Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information

Connecting Concepts of Coinage Metal Stability Across Length Scales

Kathryn A. Johnston,[†] Lisa M. Stabryla,[‡] Leanne M. Gilbertson,[‡] and Jill E. Millstone[†]*

[†]Department of Chemistry, University of Pittsburgh, 219 Parkman Avenue, Pittsburgh, PA 15260, United States

[‡]Department of Civil and Environmental Engineering, University of Pittsburgh, 3700 O'Hara Street, Pittsburgh, PA, 15261, United States

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Table S1. Compilation of data from papers that report Ag(I) ion release as a function of AgNP size. Also shown are calculations of the surface area-normalized Ag(I) ion release, where the Ag(I) ion release is shown in units of mg/m^2. In many cases, the Ag(I) ion release trends reported in these papers are as a function of AgNP diameter, and the general trend is that as the AgNP diameter decreases, the Ag(I) ion release increases. However, when examining these trends in terms of exposed surface area, some studies find that as the exposed surface area increases, the Ag(I) ion release also increases, but others find that as the exposed surface area increases, the Ag(I) ion release decreases. These discrepancies could be due to factors such as particle aggregation or coalescence as a function of time.

Reference # from main text	Conditions[a]	AgNP diameter (nm)	Initial [Ag] (ppm)	% Ag(I) ion release	[Ag(I)] released (ppm)	Total surface area per liter (m^2/L)	Surface area-normalized Ag(I) ion release (mg/m^2)
160	GA-AgNPs	5.5	5	51	2.55	0.52	4.93
		22.8		5.8	0.29	0.12	2.32
	PVP-AgNPs	4.7		62.9	3.15	0.61	5.20
		8.4		14.5	0.73	0.34	2.14
		26.3		6	0.30	0.11	2.77
		38.2		4.1	0.21	0.07	2.75
184	Acetate buffer, 24 hrs	4.8	0.05	85	0.043	5.9E-3	7.17
		60	0.05	47.4	0.024	4.74E-4	49.99
		Foil (4 x 4 x 0.127 mm)	10,700	1.10E-5	1.18E-3	0.02	0.069
186	Aerobic, 120 hrs	4.7	2	N/A	2.12	0.24	8.77
		10.5		N/A	1.25	0.11	11.57
195	28 days	4	40	69.5	27.8	5.69	4.89
		6.1		47	18.8	3.73	5.04
		8.7		21.3	8.52	2.62	3.26
197	pH 7.3, 35 days	4.9	9.8	N/A	2.17	1.14	1.91
		9.5	10.5	N/A	0.24	0.63	0.37
		19.8	10.4	N/A	0.19	0.30	0.64
198	H_2O, 80 days	6.2	7.92	15	1.19	0.73	1.63
		9.2		5.8	0.46	0.49	0.94
		12.9		3.3	0.26	0.35	0.75
		70.5		0.4	0.03	0.06	0.50
	Acetic acid, 27-34 days	6.2		41.3	3.27	0.73	4.50
		9.2		20.9	1.65	0.49	3.38
		12.9		13.6	1.08	0.35	3.08
		70.5		6.9	0.55	0.06	8.55
199	UPW, 4 hrs	11.6	1	1.3	0.013	0.05	0.27
		17.8		1.4	0.014	0.03	0.44
		47.7		0.7	7E-3	0.012	0.59
		56.5		0.6	6E-3	0.010	0.60
		94.8		0.6	6E-3	0.006	1.00
200		20	12.7	4.5	0.57	0.36	1.58

	BEGM, PVP-AgNPs, 24 hrs	110		2.5	0.32	0.07	4.83
	BEGM, citrate-AgNPs, 24 hrs	20		4.3	0.55	0.36	1.51
		110		2.2	0.28	0.07	4.25
201	Low initial [Ag]	20	0.2	N/A	0.04	6E-3	7.03
		80	1	N/A	0.06	7E-3	8.44
	Middle initial [Ag]	20	0.83	N/A	0.15	0.024	6.35
		80	2.1	N/A	0.1	0.015	6.70
	High initial [Ag]	20	1.4	N/A	0.5	0.04	12.55
		80	3.4	N/A	0.16	0.024	6.62
202	PVP-AgNPs, R2, 115 days	6.5	1	79.1	0.79	0.09	9.04
		53.4		27.7	0.28	0.01	26
	PVP-AgNPs, lake, 99 days	6.5		85.7	0.86	0.09	9.79
		53.4		7.2	0.07	0.01	6.76
204	Low initial [Ag], 337 days	19.9	0.3	N/A	0.12	9E-3	14.22
		40		N/A	0.07	4.3E-3	15.44
		80		N/A	0.03	2.1E-3	14.53
	High initial [Ag], 337 days	19.9	0.6	N/A	0.18	0.02	10.20
		40		N/A	0.12	9E-3	14.29
		80		N/A	0.05	4.3E-3	11.53
206	Citrate-AgNPs, 24 hrs	10	10	23.7	2.37	0.57	4.17
		40		7	0.7	0.14	4.92
		75		6.6	0.66	0.08	8.70
207	28 hrs	30	5	51.5	2.58	0.09	27.15
		160		40.4	2.02	0.018	113.61
		460		29.2	1.46	6E-3	236.08
208	GA-AgNPs, 24.5 hrs	5	3.21	26.8	0.86	0.37	2.36
		22		2.7	0.09	0.08	1.04
	PVP-AgNPs, 24 hrs	8		1.6	0.05	0.23	0.22
		38		3.1	0.10	0.05	2.07
209	LB, 24 hrs	9.1	12.5	7	0.88	0.78	1.12
		19.1		5.7	0.71	0.37	1.91
		43.5		4.7	0.59	0.16	3.59

[a]Abbreviations: Luria-Bertani broth (LB), gum arabic (GA), polyvinylpyrrolidone (PVP), ultra pure water (UPW), bronchial epithelial cell growth medium (BEGM), river water (R2)

Table S2. Compilation of data from papers that report Ag(I) ion release in the presence of additional small molecules in solution. Also shown are estimates of the small molecule:Ag mole ratios and the conclusions reached in these papers about how the small molecules impact Ag(I) ion release. A low molecule:Ag mole ratio does not always lead to increased Ag(I) ion release and vice versa. These discrepancies may be due to variation in the affinities of these molecules for Ag(I) ions or the reduced metal NP surface, or interactions of the molecules with one another, among other possibilities.

