Supplementary Information

A Scalable Synthesis of Highly Stable and Water Dispersible $Ag_{44}(SR)_{30}$ Nanoclusters

Lina G. AbdulHalim,[a§] Sumaira Ashraf,[b§] Khabiboulakh Katsiev,[a] Ahmad R. Kirmani, [c] Nuwan Kothalawala,[d] Dalaver H. Anjum, [e] Sikandar Abbas,[f] Aram Amassian,[d] Francesco Stellacci,[g] Amala Dass,[d] Irshad Hussain,[f]* and Osman Bakr[a]*.

[a] Division of Physical Sciences and Engineering, Solar and Photovoltaics Engineering Center, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia. E-mail: osman.bakr@ kaust.edu.sa
[b] Department of Metallurgy & Materials Engineering, Pakistan Institute of Engineering &Applied Sciences (PIEAS), Nilore, Islamabad.
[c] Materials Science and Engineering Program, Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia.
[d] Department of Chemistry and Biochemistry, University of Mississippi, University, Mississippi 38677, United States
[e] Advanced Nanofabrication Imaging and Characterization, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia
[f] Department of Chemistry, SBA School of Science & Engineering (SSE), Lahore University of Management Sciences (LUMS), DHA, Lahore Cantt – 54792, Pakistan. E-mail: ihussain@lums.edu.pk
[g] Institute of Materials, Ecole Polytechnique Federale de Lausanne, Switzerland
[§] These authors contributed equally to this work.

Experimental Section

1H NMR

Deuterated water was used as the solvent to dissolve ~10 mg clusters, then 600 µL of the solution was transferred to 5 mm NMR tube. The spectra were recorded by collecting 64 scans with a recycle relay time of 5 s. The residual solvent peaks were used as references. Exponential line broadening of 1 Hz was applied before Fourier Transformation. Bruker Topspin 2.1 software was used in all experiments to collect and analyse the data.

SV-AUC

Sample solutions (440 µL) were loaded in double-sector Epon centrepieces in a cell with quartz windows. One sector contained Ag NCs in 1M NaOH aqueous solution with a concentration adjusted so that the absorbance at the monitored wavelength (461 nm) is 0.6 OD. All SV-AUC experiments were carried out with a rotor speed of 42000 rpm at 20 ^{o}C and the entire time-course of sedimentation was recorded. 400 scans were collected for each cell among which only 100 were kept for further analysis. The cell/rotor assembly were placed in the instrument chamber and left under vacuum for at least 6 h before the start of each experiment.

HR-TEM

2 µL of Ag NCs suspended in aqueous solution was deposited on an ultrathin carbon-coated Formvar films on 200 mesh copper grids and dried in air for at least 1 h.

UV-Vis

Spectral measurements were performed using diluted aqueous solutions of the clusters in 1 cm length plastic cuvettes at 270 –1000 nm.

