

Supplementary Materials

Nitroxide-coated Silver Nanoparticles: Synthesis, Surface Physicochemistry and Antibacterial Activity

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Calculations of the surface density of DiSS (sample AR2HH(-5)).

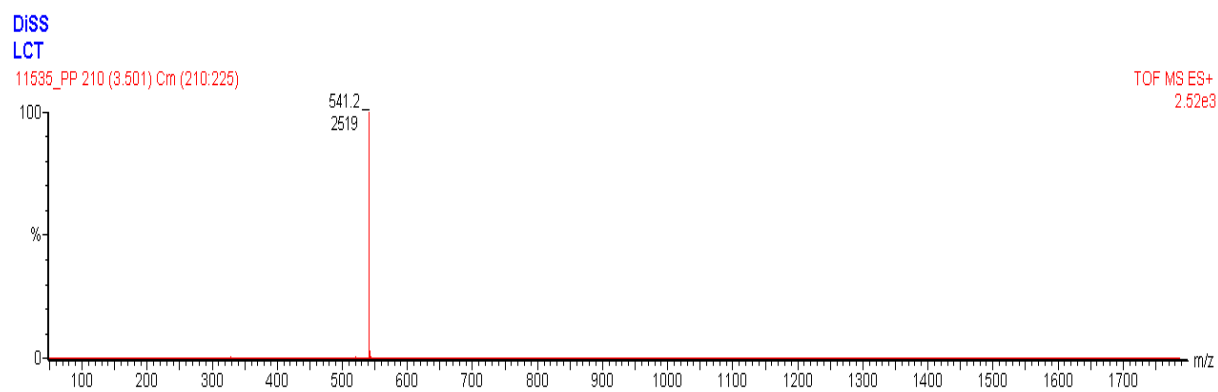


Fig. S1 ESI-MS spectrum of bisnitroxide disulfide (DiSS) as a sodium ion $[M + Na]^+$.

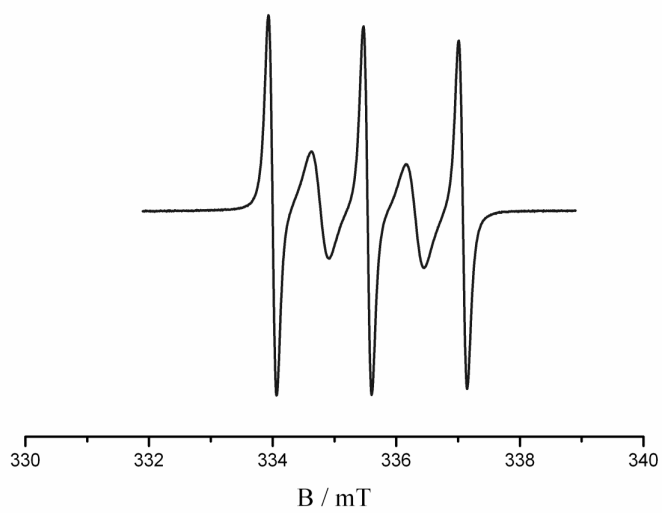


Fig. S2 ESR spectrum of DiSS (see Scheme 1) in toluene solution at 293 K.

