Removal of As³⁺, As⁵⁺, Sb³⁺, and Hg²⁺ Ions from Aqueous Solutions by Pure and Co-Precipitated Akaganeites Nanoparticles: Adsorption Kinetic Studies.

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Table SI_1. Equations of kinetic models of adsorption used to fit the experimental data. In these equations Q is the amount of adsorbate sorbed at instant t (mg g⁻¹), Q_{max} is the maximum amount of adsorbate sorbed (mg g⁻¹), t is the time (min), k'_{ad} is pseudo adsorption rate constant (unit for order 1: min⁻¹, order 2: g mg⁻¹ min⁻¹, unit for Langmuir: min⁻¹), k_d is desorption rate constant (min⁻¹), ϑ is a parameter of Bangham model, $\hbar$ is Bangham diffusion rate (mg g⁻¹ min⁻ᵛ), β, in the Elovich model, is the constant related to the extent of surface coverage and activation energy for chemisorption (g mg⁻¹) and α is the initial sorption rate (mg g⁻¹ min⁻¹).

Kinetic model	Nonlinear form
Langmuir	$Q = Q_{max}\left(\dfrac{k'_{ad}}{k'_{ad} + k_d}\right)\left(1 - e^{-\left(k'_{ad}+k_d\right)t}\right)$ (2)
Lagergren	$Q = Q_{max}\left(1 - e^{-k'_{ad}t}\right)$ (3)
Bangham	$Q = \hbar t^{\vartheta}$ (4)
Ho and McKay	$Q = \dfrac{(k'_{ad}Q^2_{max})t}{1 + k'_{ad}Q_{max}t}$ (5)
Elovich	$Q = \left(\dfrac{1}{\beta}\right)Ln(1 + \alpha\beta t)$ (6)
Simplified Elovich (1<< αβt)	$Q = \left(\dfrac{1}{\beta}\right)Ln(\alpha\beta t)$ (7)

Table SI_2. Experimental mean adsorption capacity at 60 min of a given adsorbate on a given adsorbate. This data can be related to the maximum adsorption capacity, Q_{max}.

Sample	Experimental Q_{max} (mg adsorbed adsorbate g^{-1} adsorbent)
pAk-Hg	4.12 ± 0.21
Ak60Hg-Hg	4.40 ± 0.22
Ak60Sb-Hg	5.51 ± 0.28
Ak60As-Hg	6.02 ± 0.30
pAk-Sb	18.41 ± 0.92
Ak60Hg-Sb	53.15 ± 2.66
Ak60Sb-Sb	50.99 ± 2.55
Ak60As-Sb	47.65 ± 2.38
Ak60Sb-As^{5+}	41.26 ± 2.06
Ak60As-As^{5+}	47.29 ± 2.36
pAk-As^{3+}	8.58 ± 0.43
Ak60Hg-As^{3+}	11.73 ± 0.59
Ak60Sb-As^{3+}	15.68 ± 0.78
Ak60As-As^{3+}	12.79 ± 0.64

Table SI_3. Results of the adjustment of the adsorption kinetics to the nonlinear kinetic models of Bangham, Simplified Elovich, Elovich and Lagergren. Here, $Q_{max.\ exp}$ is the mean experimental maximum amount of adsorbate sorbed (mg g^{-1}) at 60 minutes, k is the Bangham diffusion rate (mg g^{-1} s^{-v}), ϑ is a parameter in the Bangham model, α is the initial sorption rate in the Elovich model (mg g^{-1} s^{-1}), β is the constant related to the extent of surface coverage and activation energy for chemisorption in the Elovich model (g mg^{-1}), Q_{max} is the maximum amount of adsorbate adsorbed (mg g^{-1}) in the Lagergren model and finally, K'_{ad} is a pseudo adsorption rate constant (s^{-1}) in Lagergren model. E is the root mean square error. Empty cells with a dash indicate that the experimental data did not converge to the specified nonlinear models.

