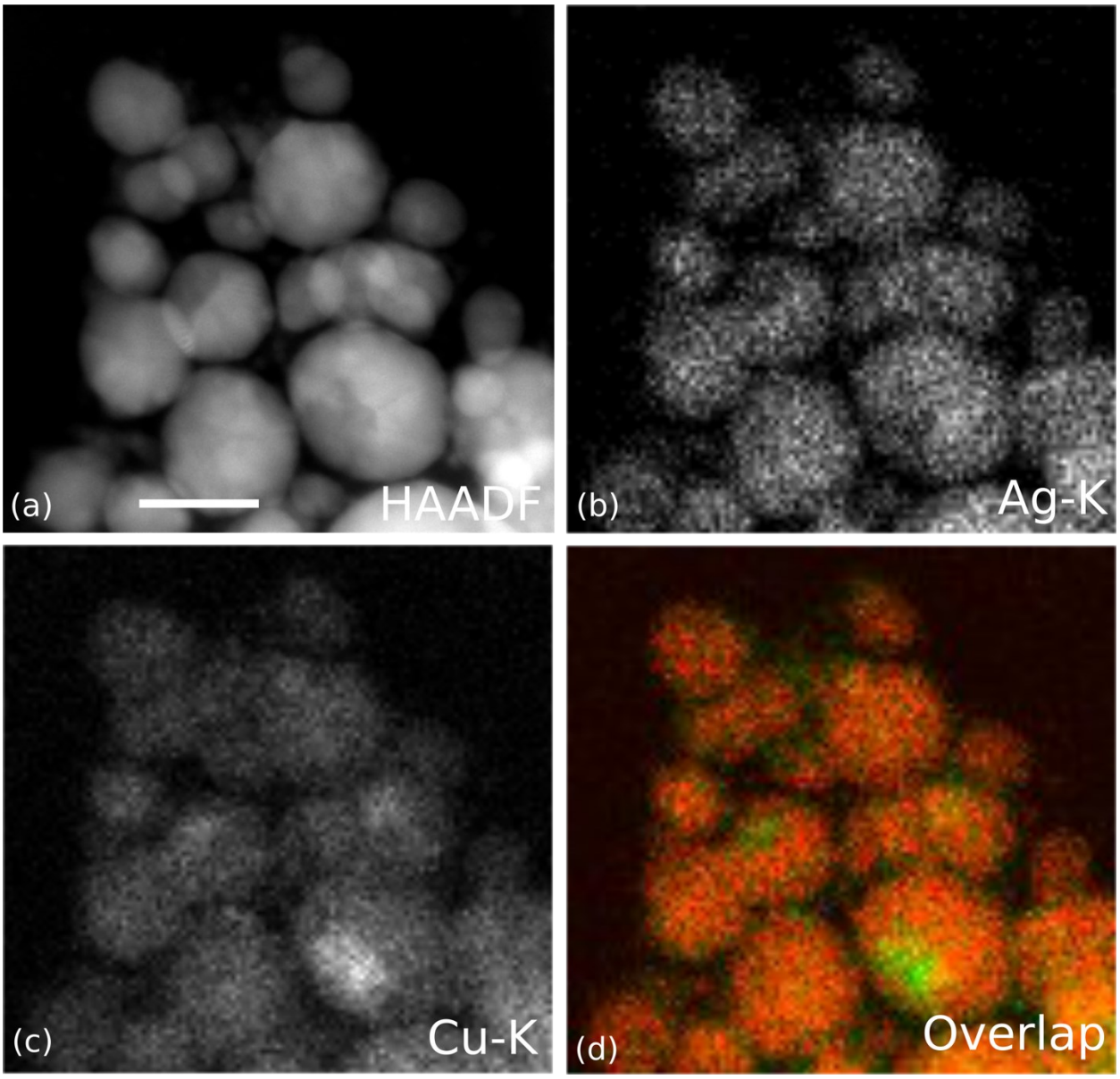

Figure S1. EDX spectrum image of AgCu bimetallic NPs. (a) Low-magnification HAADF-STEM image of AgCu9010 NPs. Elemental maps of (b) silver, (c) copper and (d) overlap elements, where green and red denote Cu and Ag, respectively. The scale bar in (a) represents 30 nm.

