Hybrid materials with antibacterial properties based on hyperbranched polyaminopropylalkoxysiloxanes embedded with Ag nanoparticles

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Supporting Information

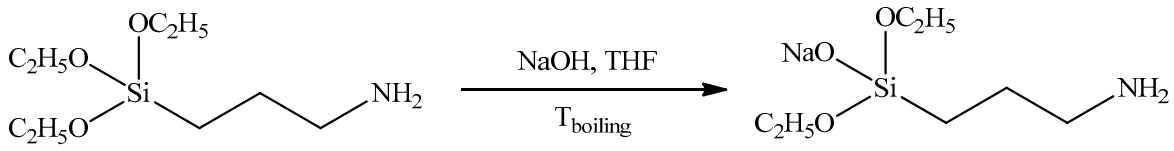

Figure S1. Scheme of synthesis of monosodium salts of (3-aminopropyl)diethoxysilanes.

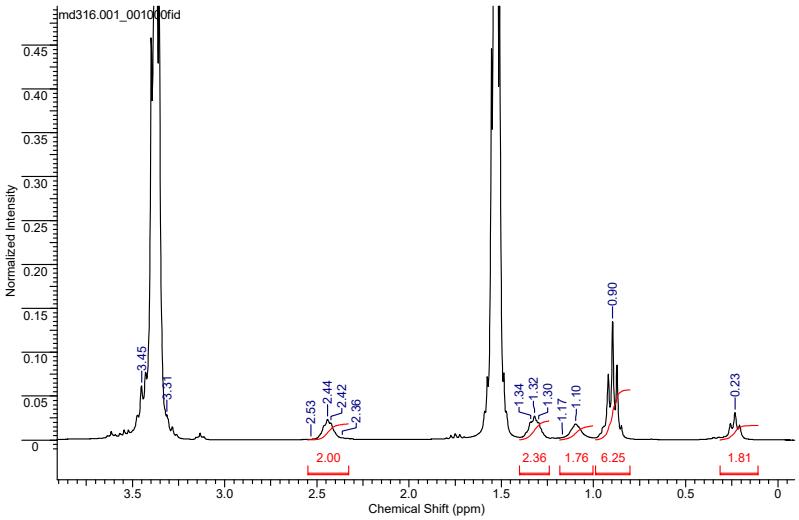

Figure S2. ^{1}H NMR Spectral data of Sodiumoxy-(3-Aminopropyl)diethoxysilane.

^{1}H NMR (300 MHz, THF) δ: 2.53-2.36 ppm (m, 2H ,-C<u>H</u>$_2$-NH$_2$), 1.34-1,30 ppm (m, 2H, -C<u>H</u>$_2$-CH$_2$-NH$_2$), 0.23 ppm (t, 2H, -Si-C<u>H</u>$_2$-, J= 7.4 Hz), 0.9 ppm (t, 6H, C<u>H</u>$_3$CH$_2$O-, J= 7 Hz), 3.45-3.31 ppm (m, 4H, CH$_3$C<u>H</u>$_2$O-) 1.17-1.1 ppm (m, 2H, -N<u>H</u>$_2$)

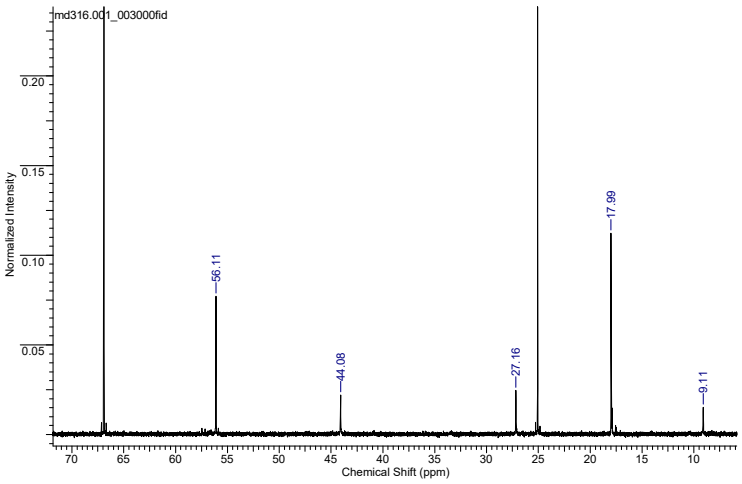

Figure S3. ^{13}C NMR Spectral data of Sodiumoxy-(3-Aminopropyl)diethoxysilane.