|		Nonlinear kinetic model of adsorption											
		Bangham			**Simplified Elovich**			**Elovich**			**Lagergren**		
Sample	Q_{max} exp.	k	ϑ	E	α	β	E	α	β	E	Q_{max}	K'_{ad}	E
pAk-Hg^{2+}	4.1	0.04 ±0.004	0.14 ±0.03	0.605	-	-	-	-	-	-	3.71 ±0.23	0.01 ±0.003	0.692
Ak60Hg-Hg^{2+}	4.4	0.05 ±0.002	0.11 ±0.02	0.301	-	-	-	-	-	-	4.10 ±0.12	0.02 ±0.002	0.335
Ak60Sb-Hg^{2+}	5.5	0.04 ±0.003	0.19 ±0.02	0.411	-	-	-	-	-	-	4.45 ±0.30	0.01 ±0.003	0.904
Ak60As-Hg^{2+}	6.0	0.08 ±0.002	0.07 ±0.01	0.251	-	-	-	-	-	-	5.46 ±0.15	0.03 ±0.01	0.508
pAk-As^{3+}	8.6	0.06 ±0.002	0.21 ±0.01	0.452	0.24 ±0.03	0.75 ±0.02	0.275	0.22 ±0.03	0.74 ±0.03	0.287	7.53 ±0.18	0.01 ±0.004	0.697
Ak60Hg-As^{3+}	11.7	0.1 ±0.002	0.17 ±0.01	0.351	1.13 ±0.19	0.68 ±0.02	0.322	1.09 ±0.18	0.68 ±0.02	0.321	9.87 ±0.27	0.01 ±0.001	1.256
Ak60Sb-As^{3+}	15.7	0.09 ±0.004	0.26 ±0.01	0.856	0.22 ±0.02	0.35 ±0.01	0.447	0.18 ±0.02	0.33 ±0.01	0.468	14.61 ±0.36	0.003 ±0.0003	1.208
Ak60As-As^{3+}	12.8	0.11 ±0.002	0.16 ±0.01	0.481	1.36 ±0.19	0.62 ±0.02	0.307	1.34 ±0.20	0.61 ±0.02	0.311	11.15 ±0.24	0.01 ±0.001	1.121
