Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Tuning the Charge Transfer Efficiency by Functionalizing Ligands in $FAPbBr_3$ Nanocrystals and Graphene Heterostructures

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Table S1: EDX analysis and percentage elemental composition of functionalized graphene.

Sample code	C		O		N		S	
	Atom %	Weight %	Atom %	Weight %	Atom %	Weight %	Atom %	Weight %
GO	54.41	50.01	45.59	49.99	-	-	-	-
GO-Ala	65.13	59.12	33.18	27.44	7.43	7.70	-	-
GO-Tyr	56.03	50.32	41.28	35.79	8.18	8.39	-	
GO-Cys	58.47	63.63	35.10	28.67	5.15	4.19	2.78	1.28

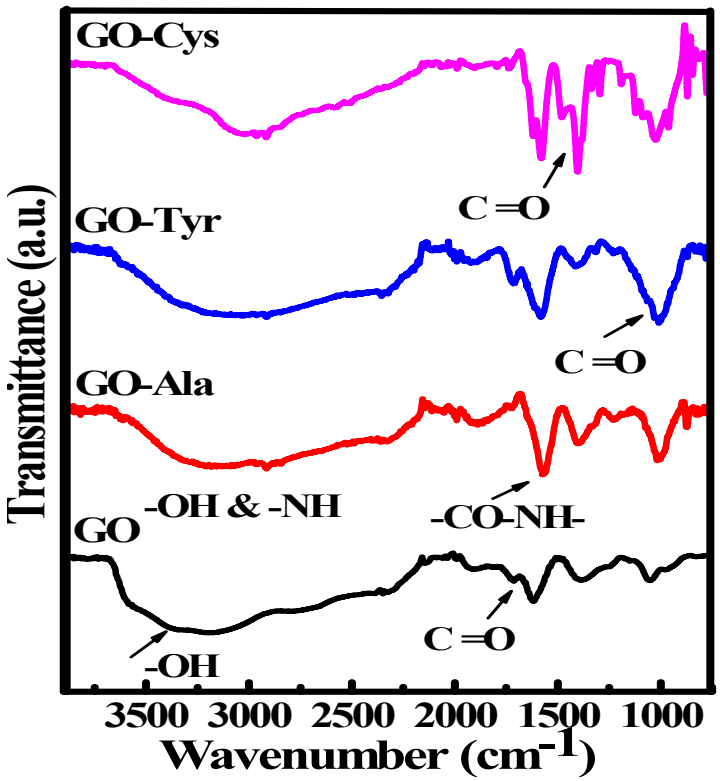

Figure S1: FTIR spectra of GO, GO-Ala, GO-Tyr, and GO-Cys.

Table S2. Vibrational modes observed in functionalized graphene.

Mode of Vibration	**Observed Peak (cm^{-1})**
Stretching vibrations of O-H and -NH group	3300
Stretching vibrations of C=O	1718
Bending vibrations of C=O	1017
Stretching vibration of C=O	1590
asymmetric $–NH_2$ stretching	871

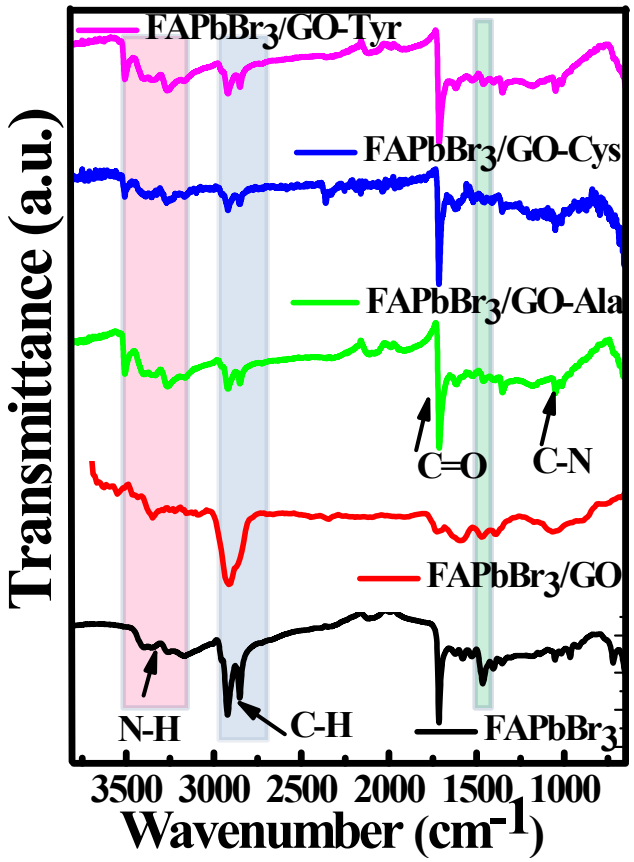

Figure S2: FTIR spectra of $FAPbBr_3$ NCs and NCs/functionalized graphene (GO, GO-Ala, GO-Cys, and GO-Tyr) heterostructures.