^{13}C NMR (THF) δ: 9.11 ppm (-Si-$\underline{C}H_2$-CH_2-), 27.16 ppm (-Si-CH_2-$\underline{C}H_2$-), 56.11 ppm (-CH_2-$\underline{C}H_2$-NH_2), 44.08 ($CH_3C\underline{H}_2O$-), 17.99 ppm ($C\underline{H}_3CH_2O$-).

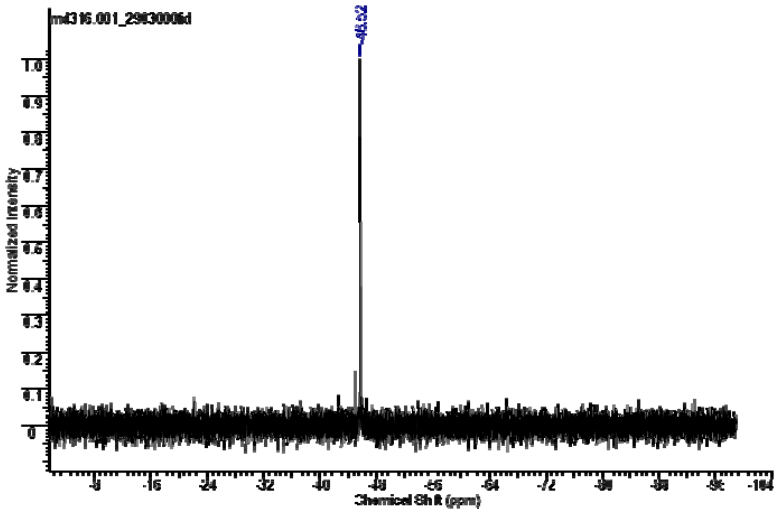

Figure S4. ^{29}Si NMR Spectral data of Sodiumoxy-(3-Aminopropyl)diethoxysilane.

^{29}Si (THF), δ: -46.52 ppm.

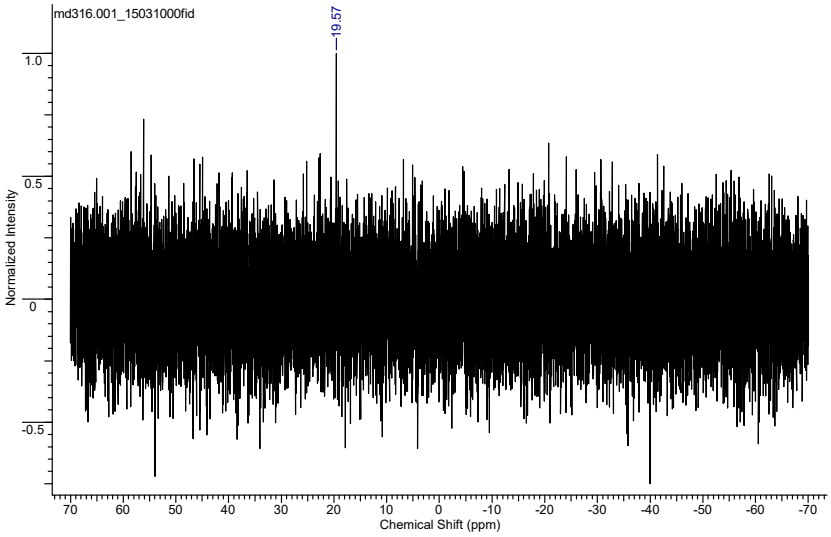

Figure S5. ^{15}N NMR Spectral data of Sodiumoxy-(3-Aminopropyl)diethoxysilan. ^{15}N (THF), δ: 19.6 ppm ($-NH_2$).