Ak60Sb-As^{5+}	41.3	0.22 ±0.01	0.29 ±0.01	1.550	0.43 ±0.02	0.13 ±0.002	0.684	0.32 ±0.01	0.12 ±0.001	0.477	37.81 ±1.04	0.002 ±0.0002	3.251
Ak60As-As^{5+}	47.3	0.31 ±0.01	0.22 ±0.01	2.181	1.52 ±0.31	0.15 ±0.01	2.253	1.31 ±0.27	0.15 ±0.01	1.134	-	-	-
pAk-Sb^{3+}	18.4	0.01 ±0.01	0.29 ±0.01	0.461	0.20 ±0.02	0.31 ±0.01	0.561	0.15 ±0.01	0.29 ±0.01	0.465	16.05 ±0.66	0.002 ±0.0	1.796
Ak60Hg-Sb^{3+}	53.1	0.41 ±0.01	0.19 ±0.01	1.577	3.23 ±0.81	0.14 ±0.01	2.241	3.02 ±0.78	0.14 ±0.01	2.216	-	-	-
Ak60Sb-Sb^{3+}	51.0	0.50 ±0.02	0.14 ±0.01	2.784	9.40 ±3.11	0.16 ±0.01	2.093	9.40 ±3.20	0.16 ±0.01	2.104	-	-	-
Ak60As-Sb^{3+}	47.6	0.53 ±0.01	0.10 ±0.004	0.890	176.56 ±45.05	0.25 ±0.01	0.672	176.49 ±45.08	0.25 ±0.01	0.672	42.22 ±0.79	0.02 ±0.002	3.222
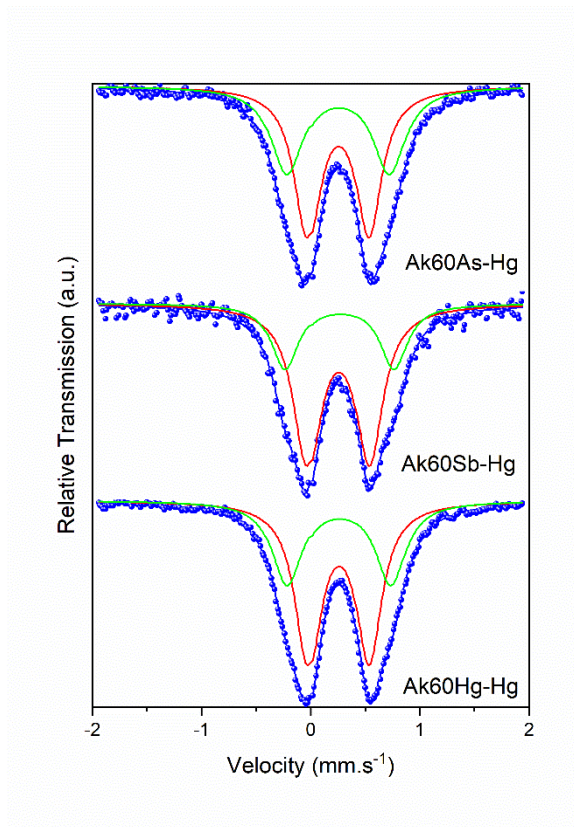
Figure SI_1. 300 K Mössbauer spectra of co-precipitated akaganeites after adsorption of Hg.
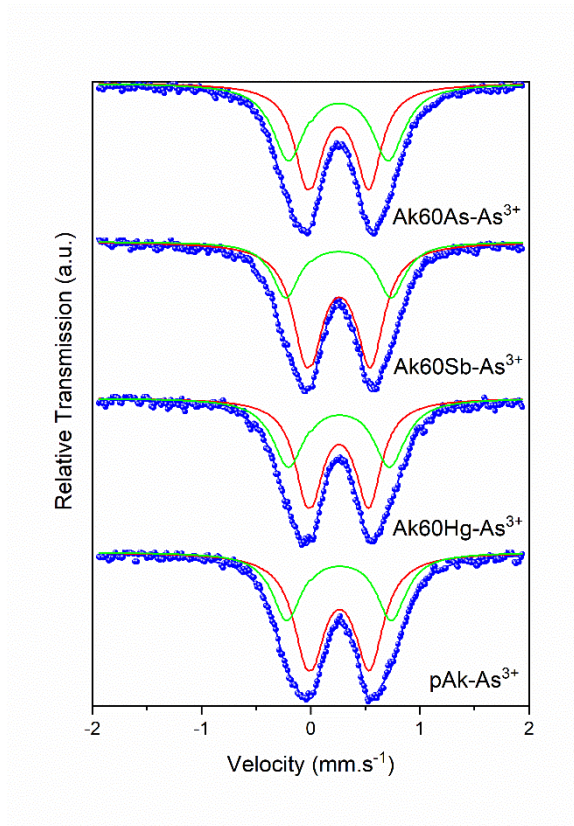
Figure SI_2. 300 K Mössbauer spectra of co-precipitated akaganeites after adsorption of As^{3+}.
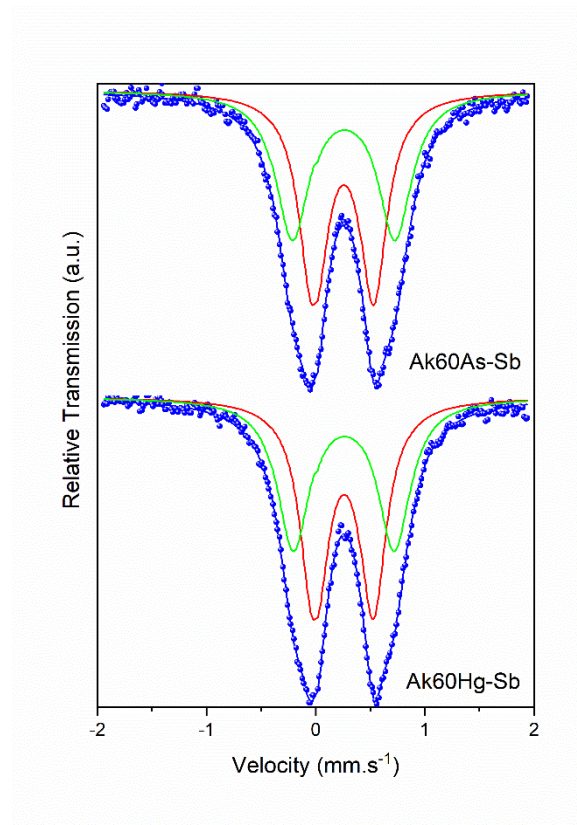
Figure SI_3. 300 K Mössbauer spectra of co-precipitated akaganeites after adsorption of Sb.
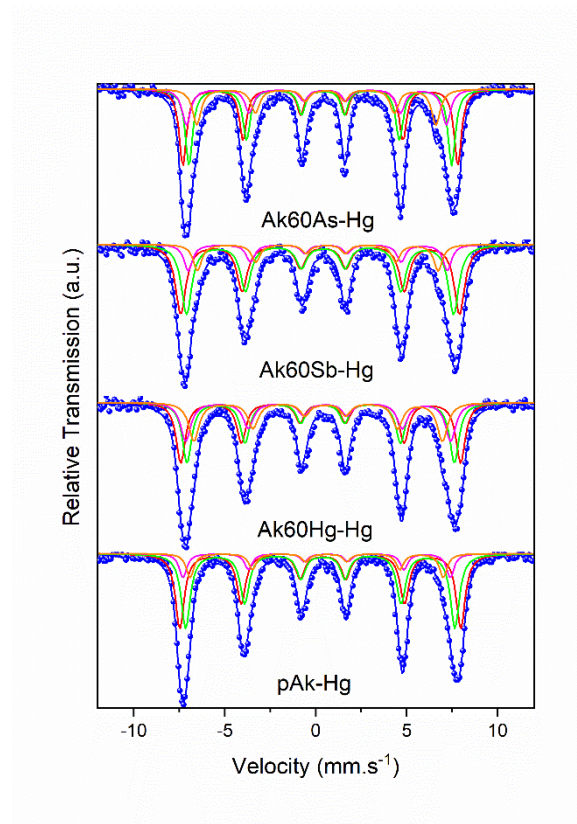