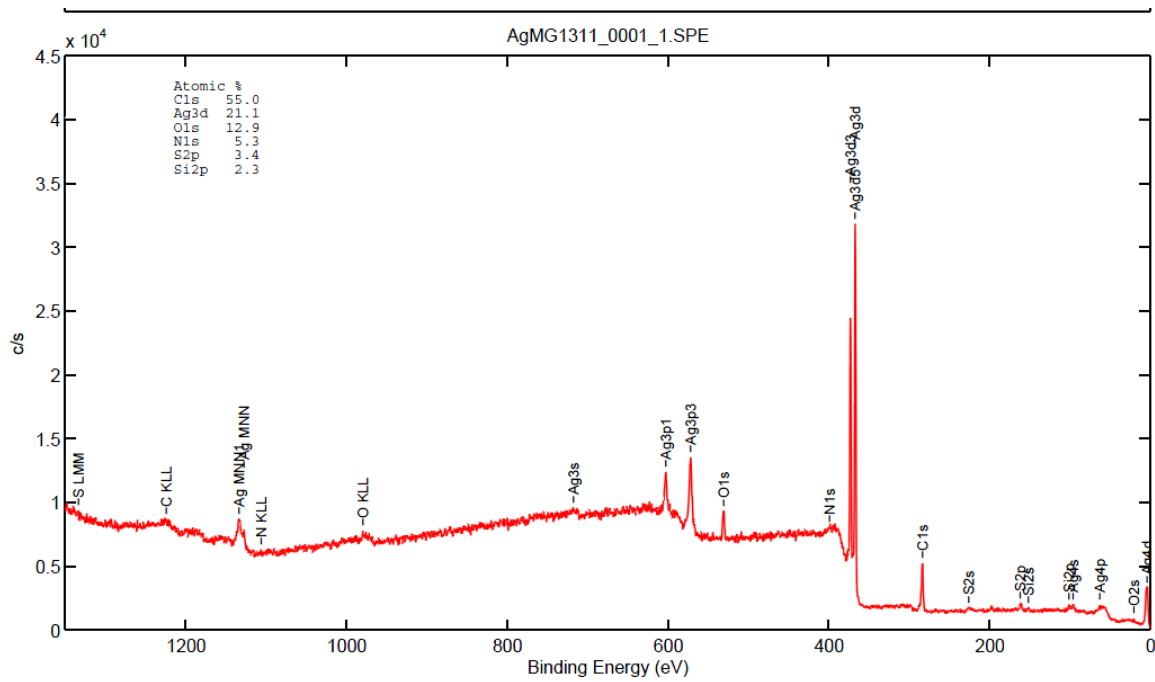


Figure S3. XPS survey spectra of the synthesized AgNPs (sample AR2HH(-5)).