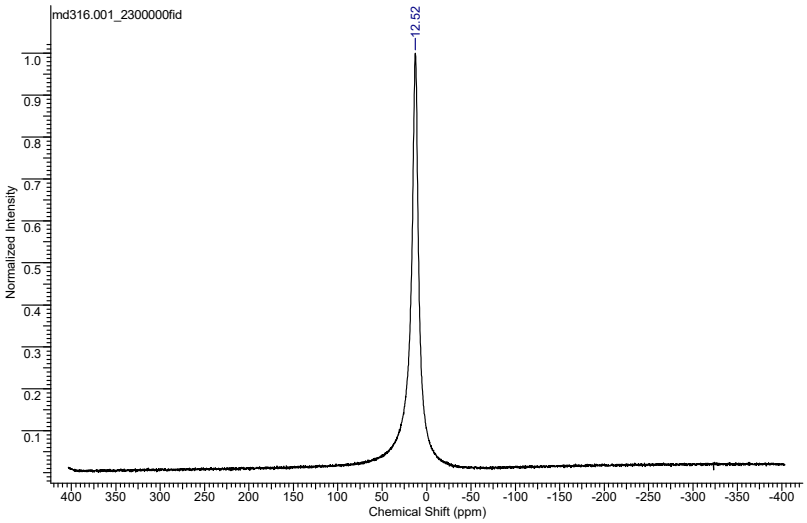

Figure S6. ^{24}Na NMR Spectral data of Sodiumoxy-(3-Aminopropyl)diethoxysilane. ^{23}Na (THF) 12.5 ppm.

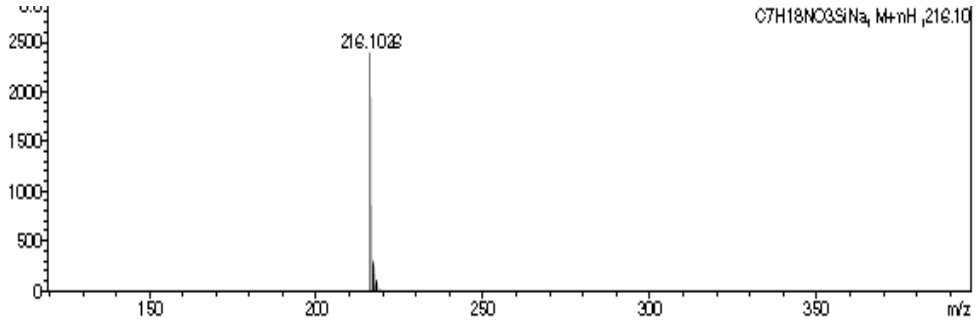

Figure S7. Mass spectra of Sodiumoxy-(3-Aminopropyl)diethoxysilane: HRMS calcd for $C_7H_{18}NNaO_3Si$: 216.1026; found: [M+nH] = 216.1024.

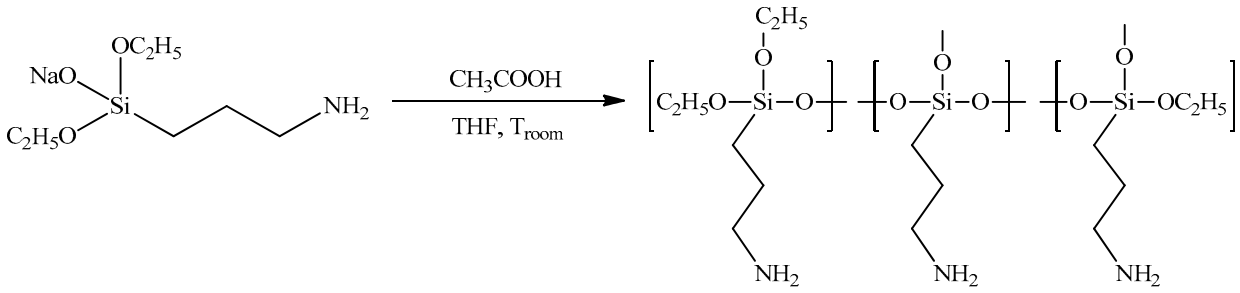

Figure S8. Scheme of synthesis of hyperbranched polyaminopropylethoxysiloxane (HBPAPES)

