Supporting Information

Highly Stable and Luminescent Formamidinium-Based Perovskite Nanocrystals' Probe for Temperature and Mercury Sensors and *In-vitro* Imaging in Live Cells

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1. Characterization techniques and sample preparations:

1.1. UV-VIS absorption and photoluminescence (PL) measurements: UV-VIS spectrophotometer UV-1900i SHIMADZU was used to record the UV-Vis absorption spectra. Ocean Insight Maya 2000 Pro high-sensitivity spectrometer was used to record the PL spectra using the excitation wavelength of λ_{ex}= 370 nm for all the samples. These synthesized FA-Cs10@O, FA-Cs10@O@P, FA-Cs10@S, and FA-Cs10@S@P NCs were diluted in toluene. Further, they were transported to a quartz cuvette for the measurements.

1.2. Powder X-ray diffraction (PXRD): The concentrated NCs dispersed in toluene were drop casted on the well-cleaned glass substrate (1x1 cm). Bruker D8 diffractometer was used to measure the PXRD with Cu-K_α (λ= 1.54 Å) as incident radiation at 40 kV and 30 mA power. PANalytical Expert's high score plus software was used to analyse the XRD data.

1.3. Transmission electron microscopy (TEM) images: All the samples in toluene with an optimum solution concentration were dropped on the carbon-coated Cu grids with 200 mesh. Jeol-JEM-2100 PLUS microscope was used to measure the TEM operated at 200 kV.

1.4. Fourier transform infrared spectroscopy (FTIR) measurement: A few microliters of concentrated NCs solutions were placed on the ATR-FTIR attenuated total reflection mode.

Bruker Alpha-T spectrometer was used to measure the FTIR spectra after the evaporation of the solvent.

1.5. X-ray photoelectron spectroscopic measurement (XPS): The XPS analysis was carried out using XPS Analytical Facility (XPS Lab), Department of Chemical Engineering, ICT-Mumbai. The NCs thin film was prepared and exposed to a beam of X-rays, which excites the atoms on the surface of the sample.

1.6. Stability tests in polar solvent, heat stability, ion migration, and ion-detection measurements: The stability tests of all the NCs in terms of polar solvent, ion migration, heat treatment and the selectivity as well as the sensitivity of the NCs towards the Hg^{2+}-ion detection was carried out by using Ocean insight Maya 2000 Pro high-sensitivity spectrometer with a 370 nm UV excitation source. All the stability tests were done in open-air atmospheric room conditions with 55- 65% humidity.

1.7. Preparation of TBA-Cl precursor solution: The TBA-Cl stock precursor solution of 0.19 mmol was prepared by dissolving 55 mg of TBA-Cl in 1 mL of toluene followed by sonication until complete dissolution of the solute. Further, we diluted the solution by taking 10 µL from stock solution in 0.5 mL of toluene and used it for our measurements.

2. **Table S1:** Comparative study for detection of mercury ions in presence of different fluorescent probes.

Name of Fluorescent probes	Linear range	Detection limit	Reference
A thio-urea based Chemo sensor	10 µM – 100 µM	11.14 µM	1
N-GQDs	2.5-800 µM	2.5 µM	2
M-CDs	0-1200 µM	5.6 µM	3
N, S-CDs	5 µM – 50 µM	1.78 µM	4
FA-Cs10@S@P NCs	0 µM – 15.4 µM	1.13 µM	This Work

3. Figures:

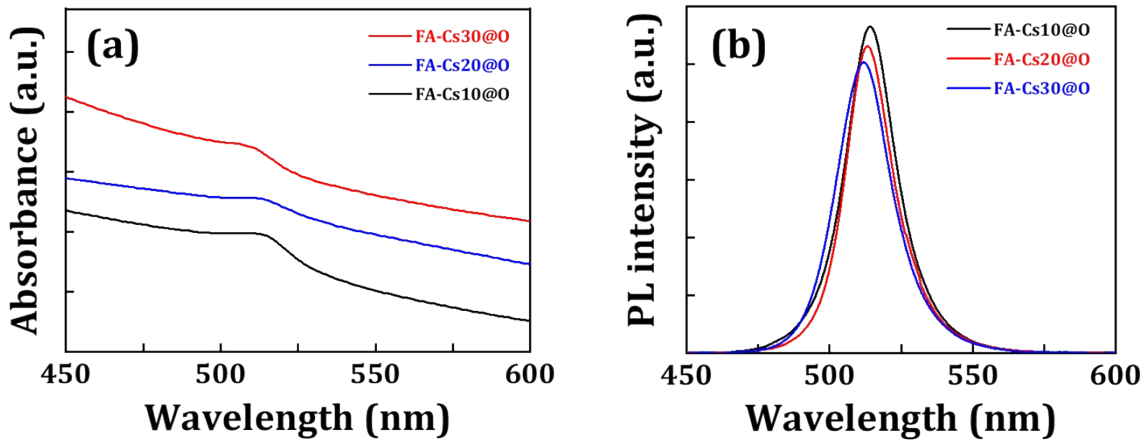

Figure S1: (a) UV-VIS and (b) PL spectra of different Cs-doped $FAPbBr_3$ NCs as represented in legends.