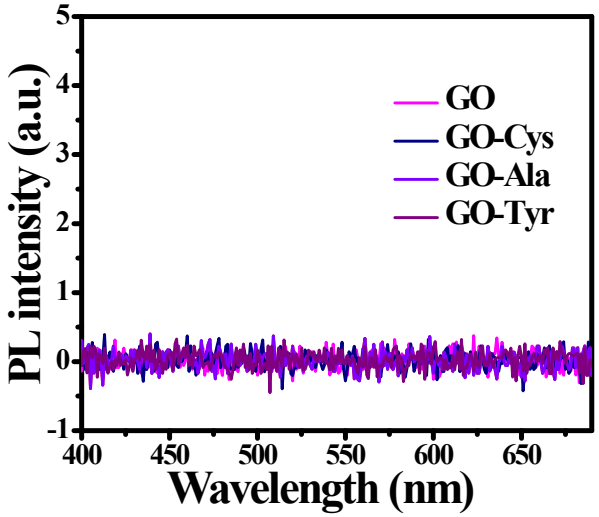

Figure S3: PL spectra of GO, GO-Cys, GO-Ala, and GO-Tyr indicating the non-emissive nature of these compounds**.**

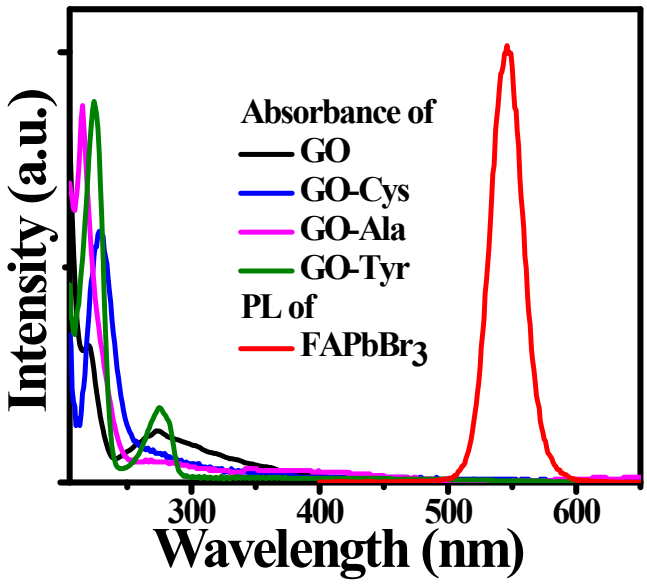

Figure S4. PL spectrum of $FAPbBr_3$ NCs in toluene solvent and UV-Vis absorption spectra of GO, GO-Cys, GO-Ala, and GO-Tyr in water.