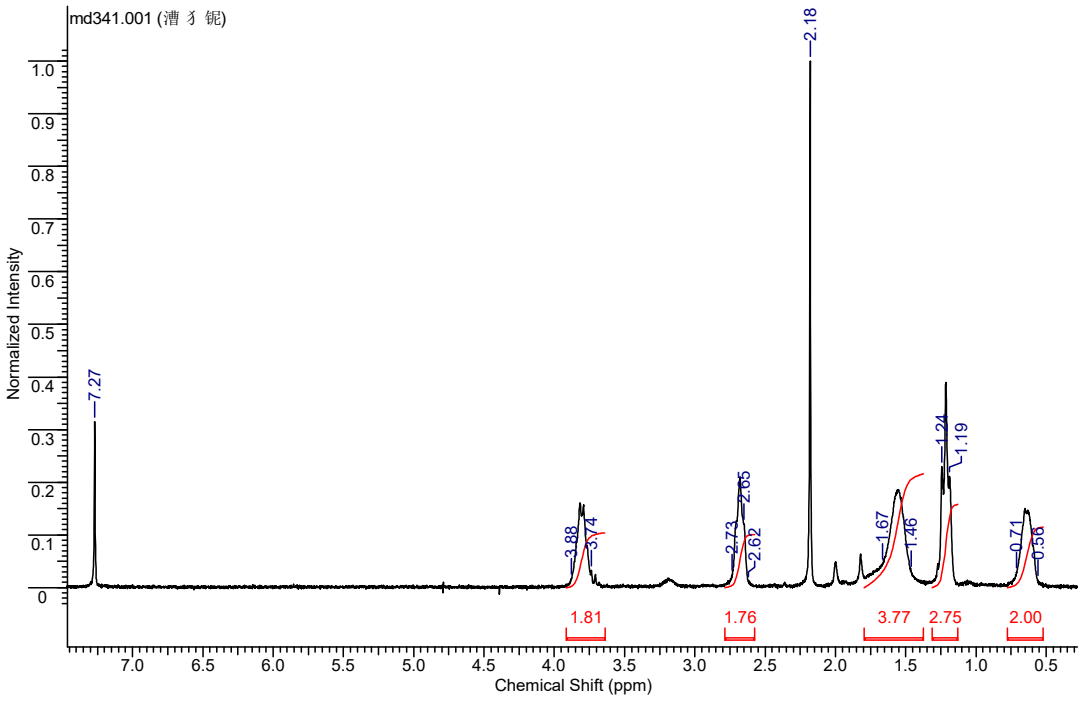

Figure S9. ^{1}H NMR Spectral data of polyaminopropylethoxysiloxane.

^{1}H NMR (300 MHz, $CDCl_3$) δ: 2.73-2.62 ppm (m, 2H ,-C<u>H</u>$_2$-NH_2), 1.67-1.46 ppm (m, 2H, -C<u>H</u>$_2$-CH_2-NH_2), 0.71-0.56 ppm (m, 2H, -Si-C<u>H</u>$_2$-), 1.24-1.19 ppm (m, 6H, C<u>H</u>$_3$$CH_2$O-), 3.88-3.74 ppm (m, 4H, CH_3C<u>H</u>$_2$O-), 1.67-1.46 ppm (m, 2H, -N<u>H</u>$_2$)