3.1. Figure S1:

3.2. Figure S2:

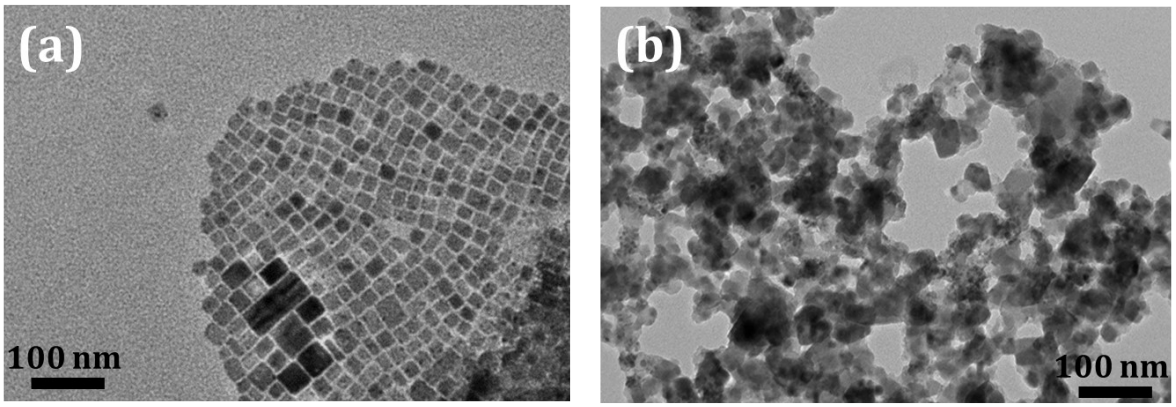

Figure S2: TEM images of (a) FA-Cs10@O@P NCs and (b) FA-Cs10@S@P NCs.

3.3. Figure S3:

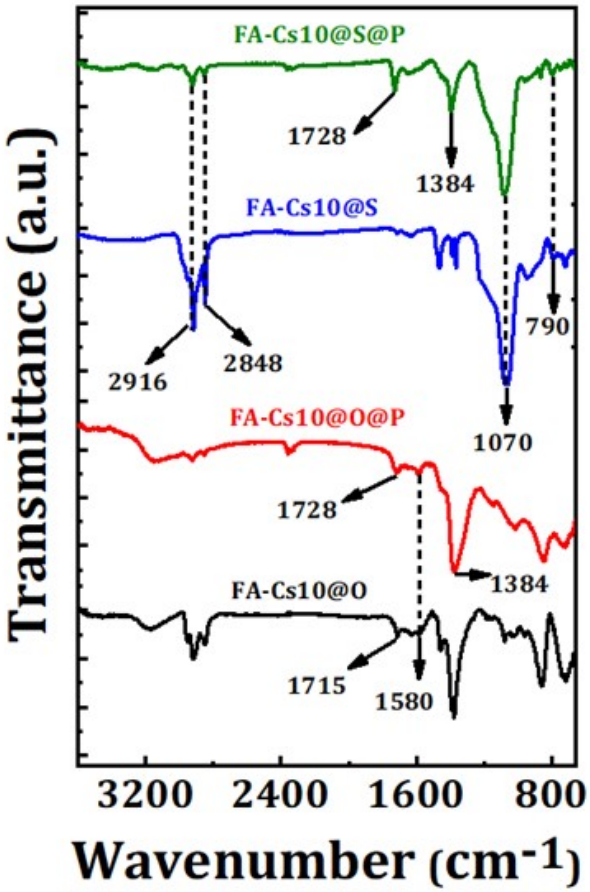

Figure S3: FTIR spectra of FA-Cs10@O (black line), FA-Cs10@O@P (red line), FA-Cs10@S (blue line), and FA-Cs10@S@P (green line) NCs.