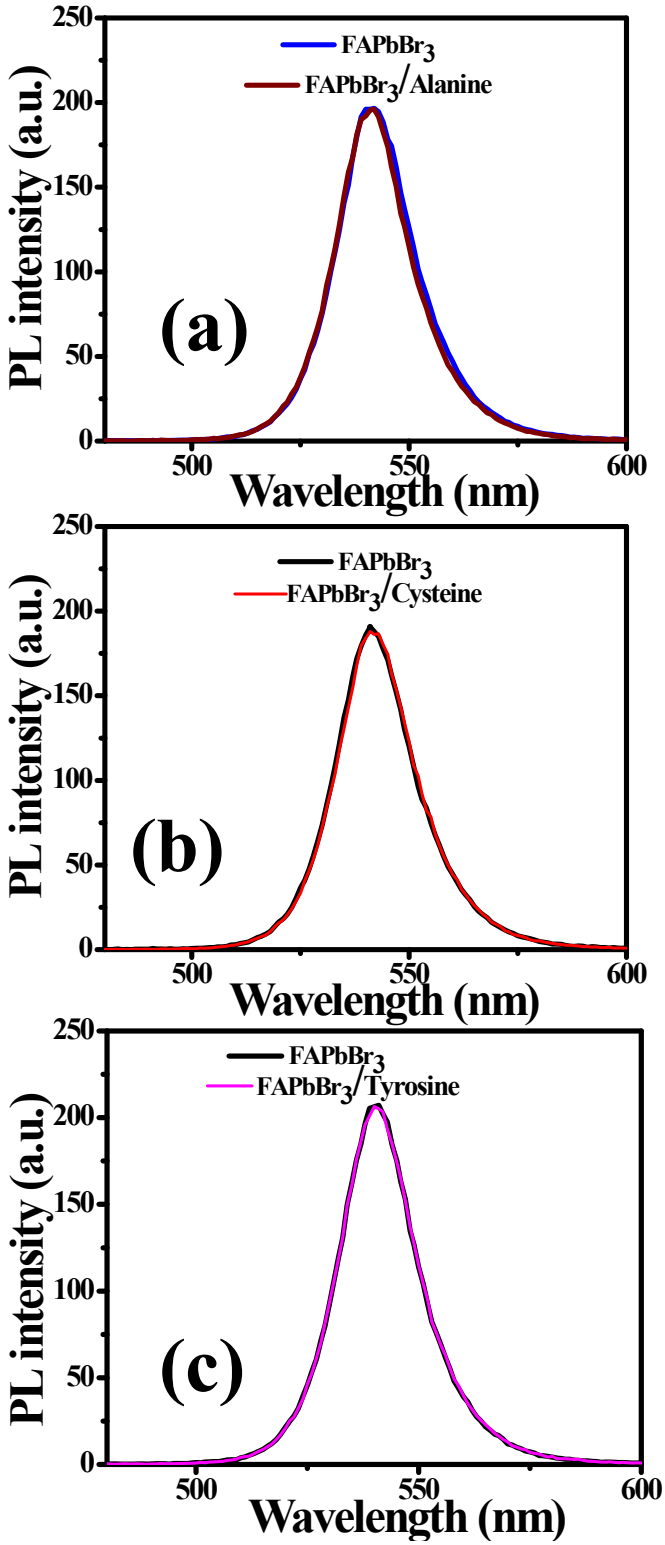

Figure S 5. (a) The PL spectra $FAPbBr_3$ NCs in toluene solution in the absence and presence of different amino acids (a) Alanine, (b) Cysteine, and (c) Tyrosine. The spectra is measured after excitation at 306 nm.