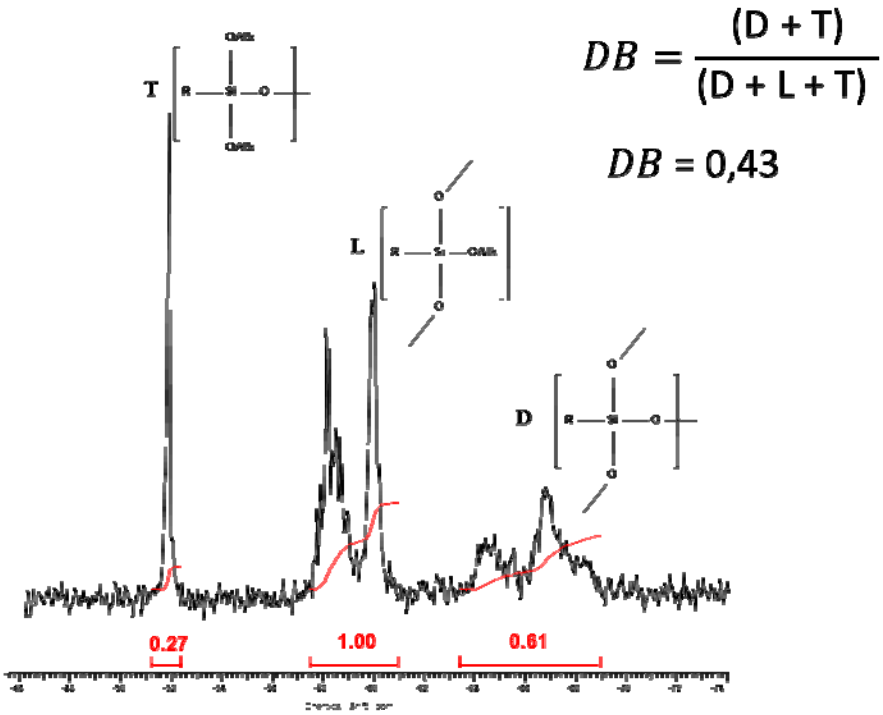

Figure S10. Degree of branching (DB) and ^{29}Si-NMR Spectral data of polyaminopropylethoxysiloxane with the addition of paramagnetic relaxation agent Chromium (III) Acetylacetonate.

^{29}Si (THF), δ: 51.89-52.3 ppm (m, R-Si$(OCH_3)_2$O-), 57.93-60.41 (m, R-Si(OCH_3)(O-)$_2$), 64.3-68.48 (m, R-Si(O-)$_3$).

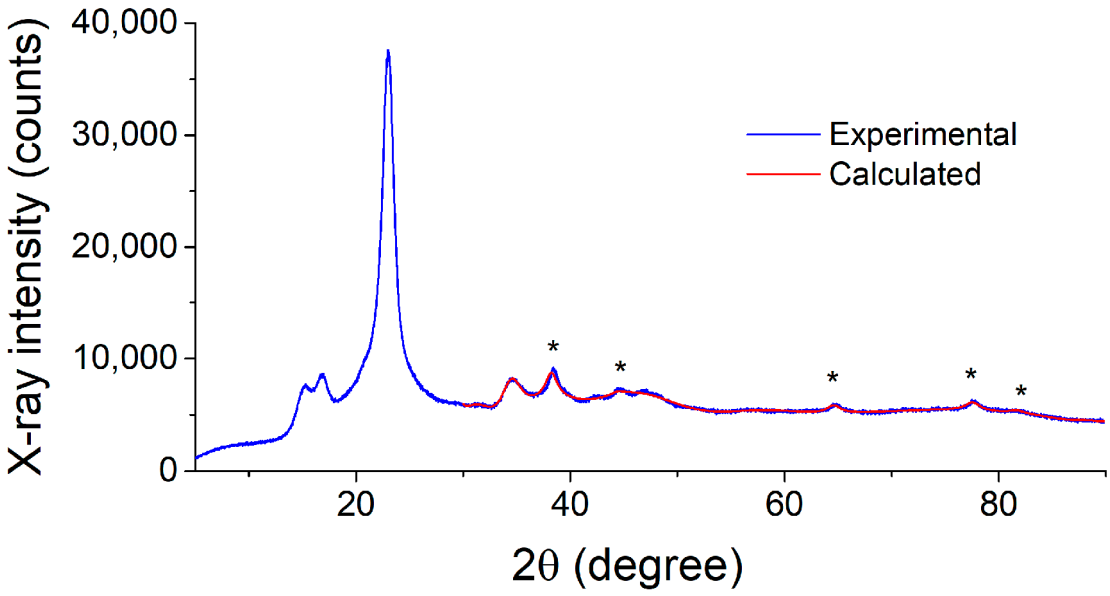

Figure S11. PXRD pattern of the Ag NPs/HBPAPES/cotton composite and its fit evidencing the presence of Ag nanoparticles. The reflections of metalic silver are marked by asterisks.