3.4. Figure S4:

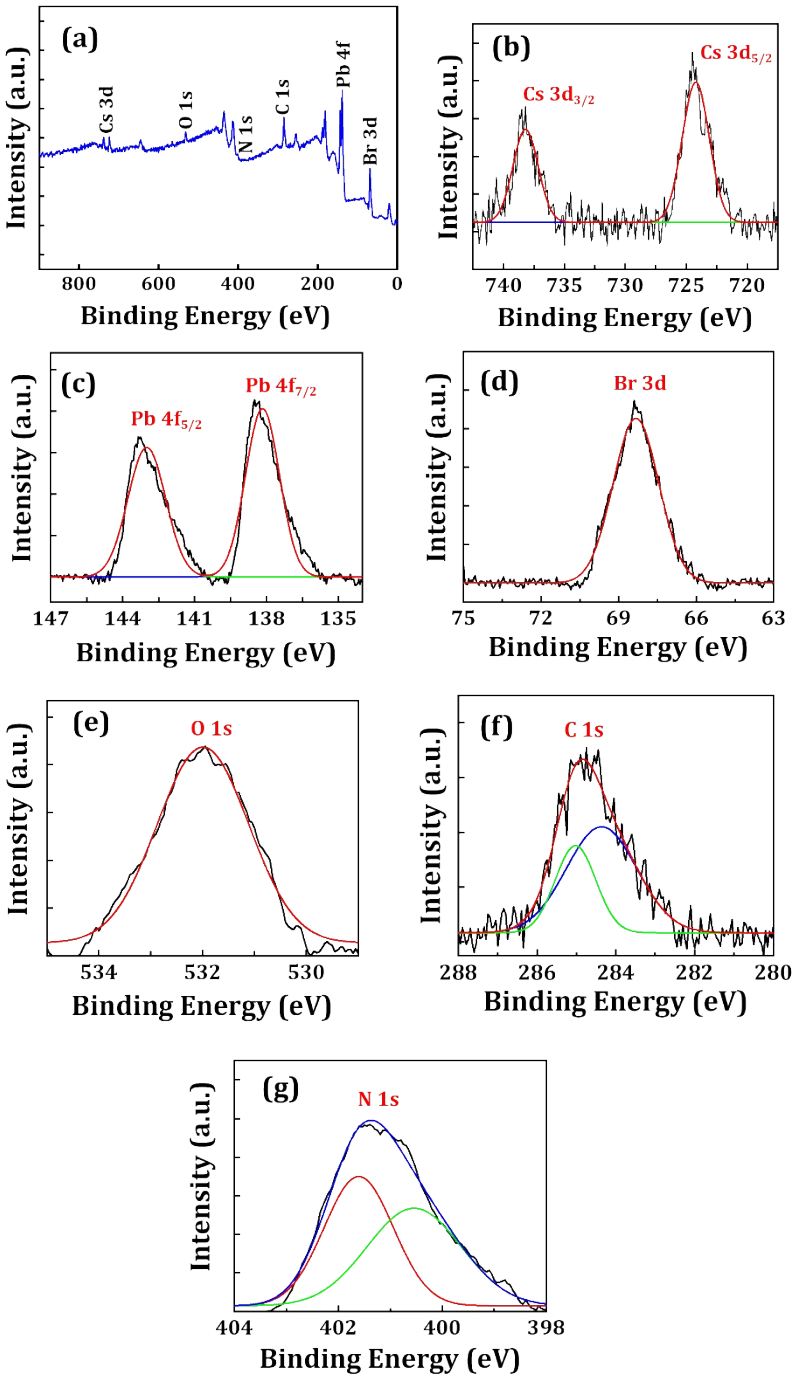

Figure S4: (a) Core XPS spectrum and HR-XPS spectra of (b) Cs 3d, (c) Pb 4f, (d) Br 3d, (e) O 1s, (f) C 1s, and (g) N 1s chemical states of FA-Cs10@O NCs.

3.5. Figure S5:

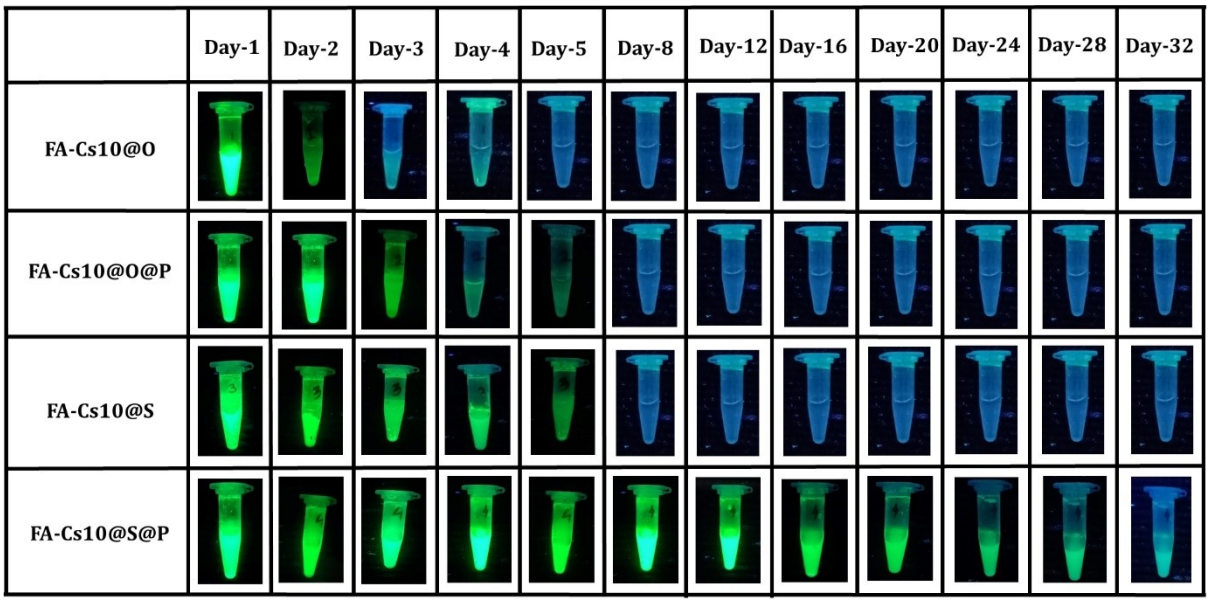

Figure S5: Photographic images of all the NCs dispersion in water for a period of 1 month while placed under a 370 nm UV lamp.