Powder XRD

The necessary FWHM fitting was done using the peak analyzer function in Origin

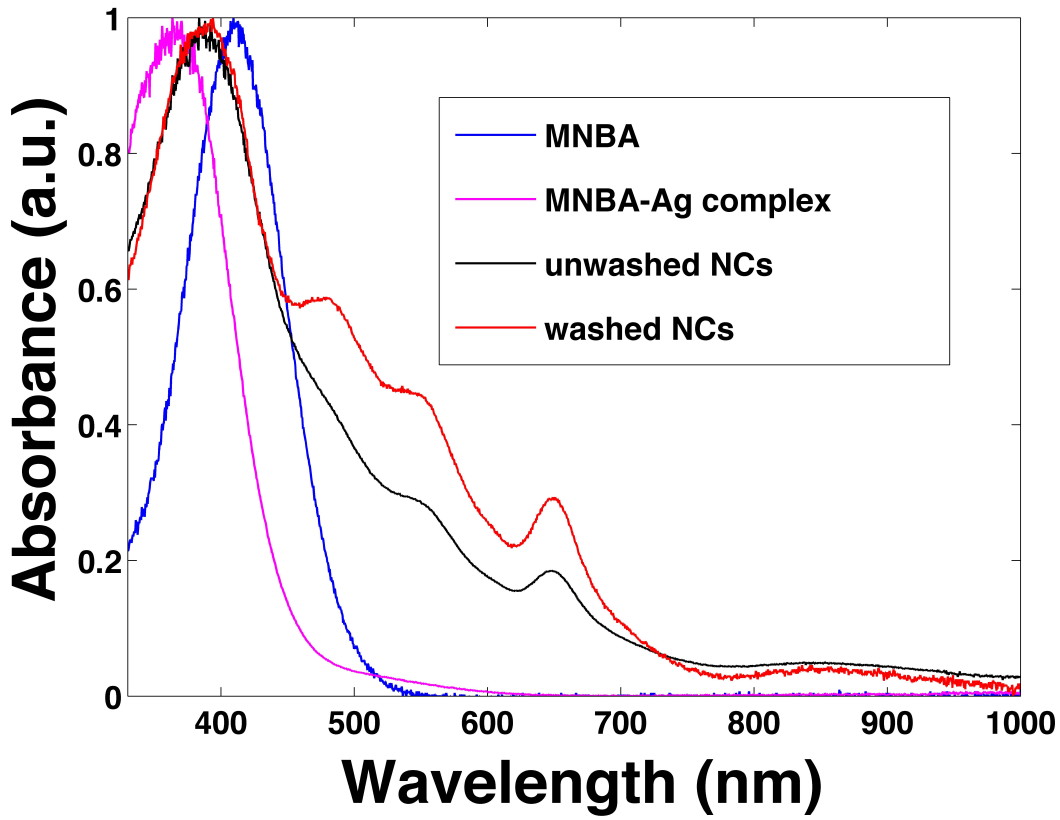

Figure S1. UV-Vis spectra of free ligands (blue), ligand-Ag complex (magenta), as-prepared NCs (black), and purified NCs (red); all in 1M NaOH aqueous solution.

.

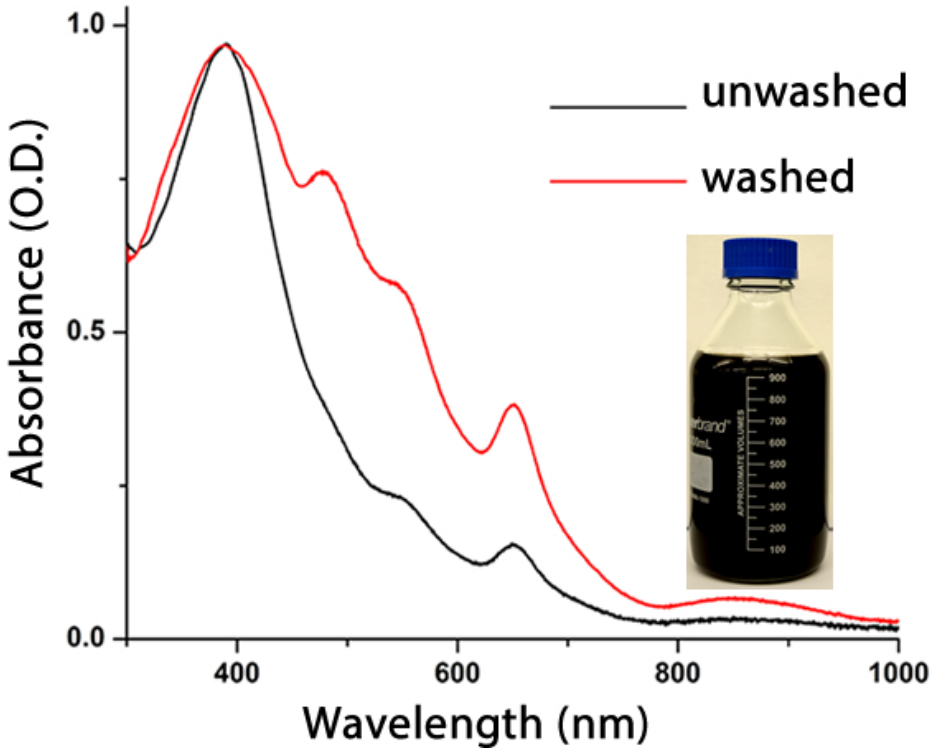

Figure S2. 40X scaled-up synthesis of $Ag_{44}(SR)_{30}$ NCs. The total amount of NCs in solution is 172 mg.