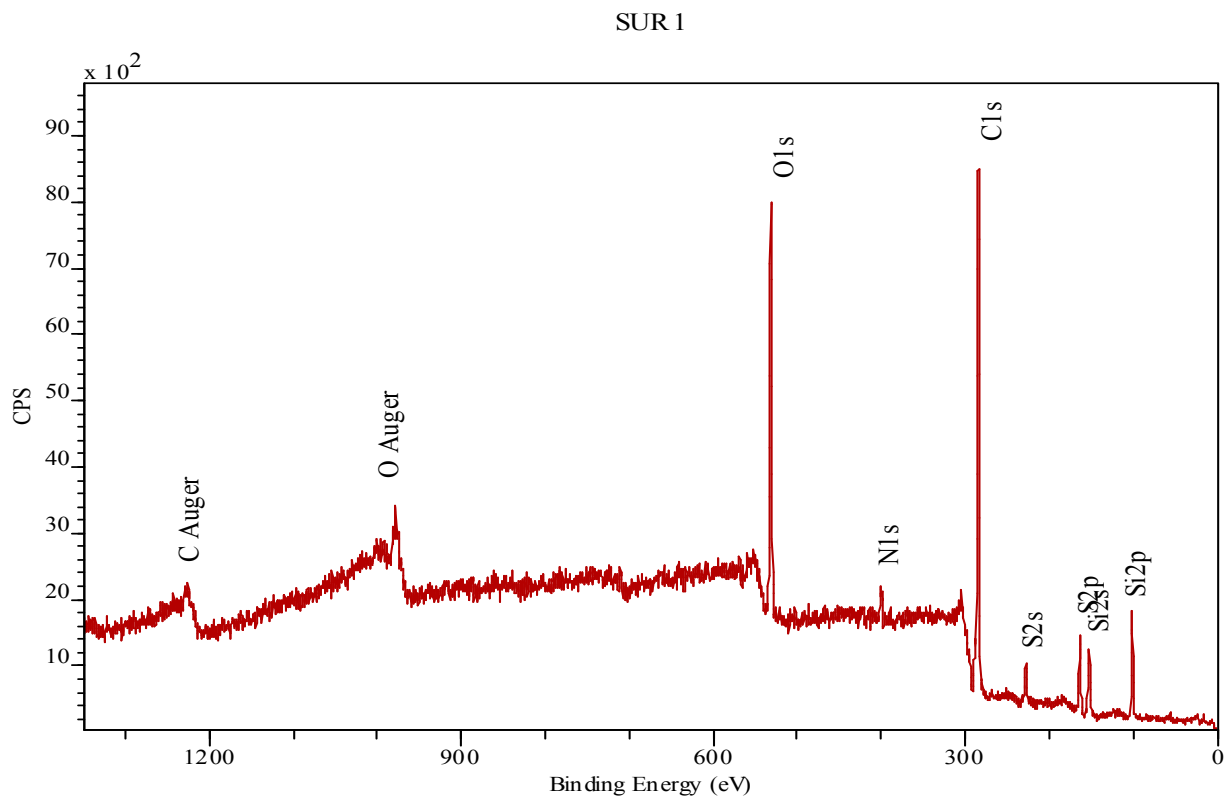


Figure S4. XPS survey spectra of DiSS (see Scheme 1).

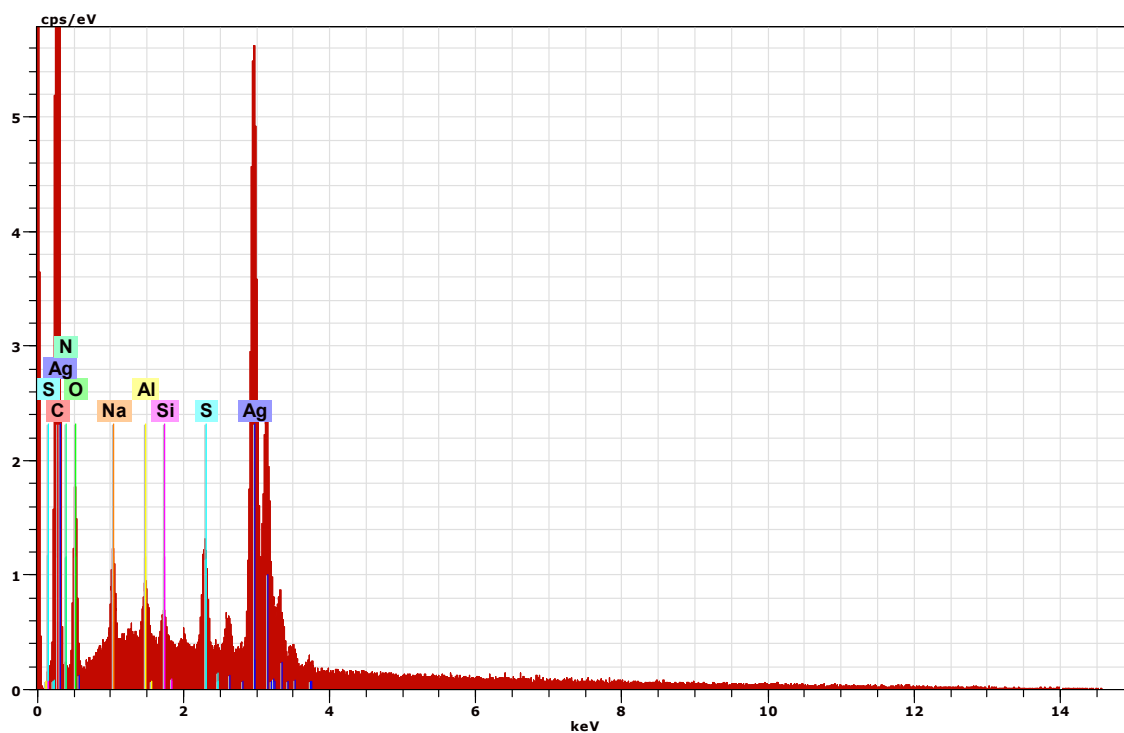


Figure S5. EDS spectrum of the synthesized AgNPs for sample AI24RT (see Table 1).