3.6. Figure S6:

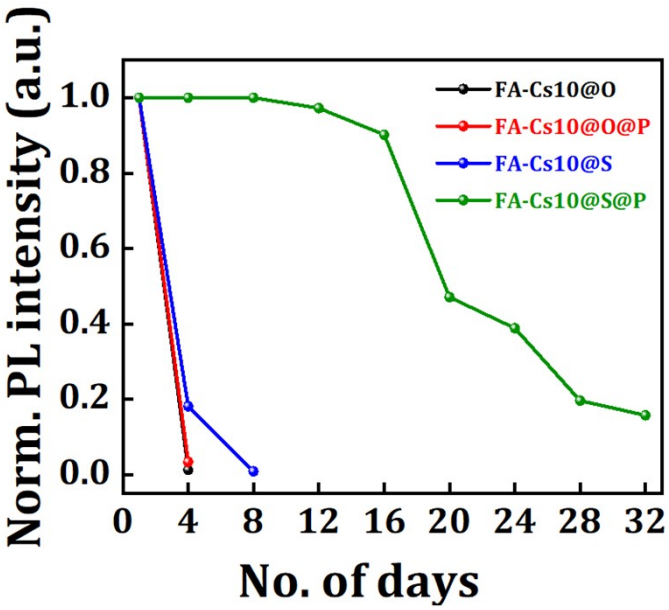

Figure S6: Change in PL intensity of all the NCs dispersed in water with respect to the number of days as represented in legend.

2.7. Figure S7:

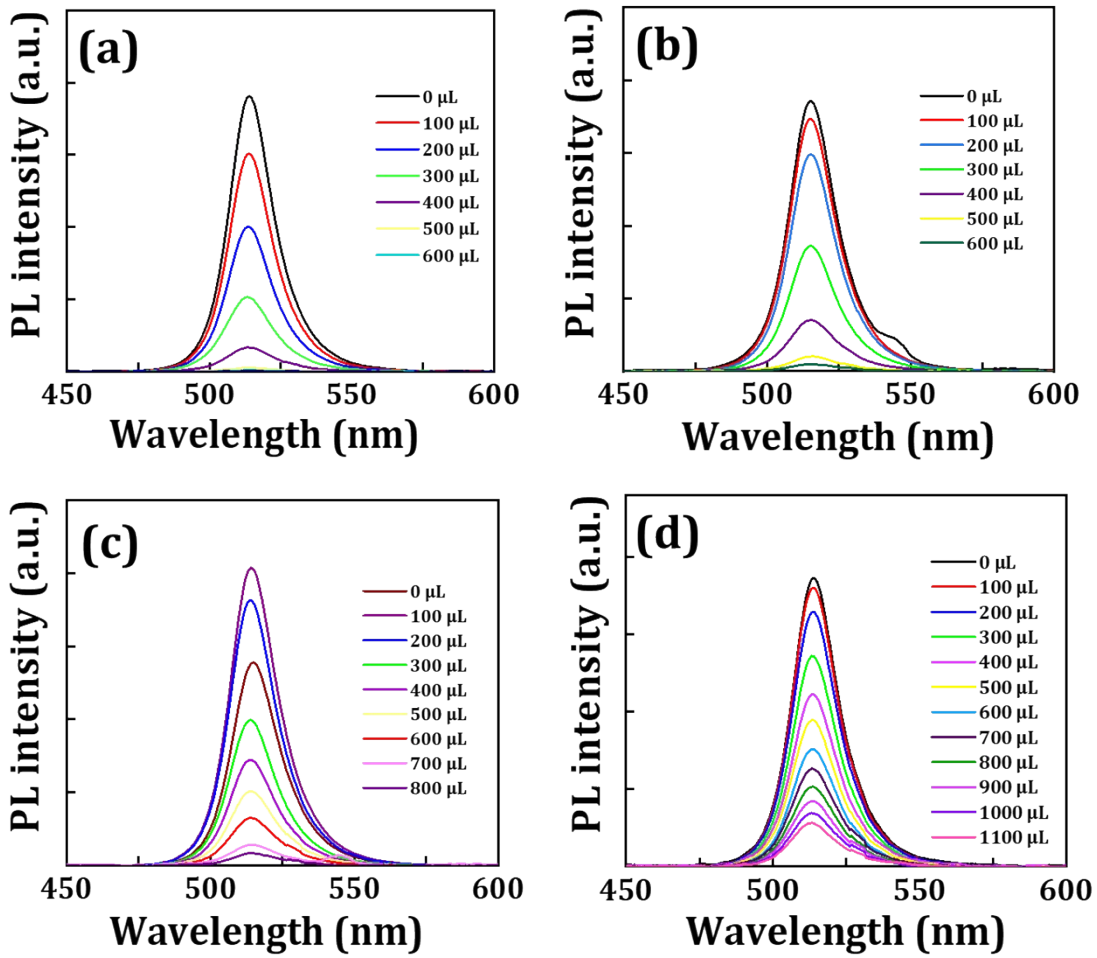

Figure S7: Change in PL spectra of (a) FA-Cs10@O, (b) FA-Cs10@O@P, (c) FA-Cs10@S, (d) FA-Cs10@S@P NCs with addition of different amount of DI water.