Figure SI_4. 77 K Mössbauer spectra of co-precipitated akaganeites after adsorption of Hg.
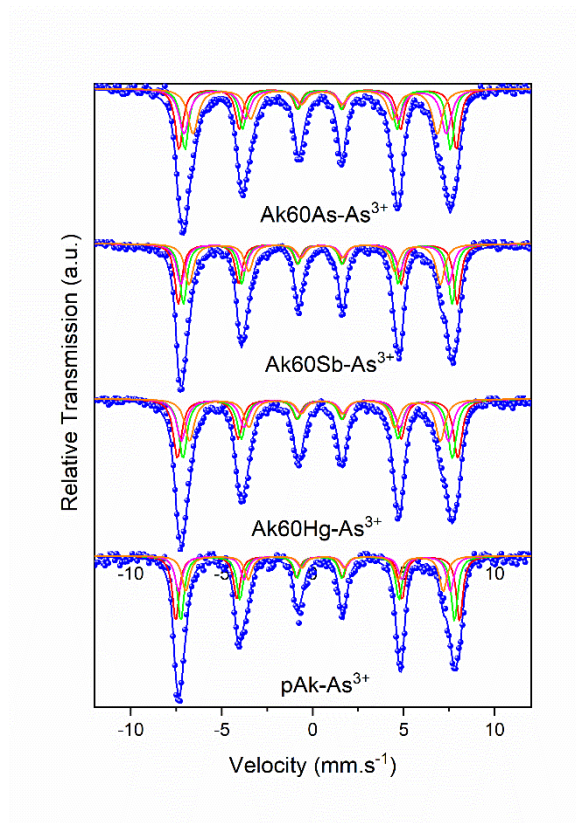
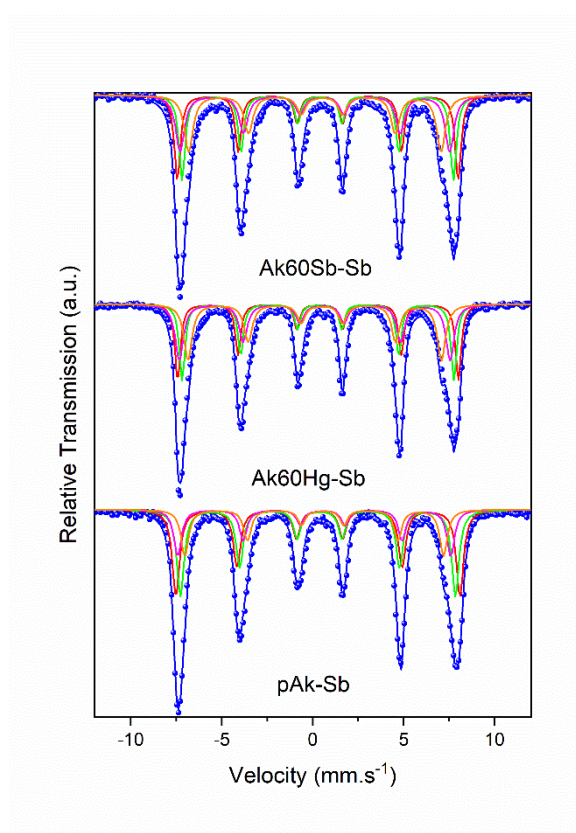**Figure SI_5.** 77 K Mössbauer spectra of co-precipitated akaganeites after adsorption of As^{3+}.