Table S1

Results of EDS analysis performed for sample AI24RTH (see Table 1 in main test).

Spectrum: Acquisition

Element	Series	unn. C [wt. %]	norm. C [wt. %]	Atom. C [at. %]	Error (1 Sigma) [wt. %]
Carbon	K-series	40.32	47.07	76.41	4.68
Oxygen	K-series	8.21	9.58	11.68	1.29
Silver	L-series	32.12	37.49	6.78	1.04
Sulfur	K-series	1.63	1.90	1.16	0.09
Silicon	K-series	0.36	0.43	0.30	0.05
Aluminium	K-series	0.62	0.72	0.52	0.06
Sodium	K-series	1.19	1.39	1.18	0.11
Nitrogen	K-series	1.22	1.42	1.98	0.38
Total:		85.67	100.00	100.00	

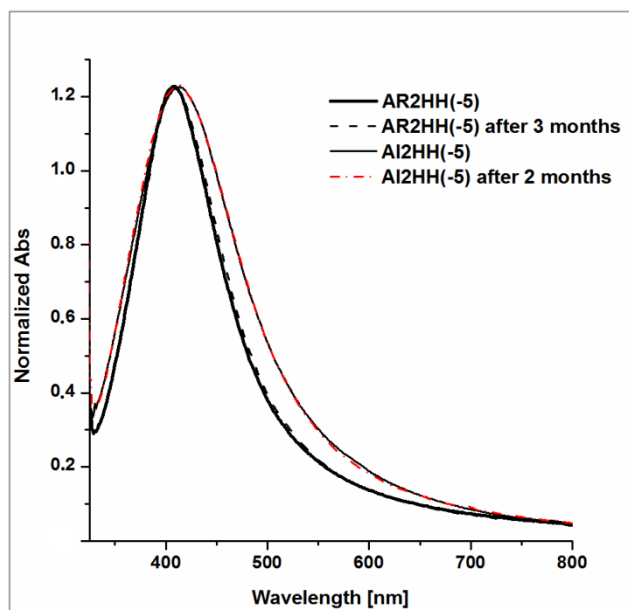


Figure S6. UV-vis absorption spectra of acetone solutions of the selected prepared samples directly after synthesis and 2 or 3 months later.

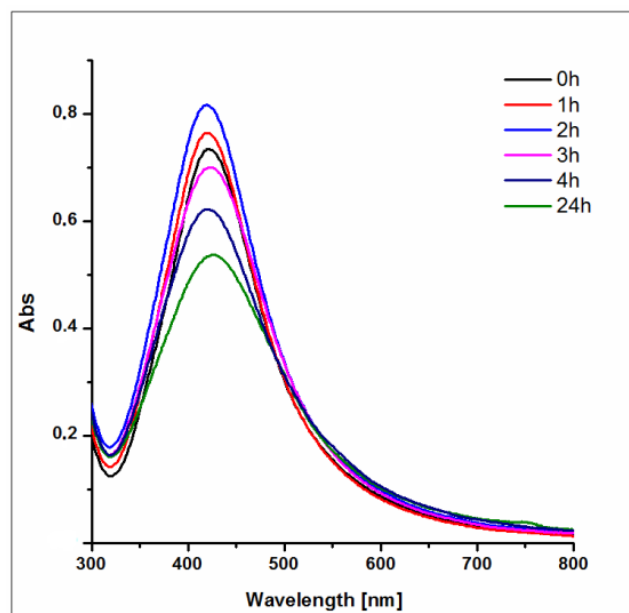


Figure S7. UV-vis spectra recorded during synthesis (solution was diluted with DMF 20 x) first spectrum was recorded after addition of all amount of NaBH_4 solution (0h) and next after a given period of time (reaction conditions the same as for AR2HH(-5) sample preparation).