2.8. Figure S8:

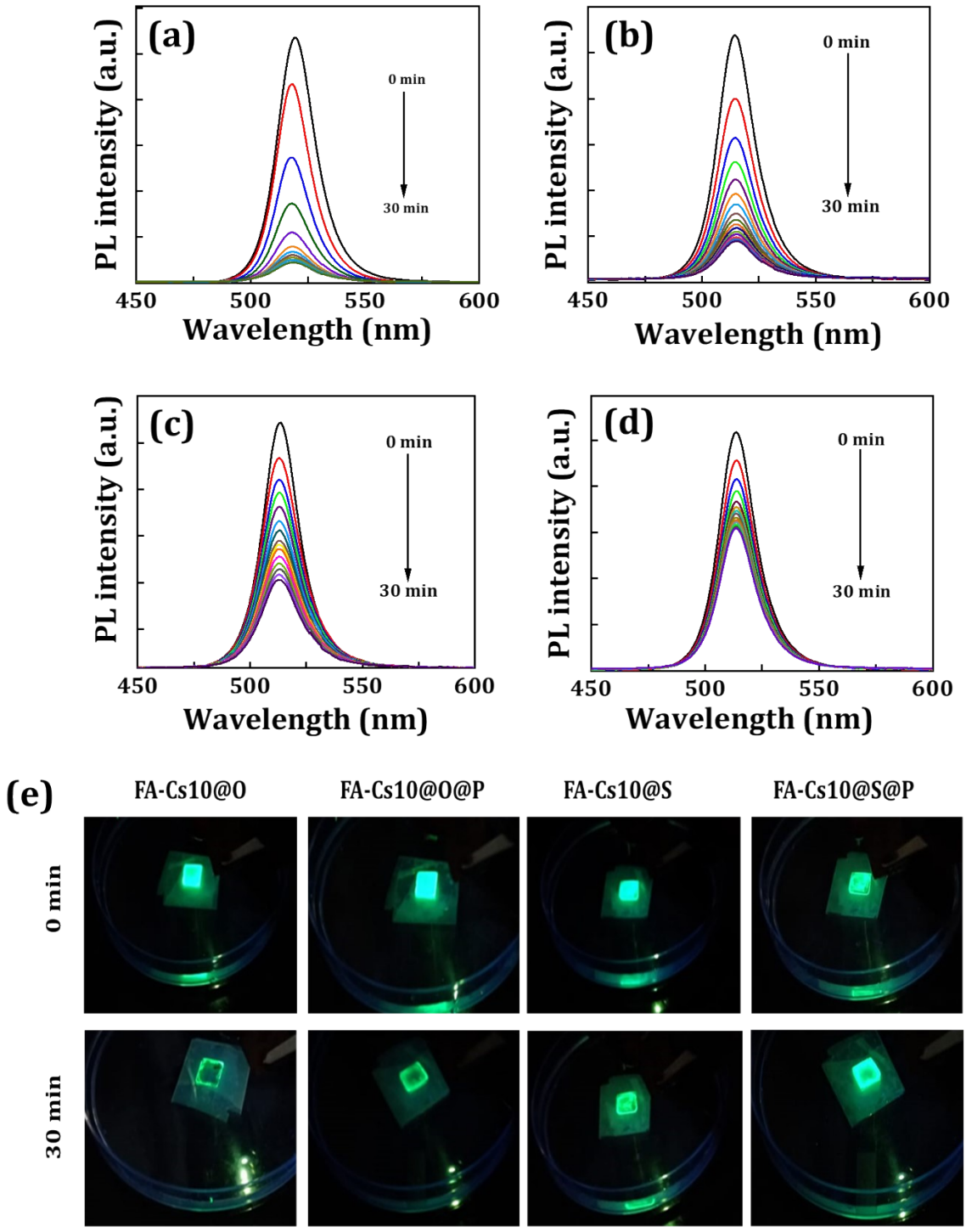

Figure S8: Variations of PL intensities of (a) FA-Cs10@O, (b) FA-Cs10@O@P, (c) FA-Cs10@S, (d) FA-Cs10@S@P NCs' films dipped in water. (e) Photographic images of all these NCs' films in water and placed under a 370 nm UV lamp.

