## Supporting information

## Uptake of Toxic Metal Ions from Water by Naked and Monolayer Protected Silver Nanoparticles: An X-ray Photoelectron Spectroscopic Investigation

M. S. Bootharaju and T. Pradeep\*

DST Unit on Nanoscience (DST UNS), Department of Chemistry and Sophisticated Analytical Instrument Facility, Indian Institute of Technology Madras, Chennai - 600 036, India.

\*E-mail: pradeep@iitm.ac.in



**Figure S1.** UV-vis absorption spectra of Ag@citrate (A) and Ag@MSA (B) nanoparticles. Insets of A and B correspond to TEM images of Ag@citrate and Ag@MSA nanoparticles, respectively.



**Figure S2.** FTIR (A) and XRD (B) patterns. The traces (a) and (b) correspond to Ag@citrate and Ag@MSA nanoparticles, respectively.



Figure S3. XPS survey spectra of Ag@citrate (a) and Ag@MSA (b) nanoparticles. Peaks due to the Mo substrate also appears in trace (a).



**Figure S4.** UV-vis spectra of Ag@citrate-Hg(II) reactions at 0.05, 0.1, 10, 50 and 100 ppm (a, b, c, d and e, respectively), after 24 h.



**Figure S5**. FTIR spectra of Ag@citrate nanoparticles treated with 10, 50 and 100 ppm Hg(II) solutions (B, C and D). The region 1850-450 alone is shown here for understanding the interaction of Hg(II) with functional groups of Ag@citrate. A is FTIR of Ag@citrate.



Figure S6. FTIR spectrum of Hg-citrate in the region 1850 - 450 cm<sup>-1</sup>.



Figure S7. SEM image (A) and EDAX spectrum (B) of Ag@citrate nanoparticles treated with 100 ppm Hg(II) solution, after 24 h. The Si peak is due to the substrate.



**Figure S8**. TEM images (left) of Ag@citrate nanoparticles treated with 0.1, 10 and 100 ppm (A, B and C) of Hg(II) ions. The uptake of mercury by nanoparticles is mapped (right of each TEM figure) and in 0.1 ppm case no mercury is observed. The elemental images are slightly rotated anticlockwise with respect to the TEM images.



**Figure S9**. The EDAX spectra of Ag@citrate nanoparticles treated with 0.1, 10 and 100 ppm (A, B and C) of Hg(II) ions. At 2.2 keV position, no mercury was seen in 0.1 ppm sample and it's presence is observed in both 10 and 100 ppm sample. The scale of the top is not the same as in others.



**Figure S10.** DLS of Ag@citrate (A) and Ag@citrate treated with 0.1, 10 and 100 ppm (B, C and D, respectively) Hg(II) solutions. The average hydrodynamic diameters are also shown. Polydispersity is observed as typical of Ag@citrate.



Figure S11. XPS survey spectrum (A), core level spectra of Hg 4f (B), O 1s (C) and C 1s (D) of Hg-citrate.





**Figure S12.** UV-vis of Ag@MSA-Hg(II) reactions at 10, 50 and 100 ppm (a, b, c and d), after 24 h. Trace a corresponds to Ag@MSA.

**Figure S13.** FTIR spectra of Ag@MSA nanoparticles treated with 10, 50 and 100 ppm Hg(II) solutions (B, C and D). The region 1850-450 alone is shown here for understanding the interaction of Hg(II) with functional groups of Ag@MSA. A is FTIR of Ag@MSA.



Figure S14. SEM image (A) and EDAX spectrum (B) of Ag@MSA nanoparticles treated with 100 ppm Hg(II) solution, after 24 h. Adventitious species (Si and Sn) in EDAX are due to the substrate.



Figure S15. O 1s spectrum of Ag@MSA nanoparticles treated with 10, 50 and 100 ppm Hg(II) solutions (traces a, b and c), after 24 h.



**Figure S16.** UV-vis (A) and IR spectra (B) of Ag@citrate-Hg(I) interaction. Spectra were collected after 24 h. Traces (a), (b), (c) and (d) in both A and B corresponds to Ag@citrate, 10, 30 and 50 ppm residues, respectively.



**Figure S17.** SEM image (A) and EDAX spectrum (B) of Ag@citrate nanoparticles treated with 50 ppm Hg(I) solution, after 24 h. Si and Sn peaks are due to the substrate.



**Figure S18.** UV-vis (A) and IR spectra (B) of Ag@MSA-Hg(I) reactions at 10, 30 and 50 ppm, after 24 h. Traces (a), (b), (c) and (d) in both A and B corresponds to Ag@MSA, 10, 30 and 50 ppm residues, respectively.



**Figure S19.** SEM image (A) and EDAX spectrum (B) of Ag@MSA nanoparticles treated with 50 ppm Hg(I) solution, after 24 h. Large aggregates are seen. Adventitious species in EDAX are due to the substrate.



Figure S20. O 1s core level XPS spectra of Ag@MSA nanoparticles treated with 10, 30 and 50 ppm Hg(I) solutions (traces a, b and c), after 24 h.



**Figure S21.** UV-vis (A) and IR spectra (B) of Ag@citrate-Cd(II) reactions at 10, 50 and 100 ppm, after 24 h. Traces (a), (b), (c) and (d) in both A and B corresponds to Ag@citrate, 10, 50 and 100 ppm residues, respectively.



**Figure S22.** SEM image (A) and EDAX spectrum (B) of Ag@citrate nanoparticles treated with 100 ppm Cd(II) solution, after 24 h. Adventitious species in EDAX are due to the substrate.



**Figure S23.** UV-vis (A) and IR spectra (B) of Ag@citrate-Pb(II) reactions at 10, 50 and 100 ppm, after 24 h. Traces (a), (b), (c) and (d) in both A and B correspond to Ag@citrate, 10, 50 and 100 ppm residues, respectively.



**Figure S24.** SEM image (A) and EDAX spectrum (B) of Ag@citrate nanoparticles treated with 100 ppm Pb(II) solution, after 24 h. Adventitious species in EDAX are due to the substrate.



**Figure S25.** UV-vis (A) and IR spectra (B) of Ag@MSA-Cd(II) reactions of 10, 50 and 100 ppm, after 24 h. Traces (a), (b), (c) and (d) in both A and B corresponds to Ag@MSA, 10, 50 and 100 ppm residues respectively.



Figure S26. SEM image (A), EDAX spectrum (B) and elemental mapping (C) of Ag@MSA nanoparticles treated with 100 ppm Cd(II) solution, after 24 h. Si peak is due to the substrate.



**Figure S27.** UV-vis (A) and IR spectra (B) of Ag@MSA-Pb(II) reactions at 10, 50 and 100 ppm, after 24 h. Traces (a), (b), (c) and (d) in both A and B corresponds to Ag@MSA, 10, 50 and 100 ppm residues, respectively.



Figure S28. SEM image (A), EDAX spectrum (B) and elemental mapping (C) of Ag@MSA nanoparticles treated with 100 ppm Pb(II) solution, after 24 h. Si and Sn peaks are due to the substrate.



Figure S29. O 1s of Ag@MSA nanoparticles treated with 10, 50 and 100 ppm of Cd(II) solutions (traces a, b and c), after 24 h.



Figure S30. O 1s of Ag@MSA nanoparticles treated with 10, 50 and 100 ppm of Pb(II) solutions (traces a, b and c), after 24 h.