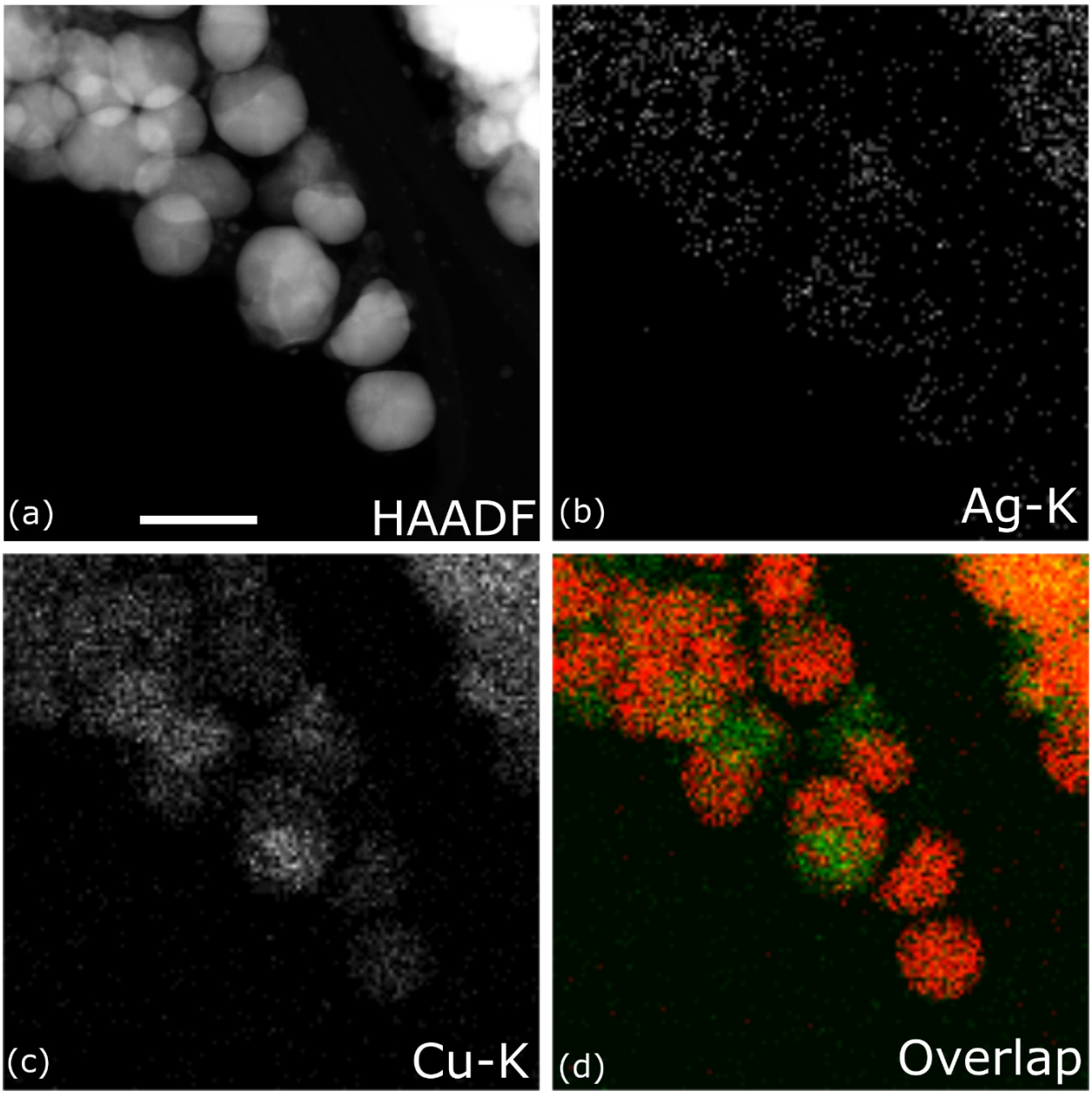

Figure S2. EDX spectrum image of AgCu bimetallic NPs. (a) Low-magnification HAADF-STEM image of AgCu5050 NPs. Elemental maps of (b) silver, (c) copper and (d) overlap elements, where green and red denote Cu and Ag, respectively. The scale bar in (a) represents 50 nm.