2.9. Figure S9:

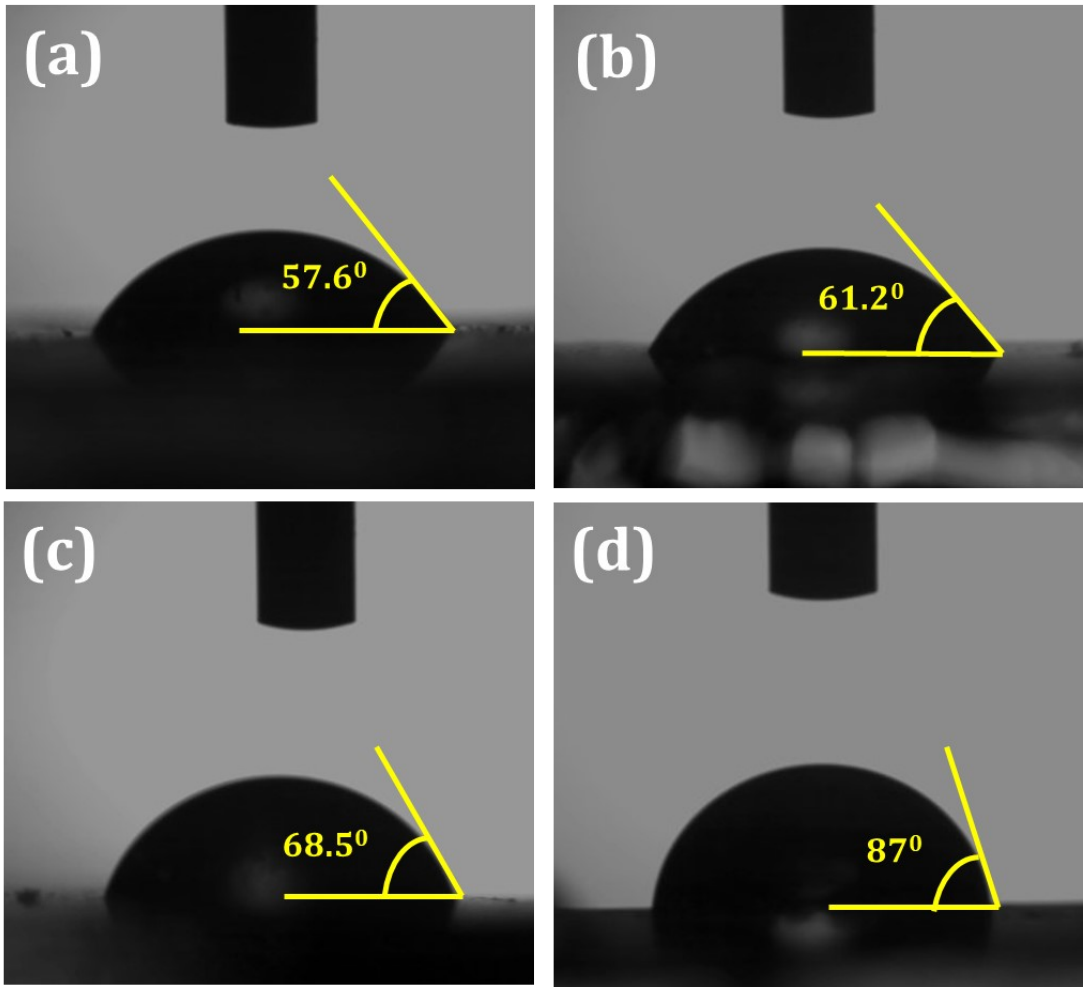

Figure S9: Contact angle measurement of (a) FA-Cs10@O, (b) FA-Cs10@O@P, (c) FA-Cs10@S, (d) FA-Cs10@S@P NCs' films.