Reference # from main text	Initial [Ag]	Molecule[a]	[Molecule][b]	Molecule:Ag mole ratio (low)[c]	Molecule:Ag mole ratio (high)[c]	Paper conclusion
184	2 mg/L	cysteine, glutathione	0.00005 – 1 mM	0.003	53.5	Decreased release
185	0.35 g/L	cysteine	1 g/L	2.52	N/A	Decreased release
267	5 μM	cysteine	1000, 10,000 nM	0.2	2	Increased release
272	27.8 μM	glutathione	16.7, 83.3, 416.3 μM	0.6	15	Increased release
293	171 μg/L	citrate	50 mg C/L	2607	N/A	Decreased release
313	8 μM	cysteine	400 μM	50	N/A	Increased release
316	370 μM	glutathione	370 μM	1	N/A	Increased release
317	5 μM	cysteine	0.2, 0.5, 2, 5 μM	0.04	1	Decreased release
318	Not reported	cysteine	0.1, 1, 10 mg/L	Not reported	Not reported	Decreased release
319	1.6 mg/mL	EDTA	0 – 800 mg/L	0.002	0.18	Decreased release
320	500 μg/L	cysteine	0.1 – 10 μM	0.02	2.14	Decreased release

[a]Abbreviation: ethylenediaminetetraacetic acid (EDTA)

[b]In some papers, these concentrations are reported in milligrams of carbon per liter. Where these units were reported, the molecule:Ag calculations done here used the molecular weight of carbon. Where these units were not used or the units were not specified, we assumed that the reported concentrations were in terms of the overall small molecule, so the molecule:Ag calculations were done using the molecular weights of the small molecules.

[c]Where there was more than one concentration of small molecule reported, we evaluate the small molecule:Ag ratio for the lowest and highest small molecule concentrations. Where only one concentration of small molecule was reported, we calculate only one small molecule:Ag ratio.

Table S3. Compilation of data from papers that report Ag(I) ion release in the presence of NOM in solution. Also shown are estimations of the NOM:Ag mole ratios and the conclusions reached in these papers about how NOM impacts Ag(I) ion release. Some of these papers seem to observe a trend where a low NOM:Ag mole ratio leads to increased Ag(I) ion release and a high NOM:Ag mole ratio leads to decreased Ag(I) ion release.

Reference # from main text	Initial [Ag]	NOM type[a]	[NOM][b]	NOM:Ag mole ratio (low)[c]	NOM:Ag mole ratio (high)[c]	Paper conclusion
187	0.05 mg/L	SRHA	5 – 50 mg/L	10.7	107	Decreased release
216	5 mg/L	PLFA[d]	600 mg/L	9.9	N/A	Decreased release
224	2.8 µg/L	SRDOC	1.46 mg C/L	4649	N/A	Decreased release
224	11.5 µg/L	SRDOC	10.43 mg C/L	8087	N/A	Decreased release
293	171 µg/L	SRFA	300 mg C/L	15,643	N/A	Decreased release
318	Not reported	DOC	10 – 25 mg/L	Not reported	Not reported	Increased release
319	1 mg/mL	alginate	2 – 333 mg C/L	0.018	3	Decreased release
321	5 mg/L	PLFA	1 – 10 mg C/L	0.2	2	Increased release
322	1 mg/L	BSA	600 mg/L	0.97	N/A	Increased release
322	1.6 mg/L	alginate[e]	600 mg/L	0.1	4	Decreased release
323	100 µg/L	PLFA[d]	30 mg/L	24.7	N/A	Increased release
324	1 mg/L	Suwanee River NOM	10 – 80 mg/L	1.07	8.56	Decreased release

[a]Abbreviations: Pony Lake fulvic acid (PLFA), bovine serum albumin (BSA), dissolved organic carbon (DOC), Suwannee River humic acid (SRHA), Suwannee River dissolved organic carbon (SRDOC), Suwannee River fulvic acid (SRFA)

[b]It is most common for the concentrations of these NOM molecules to be reported in milligrams of carbon per liter. Where these units were reported, the NOM:Ag calculations done here used the molecular weight of carbon. Where these units were not used or the units were not specified, we assumed that the reported concentrations were in terms of the overall NOM species, so the NOM:Ag calculations were done using estimated molecular weights of the NOM species.

[c]Where there was more than one concentration of NOM reported, we evaluate the NOM:Ag ratio for the lowest and highest NOM concentrations. Where only one concentration of NOM was report, we calculate only one NOM:Ag ratio.

[d]PLFA molecular weight ≈ 1300 Da[1]

[e]Alginate molecular weight = 10,000 – 600,000 Da

References

1. A. Brown, D. M. McKnight, Y.-P. Chin, E. C. Roberts and M. Uhle, Chemical characterization of dissolved organic material in Pony Lake, a saline coastal pond in Antarctica, *Mar. Chem.*, 2004, **89**, 327-337.