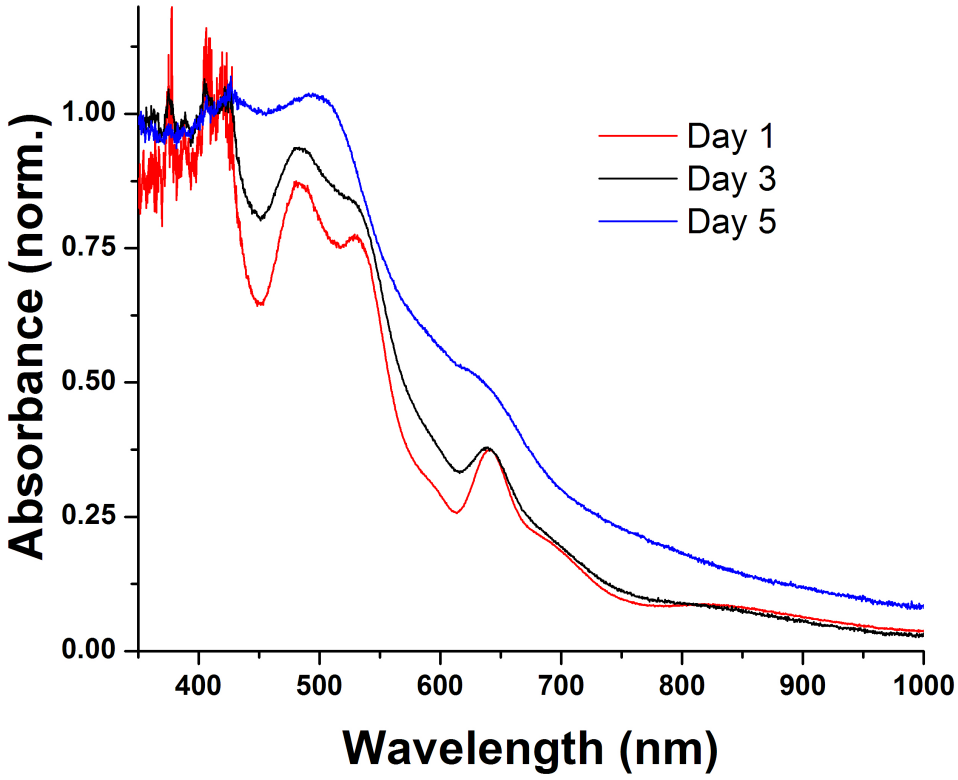

Figure S3. UV-Vis absorption spectra of 3-MBA Ag NCs with time.

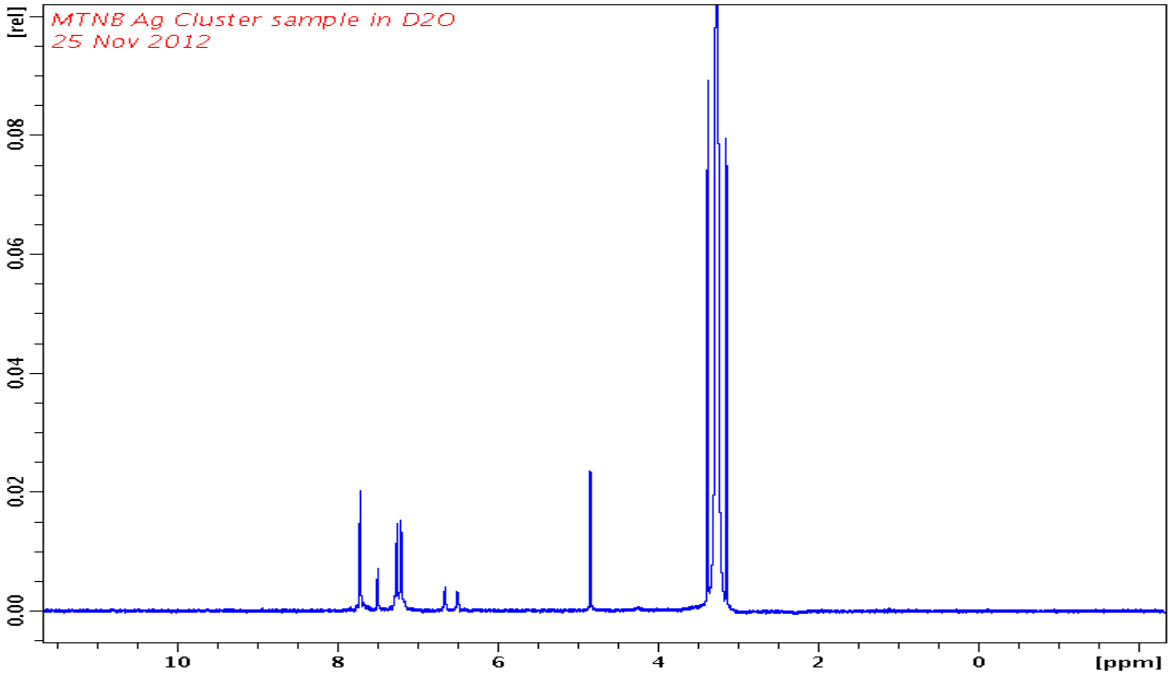

Figure S4. Full 1H NMR Spectrum for Ag NCs in 1M NaOH in D2O solution.

For aromatic region, the chemical shifts for the Ag NCs are at: 7.7109, 7.4903, 7.2604, 7.2022, 7.1869, 6.6597, 6.6444, 6.4942, and 6.4789.