Figure SI_6. 77 K Mössbauer spectra of co-precipitated akaganeites after adsorption of Sb.

Table SI_4. Values of hyperfine parameters derived from the fits of the 300 K Mössbauer spectra for co-precipitated akaganeites before and after adsorption of different pollutants. Isomer shift (δ), quadrupole splitting (Δ), linewidth ($\Gamma/2$) and relative adsorption area (A).

Sample	Components	δ (mm/s)	Δ (mm/s)	Γ/2 (mm/s)	Area (%) ±2
pAk	D1	0.38±0.01	0.54±0.01	0.15±0.01	60
	D2	0.39±0.01	0.94±0.01	0.17±0.01	40
pAk-As^{3+}	D1	0.38±0.01	0.54±0.01	0.16±0.01	62
	D2	0.38±0.01	0.95±0.02	0.16±0.01	38
Ak60Hg	D1	0.38±0.002	0.55±0.01	0.16±0.002	62
	D2	0.38±0.002	0.94±0.01	0.18±0.01	38
Ak60Hg-Hg	D1	0.38±0.01	0.55±0.01	0.14±0.01	62
	D2	0.38±0.01	0.94±0.01	0.17±0.01	38
Ak60Hg-Sb	D1	0.38±0.01	0.53±0.01	0.15±0.01	53
	D2	0.38±0.01	0.91±0.01	0.18±0.01	47
Ak60Hg-As^{3+}	D1	0.38±0.01	0.54±0.01	0.15±0.01	56
	D2	0.38±0.01	0.91±0.01	0.18±0.01	44
Ak60Sb	D1	0.38±0.01	0.54±0.00	0.17±0.01	65
	D2	0.38±0.01	0.95±0.01	0.18±0.01	35
Ak60Sb-Hg	D1	0.37±0.01	0.56±0.01	0.15±0.01	70
	D2	0.39±0.01	0.99±0.01	0.15±0.01	30
Ak60Sb-As^{3+}	D1	0.38±0.01	0.56±0.01	0.16±0.01	69
	D2	0.38±0.01	0.95±0.01	0.15±0.01	31
Ak60As	D1	0.38±0.01	0.56±0.01	0.17±0.01	59
	D2	0.38±0.01	0.94±0.01	0.20±0.01	41
Ak60As-Hg	D1	0.37±0.01	0.55±0.01	0.14±0.01	57
	D2	0.37±0.01	0.93±0.01	0.18±0.01	43
Ak60As-Sb	D1	0.37±0.01	0.54±0.01	0.15±0.01	53
	D2	0.38±0.01	0.93±0.01	0.19±0.01	47
Ak60As-As^{3+}	D1	0.37±0.01	0.54±0.01	0.14±0.01	52
	D2	0.38±0.01	0.90±0.01	0.18±0.01	48

Table SI_5. Values of hyperfine parameters derived from the fits of the 77 K Mössbauer spectra for co-precipitated akaganeites before and after adsorption of different pollutants. Isomer shift (δ), quadrupolar shift (2ε), hyperfine field (B_{hf}) and relative adsorption area (A).