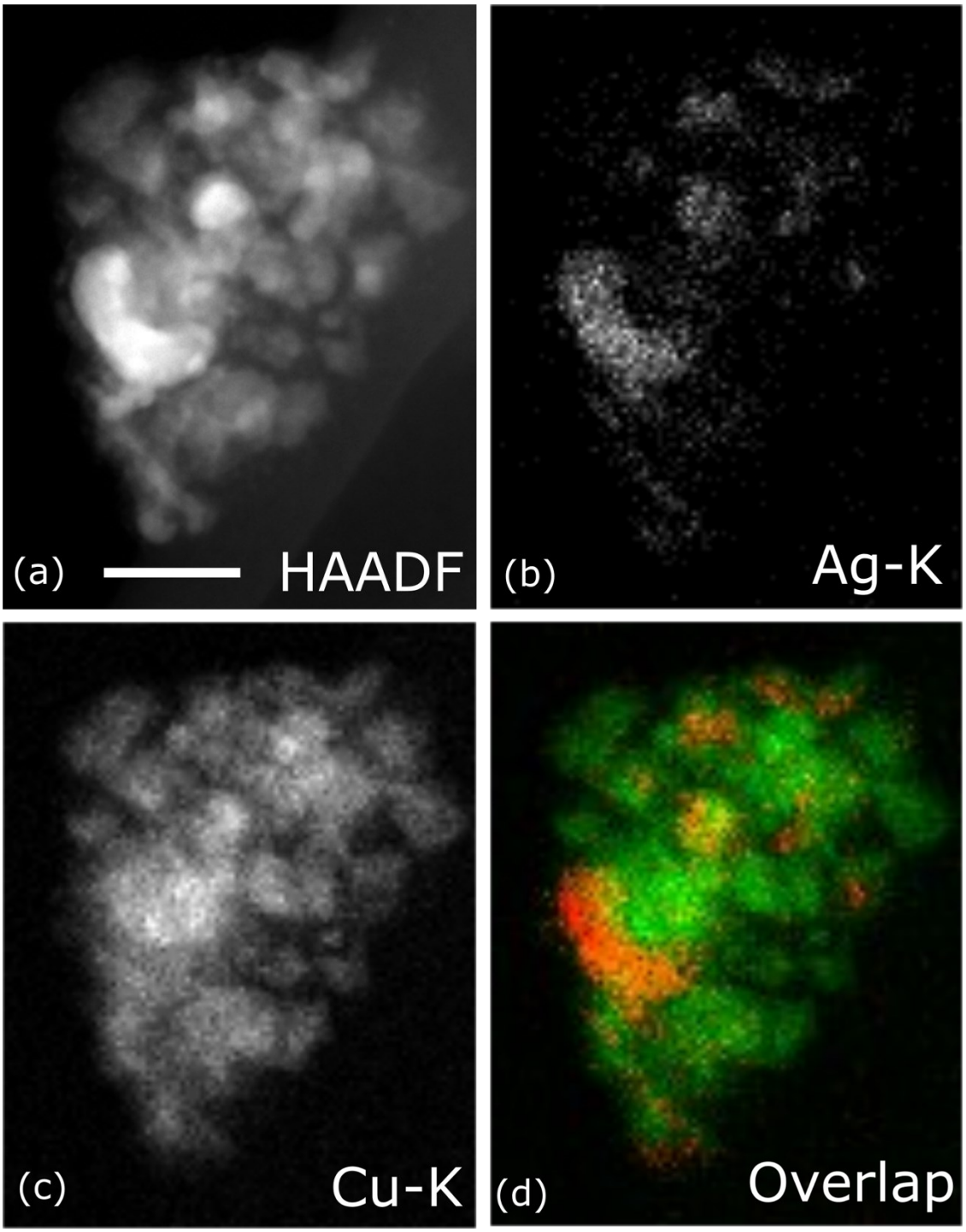

Figure S3. EDX spectrum image of AgCu bimetallic NPs. (a) Low-magnification HAADF-STEM image of AgCu1090 NPs. Elemental maps of (b) silver, (c) copper and (d) overlap elements, where green and red denote Cu and Ag, respectively. The scale bar in (a) represents 30 nm.