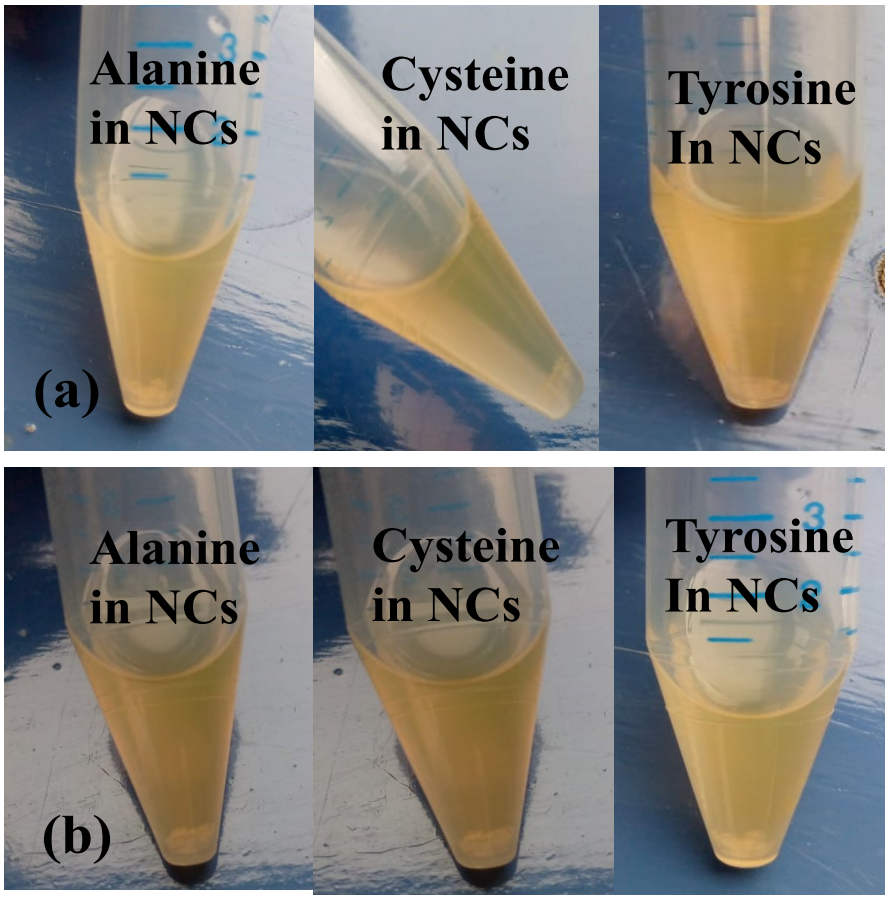

Figure S 6. Amino acids (Alanine, Cysteine, and Tyrosine) in the solution of NCs in toluene, (a) Before stirring and (b) After a stirring of half an hour.

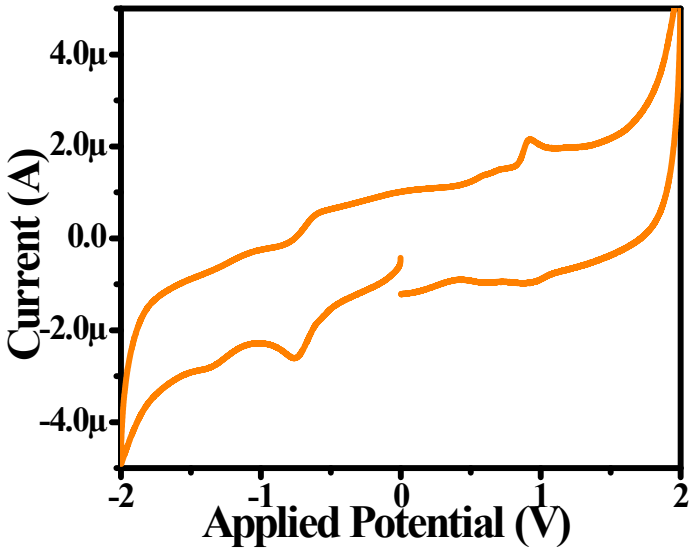

Figure S7. CV of $FAPbBr_3$ NCs with supporting electrolyte of $TBAPF_6$ (50 mM) in toluene:acetonitrile (4:1) solution.