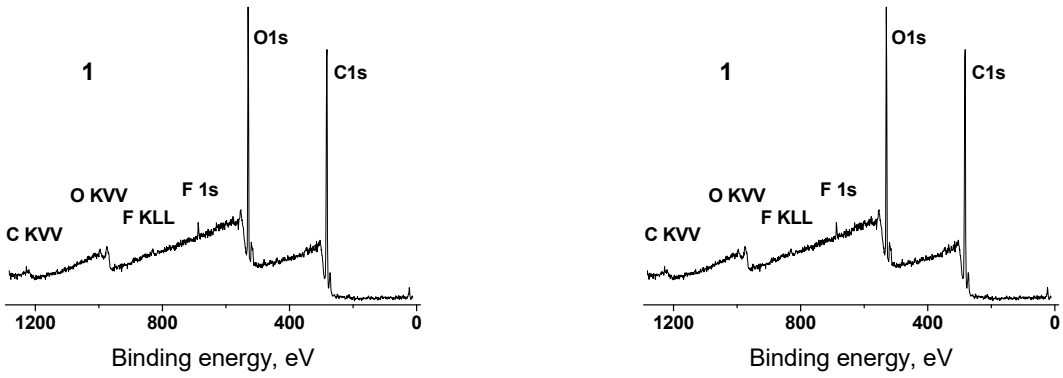

Figure S12. Survey XPS spectra of the cotton (**1**) and Ag NPs/HBPAPES/cotton (**2**) samples.

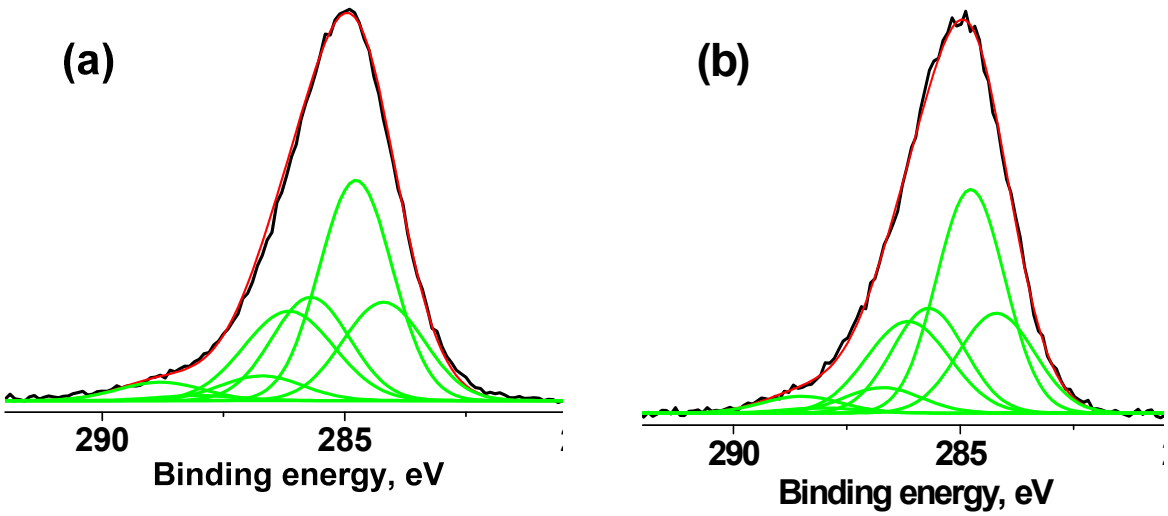

Figure S13. The C 1s spectra of the Ag NPs/HBPAPES/cotton sample: measured at U_b=0 (a) and 7 V (b) fitted in accordance to chemical structure formulas of silane and cotton.

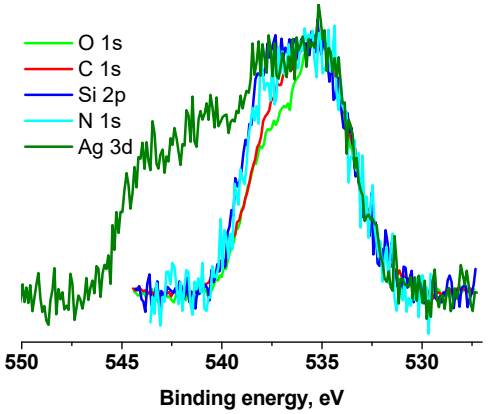

Figure S14. The O 1s, C 1s, Si 2p, N 1s and Ag 3d spectra of the Ag NPs/HBPAPES/cotton sample measured at U_b= -7 V. The figure demonstrates a coincidence of low-energy edges of all spectra which evidences on similar physical nature of low energy states.