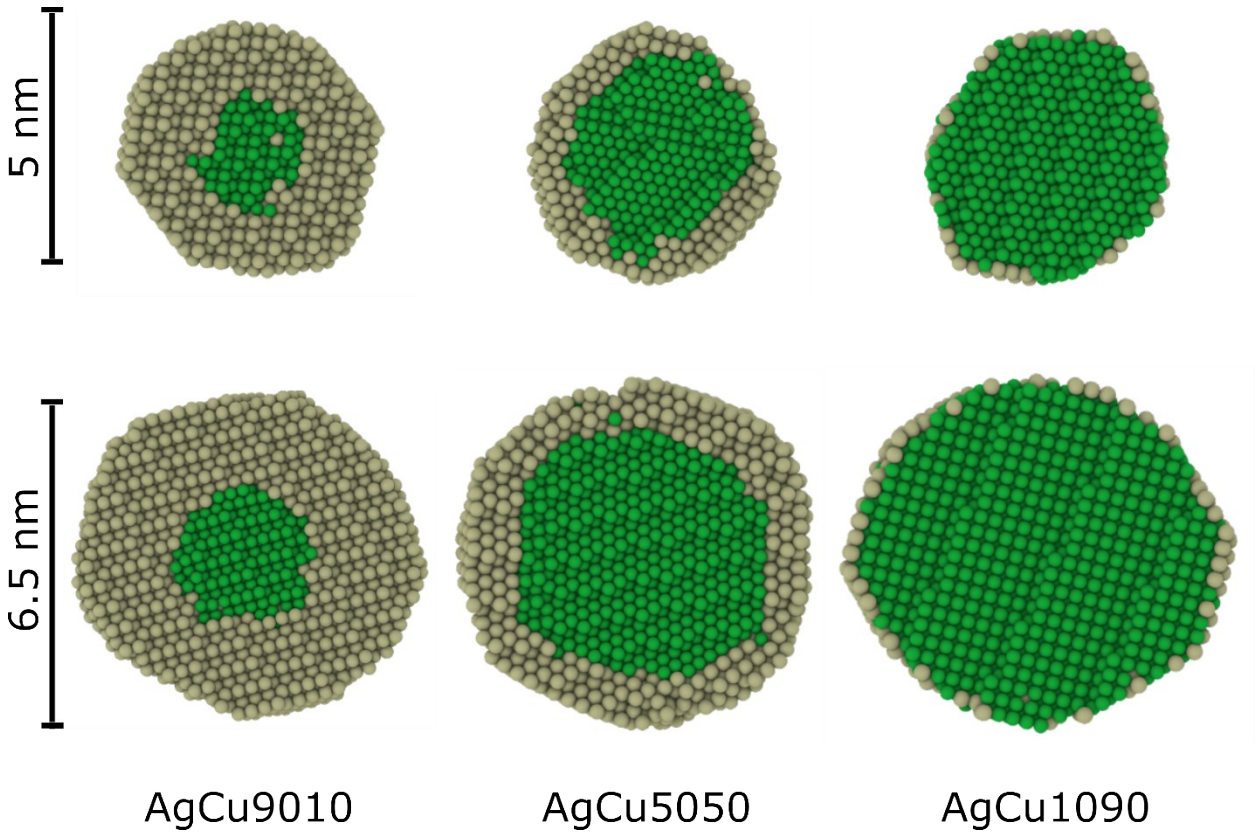

Figure S4. Cross section of the most stable atomic configuration along all sizes and concentrations of AgCu bimetallic NPs.