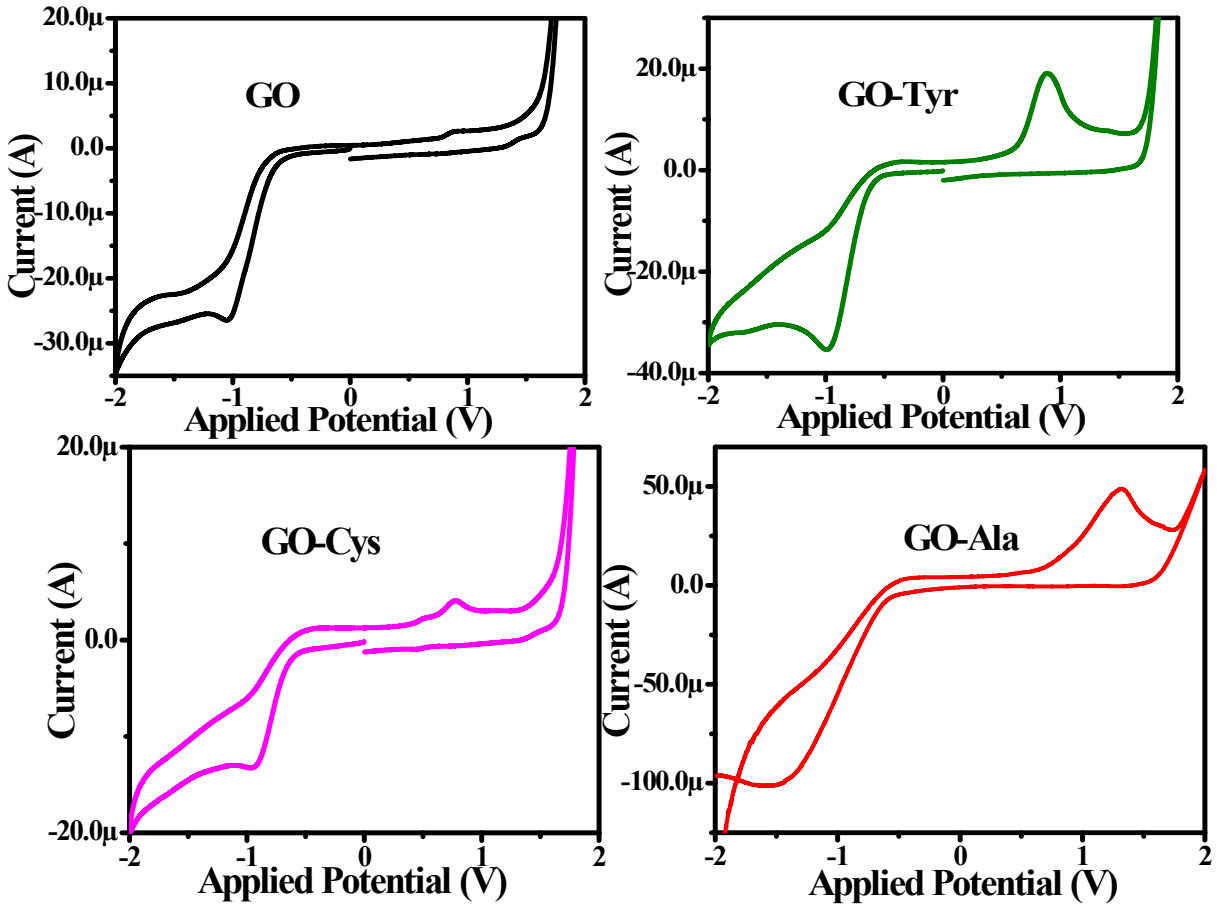

Figure S8. (a) CV of GO, (b) GO-Tyr, (c) GO-Cys, and (d) GO-Ala with supporting electrolyte of $TBAPF_6$ (50 mM) in toluene:acetonitrile (4:1) solution.

Characterization of $FAPbBr_3$ NCs

Figure S 9 (a) presents the TEM micrograph of the NCs indicating the spherical morphology of the synthesized NCs, while Figure S 9 (b) represents the HRTEM micrograph of the NCs consisting a fringe spacing of 0.22 nm that is assigned to the (211) reflection plane of the cubic crystal. In figure S 9(c), SAED pattern displays the bright circular rings suggesting the crystallinity of the samples. The XRD pattern of the prepared NCs (figure S 9(d)) is well indexed with the cubic crystalline phase of $FAPbBr_3$. The UV-Vis absorption and PL spectrum of the NCs is displayed in figure S10. The UV-Vis absorption spectrum exhibits an excitonic peak at 532 nm

and stokes shifted PL at 544 nm. The results of the NCs are well matched with the previous report[1] and hence confirm the successful formation of NCs.