2.10. Figure S10:

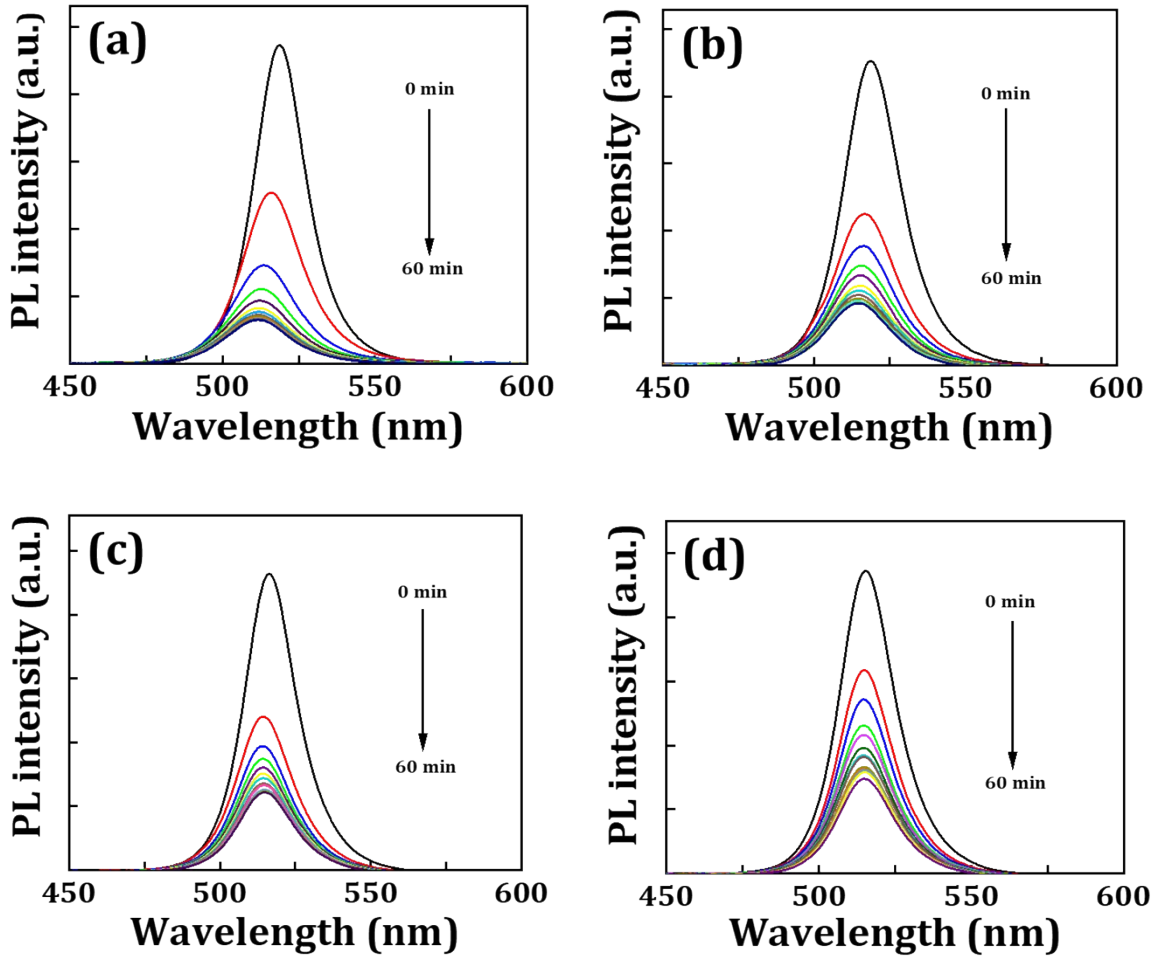

Figure S10: Variations of PL intensities of (a) FA-Cs10@O, (b) FA-Cs10@O@P, (c) FA-Cs10@S, (d) FA-Cs10@S@P NCs' films while kept on a hotplate at 80 °C.

2.11. Figure S11:

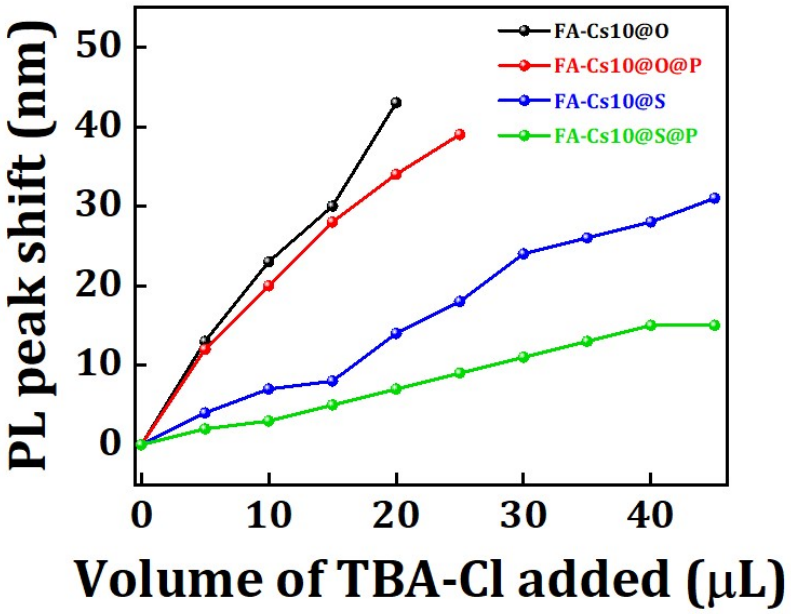

Figure S11: Change in PL peak position of all the NCs' solutions in toluene with the addition of different amounts of TBA-Cl precursor solutions as shown in legend.

2.12. Figure S12:

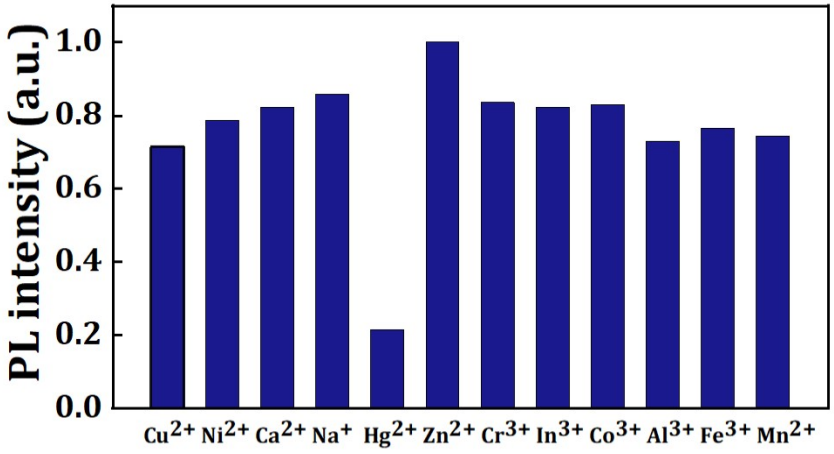

Figure S12: Histogram of the change in PL intensity of FA-Cs10@S@P NCs after adding different metal ions.