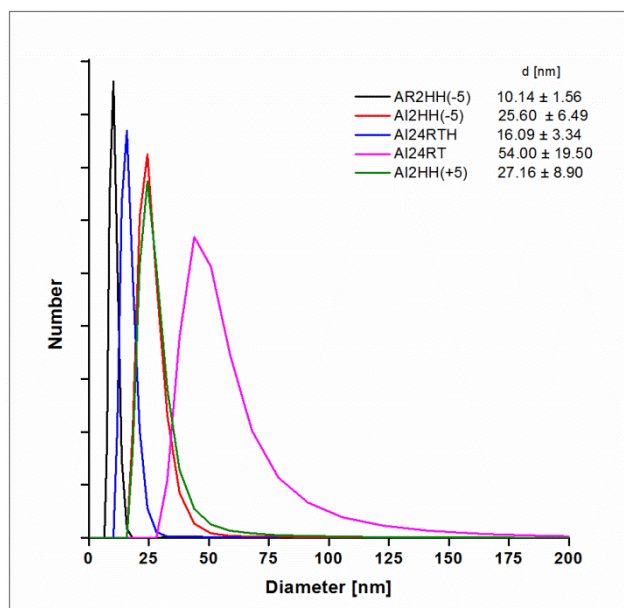


Fig.S8 The number averaged hydrodynamic diameter distribution of the synthesized N-AgNPs obtained from DLS measurements.

Table S2

Binding Energy Values, full width at half maximum (FWHM) of peaks and atomic concentrations derived from XPS analysis of DiSS (see Scheme 1 in main text).

Orbital	Position [eV]	FWHM [eV]	Concentration [atom %]
N 1s	399.6	2.057	3.22
O 1s	530.2	1.338	0.98
	531.9	1.338	17.3
	533.3	1.338	3.70
S 2p _{3/2}	163.6	1.247	1.97
	166.8	2.205	0.48
S 2p _{1/2}	164.8	1.247	0.98
	168.0	2.205	0.24
C 1s	284.6	1.323	44.2
	285.9	1.323	14.1
	287.1	1.014	1.22
	288.9	1.014	2.82

Calculations of the surface density of DiSS (sample AR2HH(-5))

$r = 3.5 \text{ nm}$; $V = 1.8 \times 10^{-19} \text{ cm}^3$; ($\rho = 10.5 \text{ g cm}^{-3}$); $m = 1.88 \times 10^{-18} \text{ g}$; $S = 153.86 \text{ nm}^2$, $N_{\text{Ag}} = 10\ 510$

TGA: 80% Ag, 20% DiSS; mass of DiSS per one nanoparticle $m = 4.78 \times 10^{-19} \text{ g}$; $N_{\text{ligands}} = 548$;

$d_{\text{ligands}} = 3.5 \text{ nm}^2$

XPS (S2s): Ag 23.7 % (atom %), S 2.5 %; $N_{\text{Ag}}/N_{\text{ligand}} = 18.9$; $N_{\text{ligands}} = 556$; $d_{\text{ligands}} = 3.6 \text{ nm}^2$

XPS (N1s): Ag 23.7 % (atom %); N 2,8%; $N_{\text{Ag}}/N_{\text{ligand}} = 16.9$; $N_{\text{ligands}} = 621$; $d_{\text{ligands}} = 4.0 \text{ nm}^2$

XPS (C1s): Ag 23.7 % (atom %); C 52.4%; $N_{\text{Ag}}/N_{\text{ligand}} = 10.9$; $N_{\text{ligands}} = 964$; $d_{\text{ligands}} = 6.2 \text{ nm}^2$

XPS (O1s): Ag 23.7 % (atom %); O 13.6%; $N_{\text{Ag}}/N_{\text{ligand}} = 10.4$; $N_{\text{ligands}} = 1005$; $d_{\text{ligands}} = 6.5 \text{ nm}^2$

where: nanoparticle radius, V – nanoparticle volume (idealized nanosphere), ρ - silver density, m – nanoparticle mass, S – nanoparticle surface, d_{ligands} – DiSS area density