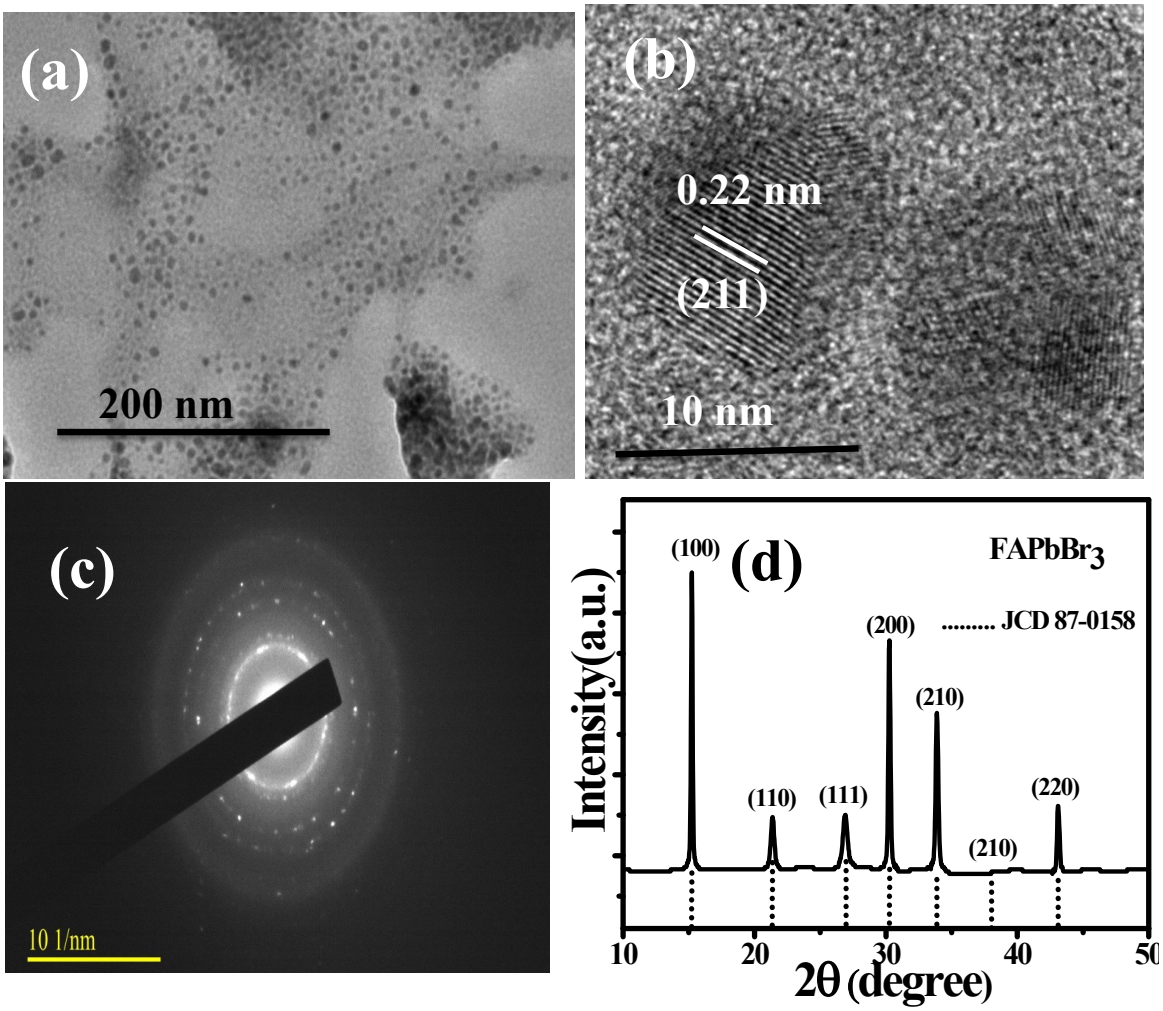

Figure S9. (a) TEM micrograph, (b) High-resolution TEM micrograph (c) SAED pattern and (d) XRD pattern of $FAPbBr_3$ NCs.