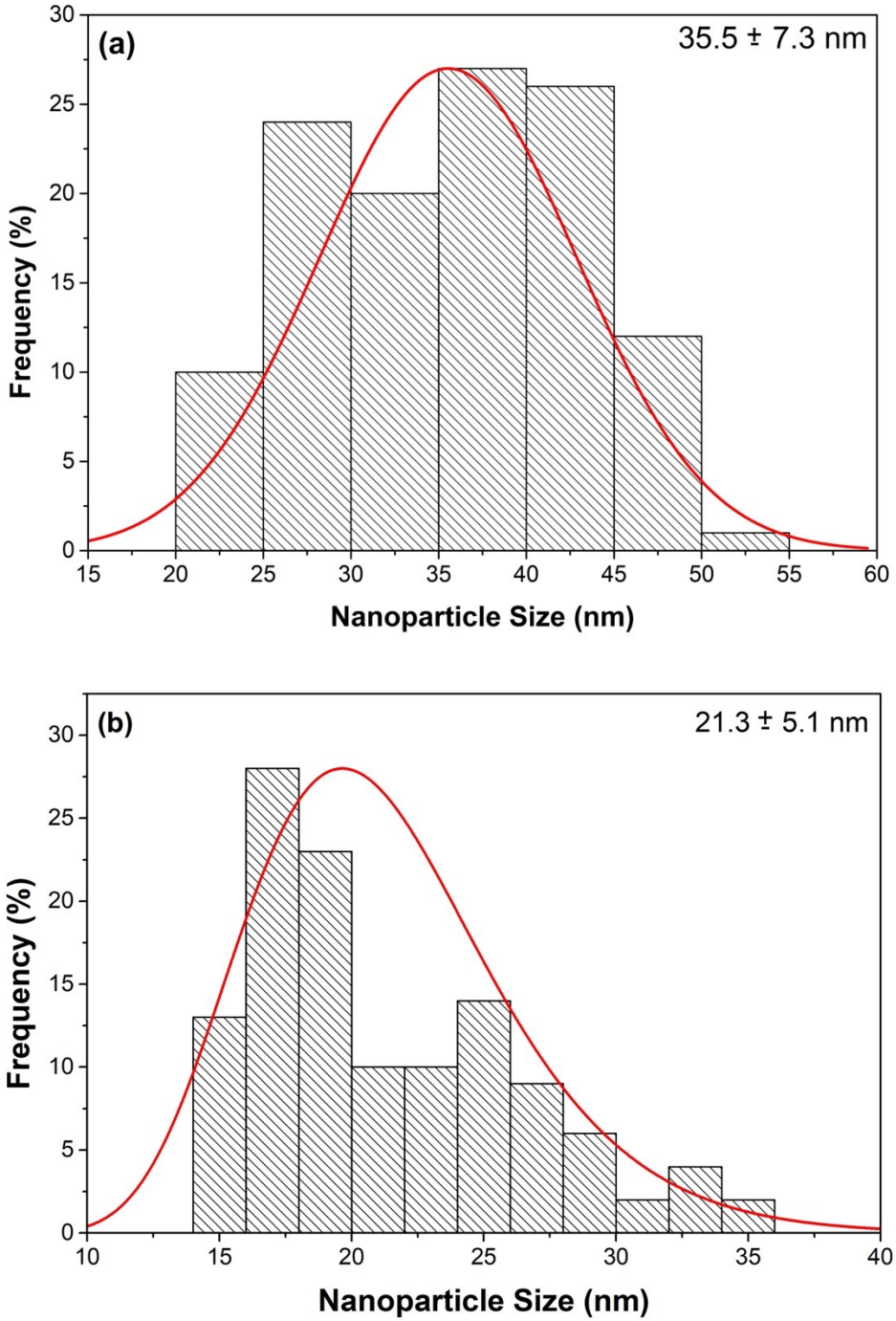

Figure S5. Size distribution graphs for AgCu5050 (a) and AgCu9010 (b). Each graph was built considering the measurement of 120 NPs randomly chosen from 4 different micrographs taken from distinct regions of the TEM grid. The data were fit using a normal and lognormal functions for (a) and (b), respectively.