Sample	S1				S2				S3				S4			
	δ (mm/s)	2ε (mm/s)	B (T)	Area (%) ±2	δ (mm/s)	2ε (mm/s)	B (T)	Area (%) ±2	δ (mm/s)	2ε (mm/s)	B (T)	Area (%) ±2	δ (mm/s)	2ε (mm/s)	B (T)	Area (%) ±2
pAk	0.50 ±0.01	-0.09 ±0.01	48 ±0.5	28	0.50 ±0.01	-0.09 ±0.01	46.5 ±0.8	28	0.47 ±0.01	-0.39 ±0.02	46.3 ±2.0	22	0.47 ±0.01	-0.39 ±0.02	44.0 ±1.2	22
pAk-Hg	0.48 ±0.01	-0.14 ±0.01	47.7 ±0.1	39	0.48 ±0.01	-0.14 ±0.01	45.7 ±0.1	39	0.47 ±0.01	-0.53 ±0.04	45.4 ±29	11	0.47 ±0.01	-0.53 ±0.04	43.0 ±20	11
pAk-Sb	0.49 ±0.01	-0.09 ±0.01	48.2 ±0.1	32	0.49 ±0.01	-0.09 ±0.01	46.7 ±0.1	32	0.47 ±0.01	-0.47 ±0.02	46.4 ±21	18	0.47 ±0.01	-0.47 ±0.02	43.9 ±12	18
pAk-As^{3+}	0.48 ±0.01	-0.10 ±0.02	48.2 ±0.1	31	0.48 ±0.01	-0.10 ±0.02	46.5 ±0.1	31	0.50 ±0.01	-0.48 ±0.03	46.1 ±24	19	0.50 ±0.01	-0.48 ±0.03	43.7 ±16	19
Ak60Hg	0.48 ±0.01	-0.13 ±0.01	47.2 ±0.5	30	0.48 ±0.01	-0.13 ±0.01	45.6 ±0.6	30	0.46 ±0.01	-0.40 ±0.02	45.1 ±1.7	20	0.46 ±0.01	-0.40 ±0.02	42.3 ±1.04	20
Ak60Hg-Hg	0.49 ±0.01	-0.12 ±0.02	47.5 ±0.1	29	0.49 ±0.01	-0.12 ±0.02	45.4 ±13	29	0.49 ±0.01	-0.39 ±0.03	45.0 ±31	21	0.49 ±0.01	-0.39 ±0.03	42.2 ±19	21
Ak60Hg-Sb	0.50 ±0.01	-0.09 ±0.01	47.7 ±0.1	24	0.50 ±0.01	-0.09 ±0.01	46.1 ±0.1	24	0.46 ±0.01	-0.40 ±0.02	46.0 ±18	26	0.46 ±0.01	-0.40 ±0.02	43.0 ±10	26
Ak60Hg-As^{3+}	0.49 ±0.01	-0.11 ±0.02	47.6 ±0.1	28	0.49 ±0.01	-0.11 ±0.02	45.7 ±11	28	0.47 ±0.01	-0.38 ±0.02	45.3 ±25	22	0.47 ±0.01	-0.38 ±0.02	42.5 ±15	22
Ak60Sb	0.50 ±0.004	-0.14 ±0.01	47.2 ±0.5	30	0.50 ±0.004	-0.14 ±0.01	47.2 ±0.5	30	0.47 ±0.01	-0.41 ±0.04	45.1 ±1.6	20	0.47 ±0.01	-0.41 ±0.04	42.3 ±1.0	20
Ak60Sb-Hg	0.48 ±0.01	-0.17 ±0.01	47.3 ±0.1	38	0.48 ±0.01	-0.17 ±0.01	45.3 ±11.0	38	0.49 ±0.01	-0.44 ±0.03	43.9 ±27	12	0.49 ±0.01	-0.44 ±0.03	40.8 ±19	12
Ak60Sb-Sb	0.49 ±0.01	-0.12 ±0.01	47.7 ±0.1	26	0.49 ±0.01	-0.12 ±0.01	46.1 ±0.1	26	0.47 ±0.01	-0.39 ±0.02	45.7 ±21	24	0.47 ±0.01	-0.39 ±0.02	42.8 ±12	24
Ak60Sb-As^{3+}	0.50 ±0.01	-0.12 ±0.01	47.3 ±0.1	28	0.50 ±0.01	-0.12 ±0.01	45.6 ±0.1	28	0.46 ±0.01	-0.38 ±0.02	45.5 ±20	22	0.46 ±0.01	-0.38 ±0.02	42.6 ±13	22
Ak60As	0.48 ±0.01	-0.14 ±0.01	46.7 ±0.7	27	0.48 ±0.01	-0.14 ±0.01	44.9 ±0.8	27	0.45 ±0.01	-0.38 ±0.02	44.2 ±2.5	23	0.45 ±0.01	-0.38 ±0.02	41.1 ±1.5	23
Ak60As-Hg	0.48 ±0.01	-0.15 ±0.01	46.7 ±0.1	32	0.48 ±0.01	-0.15 ±0.01	44.6 ±0.1	32	0.42 ±0.01	-0.46 ±0.03	44.1 ±22	18	0.42 ±0.01	-0.46 ±0.03	40.5 ±15	18
Ak60As-As^{3+}	0.49 ±0.01	-0.12 ±0.02	47.1 ±0.1	25	0.49 ±0.01	-0.12 ±0.02	45.1 ±10	25	0.47 ±0.01	-0.36 ±0.02	44.5 ±29	25	0.47 ±0.01	-0.36 ±0.02	41.4 ±16	25