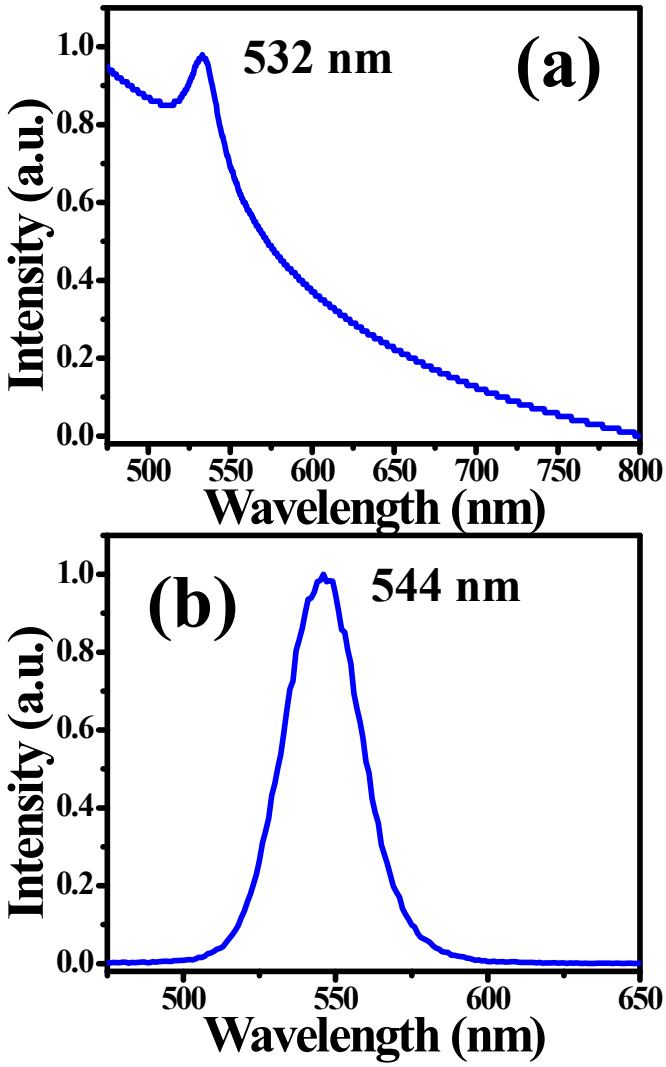

Figure S 10. (a) UV-Vis absorption and (b) PL spectra of 1 g/L solution of $FAPbBr_3$ NCs in toluene.

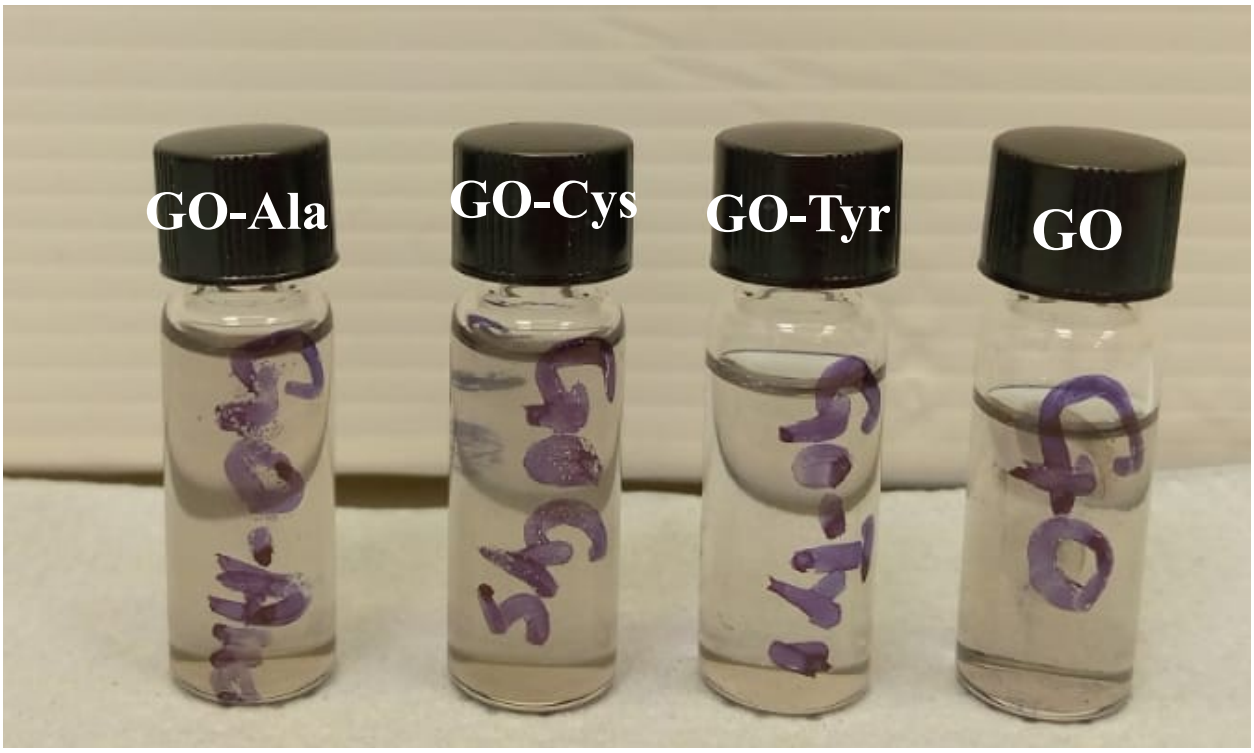

Figure S 11. (a) 0.1 mg/mL dispersion of GO, GO-Ala, GO-Tyr, and GO-Cys in toluene.

References

1 F. Di Stasio, I. Ramiro, Y. Bi, S. Christodoulou, A. Stavrinadis and G. Konstantatos, *Chem. Mater.*, 2018, **30**, 6231–6235.