2.13. Figure S13:

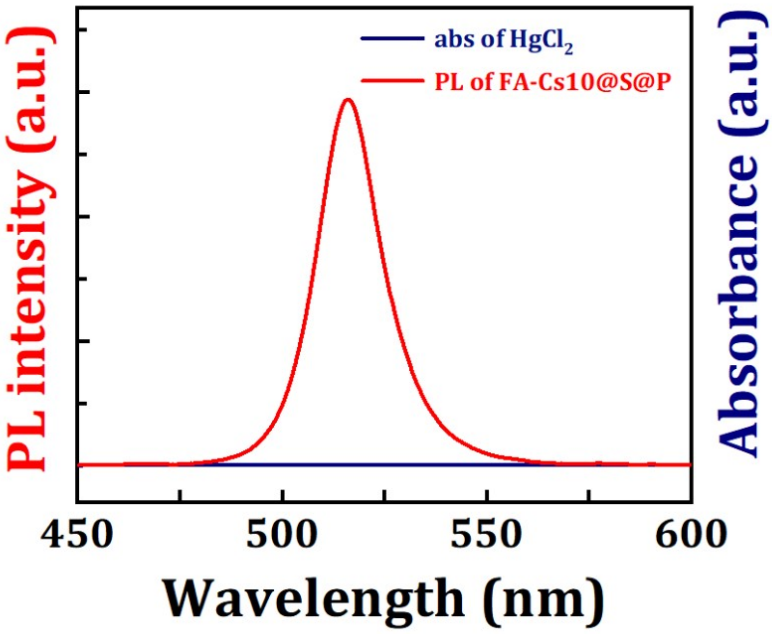

Figure S13: PL spectrum of FA-Cs10@S@P NCs solution (red line) and absorption spectrum of $HgCl_2$ solution (blue line).

2.14. Figure S14:

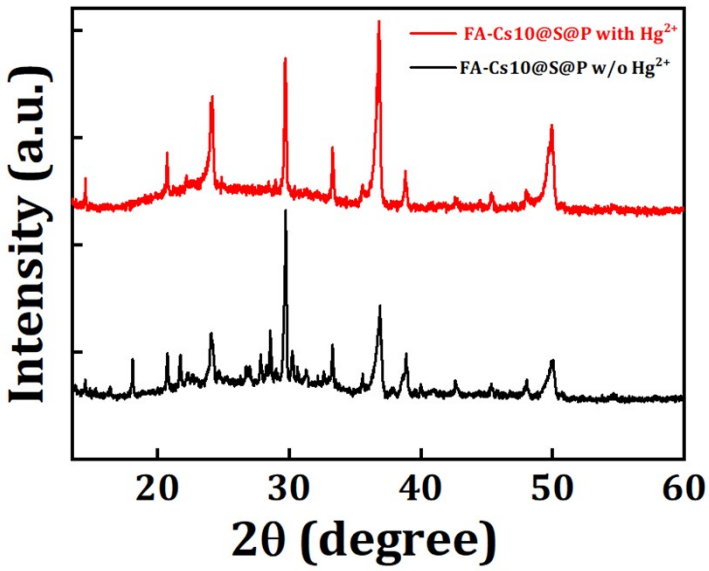

Figure S14: XRD pattern of FA-Cs10@S@P NCs in the absence and presence of Hg^{2+}-ions as shown in legend.

2.15. Figure S15:

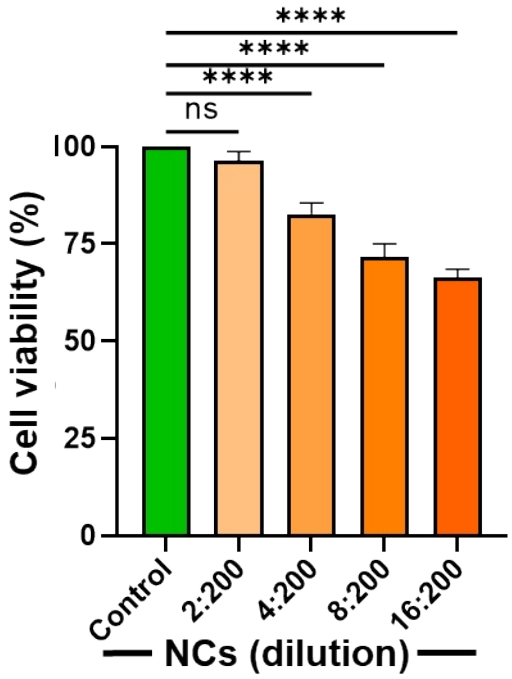

Figure S15: Cytotoxicity assessments of FA-Cs10@S@P NCs by MTT assay. 3T3L-1 cells were exposed to different dilutions (2:200, 4:200, 8:200, and 16:200) of NCs for 24 hours and cell viability was analyzed. The data are reported as percentage survival of the untreated cells. Cells exposed to 2:200 dilutions of NCs exhibits non-cytotoxic behavior. Each bar represents Mean with standard deviation (n=6). Statistical significance was calculated in GraphPad Prism9 using Oneway ANOVA test, $P<0.0001$ shown as **** and $P>0.1$ as ns (non-significant).

References:

1. A. K. Manna, J. Mondal, R. Chandra, K. Rout and G. K. Patra, *Journal of Photochemistry and Photobiology A: Chemistry*, 2018, **356**, 477-488.
2. Y. Liu, X. Tang, M. Deng, Y. Cao, Y. Li, H. Zheng, F. Li, F. Yan, T. Lan and L. Shi, *Microchimica Acta*, 2019, **186**, 1-8.
3. P. Zhu, S.-L. Hou, Z. Liu, Y. Zhou, P. J. J. Alvarez, W. Chen and T. Zhang, *Environmental Science & Technology*, 2024.
4. M. Pajewska-Szmyt, B. Buszewski and R. Gadzała-Kopciuch, *Materials chemistry and Physics*, 2020, **242**, 122484.