Table SI_6. Mean values of hyperfine parameters derived from the fits of the 300 K Mössbauer spectra for co-precipitated akaganeites before and after adsorption of different pollutants. Isomer shift (δ), quadrupole splitting (Δ) and linewidth ($\Gamma/2$).

Sample	Mean δ (mm/s)	Mean Δ (mm/s)	Mean Γ/2 (mm/s)
pAk	0.38	0.70	0.16
pAk-As^{3+}	0.38	0.70	0.16
Ak60Hg	0.38	0.70	0.16
Ak60Hg-Hg	0.38	0.70	0.15
Ak60Hg-Sb	0.38	0.71	0.16
Ak60Hg-As^{3+}	0.38	0.70	0.6
Ak60Sb	0.38	0.69	0.17
Ak60Sb-Hg	0.38	0.69	0.15
Ak60Sb-As^{3+}	0.38	0.68	0.15
Ak60As	0.38	0.72	0.18
Ak60As-Hg	0.37	0.71	0.16
Ak60As-Sb	0.37	0.72	0.17
Ak60As-As^{3+}	0.37	0.71	0.16

Table SI_7. Mean values of hyperfine parameters derived from the fits of the 77 K Mössbauer spectra for co-precipitated akaganeites before and after adsorption of different pollutants. Isomer shift (δ), quadrupolar shift (2ε), linewidth (Γ/2) and hyperfine field (B$_{hf}$).

Sample	Mean δ (mm/s)	Mean 2ε (mm/s)	Mean Γ/2 (mm/s)	Mean B$_{hf}$ (T)
pAk	0.49	-0.22	0.21	46.3
pAk-Hg	0.48	-0.23	0.29	46.1
pAk-Sb	0.48	-0.23	0.25	46.6
pAk-As^{3+}	0.49	-0.24	0.23	46.4
Ak60Hg	0.47	-0.24	0.23	45.3
Ak60Hg-Hg	0.49	-0.23	0.32	45.3
Ak60Hg-Sb	0.49	-0.25	0.23	45.6
Ak60Hg-As^{3+}	0.48	-0.23	0.29	45.4
Ak60Sb	0.49	-0.25	0.23	45.8
Ak60Sb-Hg	0.49	-0.24	0.33	45.4
Ak60Sb-Sb	0.48	-0.25	0.25	45.6
Ak60Sb-As^{3+}	0.48	-0.24	0.26	45.4
Ak60As	0.47	-0.25	0.25	44.4
Ak60As-Hg	0.46	-0.26	0.26	44.5
Ak60As-As^{3+}	0.48	-0.24	0.29	44.5