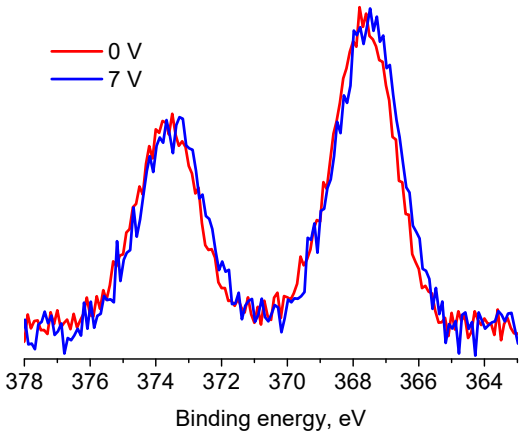

Figure S15. The Ag 3d spectra of the Ag NPs/HBPAPES/cotton sample measured at U_b = 0 V and U_b= 7 V.

Table S1. Quantification data (at. %) of the cotton and Ag NPs/HBPAPES/cotton samples recorded at various bias voltages

Sample	U_b	C	O	N	Ag	Si
Cotton	-7 V	66.1	33.9			
	0 V	67.3	32.7			
	7 V	67.8	32.2			
Ag NPs/HBPAPES/cotton	-7 V	74.1	18.6	2.7	0.6	4.1
	0 V	73.4	19.1	2.7	0.6	4.2
	7 V	74.9	17.9	2.4	0.5	4.3

Table S2. Parameters of components in C 1s and O 1s photoelectron spectra of the cotton sample: E_b – binding energy, W – peak width and I_{rel} – relative intensity.

		C 1s				O 1s			
	Peak	C1	C2	C3	C4	O1	O2	O3	O4
U_b	Parameter	C-C/C-H	C-OH	O-C-O	C(O)O	C(O*)O	C-OH	O-C-O	C(O)O*
7 V	E_b, eV	285.38	286.73	288.06	288.84	531.3	532.9	533.48	534.3
	W, eV	2.1	2.1	2.1	2.1	1.8	1.8	1.8	1.8
	I_{rel}	0.18	0.54	0.11	0.18	0.13	0.45	0.30	0.13
0 V	E_b, eV	285.38	286.73	288.06	288.76	531.3	532.91	533.49	534.3
	W, eV	2.1	2.1	2.1	2.1	1.8	1.8	1.8	1.8
	I_{rel}	0.22	0.51	0.10	0.17	0.11	0.47	0.31	0.11
-7 V	E_b, eV	285.53	286.73	288.06	288.76	531.44	532.93	533.51	534.00
	W, eV	2.1	2.1	2.1	2.1	1.8	1.75	1.79	1.8
	I_{rel}	0.19	0.53	0.11	0.17	0.13	0.44	0.30	0.13

Table S3. Parameters of peaks in C 1s photoelectron spectra of Ag NPs/HBPAPES/cotton: E_b – binding energy, W – peak width and I_{rel} – relative intensity.

		C 1s							Si $2p_{3/2}$			N 1s		Ag $3d_{5/2}$	Ag $3d_{3/2}$
U_b	Group	C-Si	C-C/C-H	C-N	C-O-Si	C-OH	O-C-O	C(O)O	Si^{4+}	Si^{3+}	Si^{4+}*	C-NH_2	*	Ag^{2+}	Ag^{2+}
0 V	E_b, eV	284.2	284.8	285.7	286.2	286.7	288.0	288.8	102.4	104.1		399.1	400.9	367.7	373.7
	W, eV	1.68	1.5	1.60	1.85	1.7	1.7	1.75	1.8	1.8		1.92	1.92	1.97	2.04
	I_{rel}	0.18	0.36	0.18	0.18	0.05	0.01	0.04	0.9	0.1		0.81	0.10	0.59	0.41
7 V	E_b, eV	284.2	284.8	285.7	286.2	286.7	288.0	288.5	102.3	103.9	99.8	399.0	401.2	367.6	373.5
	W, eV	1.68	1.50	1.60	1.83	1.7	1.7	1.75	1.8	1.8	1.8	1.88	1.89	1.96	2.00
	I_{rel}	0.18	0.36	0.18	0.18	0.05	0.01	0.03	0.77	0.12	0.11	0.88	0.12	0.6	0.4

* - differential charging