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Sensitization of near-infrared Ln^{III} [Ln = Yb or Nd] ions using water-soluble, band gap tuneable 3-MPA capped CdS nanoparticles

Ana de Bettencourt-Dias,* Rodney A. Tigaa

Department of Chemistry, University of Nevada, Reno, NV 89557-216, U. S. A.

Table of Contents

1 EDX and TEM

Table S1. Elemental composition by EDX of the 3-MPA-NPs and 3-MPA-Ln-NPs.

Sample	C %	O %	S %	Cd %	Yb/Nd %
30 min NPs	43.53	36.40	12.54	7.54	
30 min NP-Yb	62.93	18.10	7.05	5.06	6.86
30 min NP-Nd	62.65	11.82	1.07	1.90	22.56
50 min NPs	65.39	11.00	12.89	10.72	
50 min NP-Yb	62.01	13.33	12.62	8.83	3.22
50 min NP-Nd	40.94	26.66	22.72	1.35	8.33
120 min NPs	65.00	16.24	18.29	0.47	
120 min NP-Yb	29.44	27.72	23.42	14.31	5.12
120 min NP-Nd	53.13	23.13	10.61	8.96	4.17

Table S2. Average sizes of the 3-MPA-NPs and their Ln^{III} systems 3-MPA-Ln-NPs determined from TEM measurements.

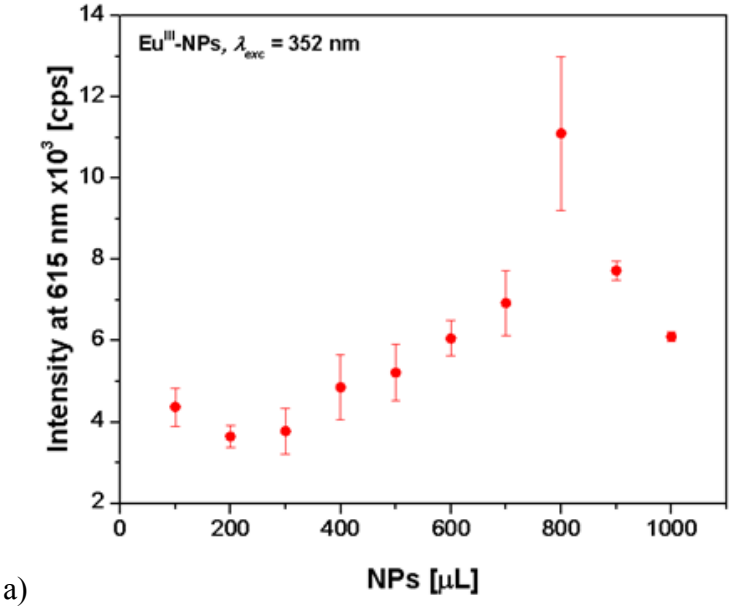
Sample	NP [nm]	Nd^{III}-NP [nm]	Yb^{III}-NP [nm]
30 min	3.5±0.2	3.9±0.3	4.0±0.6
50 min	3.1±0.3	3.7±0.5	3.3±0.2
120 min	3.6±0.6	3.7±0.4	4.2±0.1

2 FT-IR

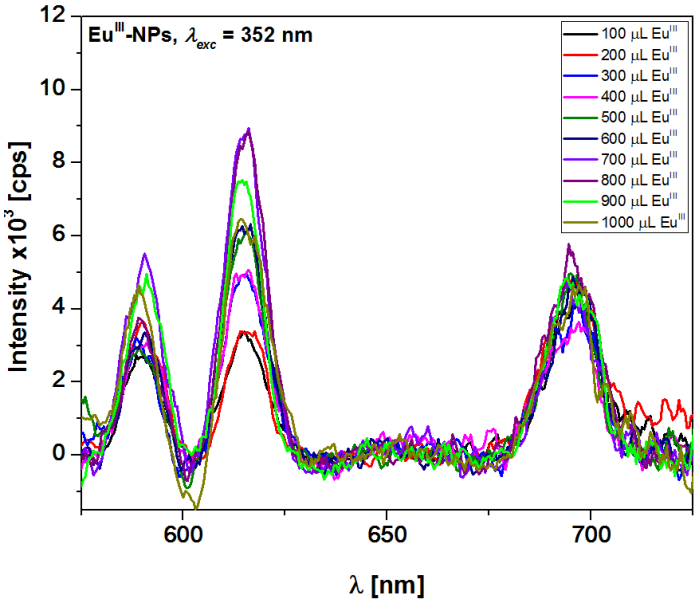
Table S3. The vibrational energies of the symmetric (ν_s) and asymmetric (ν_{as}) carboxylate vibrations of the 3-MPA-NP and 3-MPA-LnNP systems.

CdS NPs	30 min [cm^{-1}]	50 min [cm^{-1}]	120 min [cm^{-1}]
Na^{I}-NPs	ν_{as} = 1554 ν_s = 1395	ν_{as} = 1554 ν_s = 1395	ν_{as} = 1556 ν_s = 1398
Nd^{III}-NP	ν_{as} = 1532 ν_s = 1405	ν_{as} = 1533 ν_s = 1402	ν_{as} = 1538 ν_s = 1408
Yb^{III}-NP	ν_{as} = 1538 ν_s = 1402	ν_{as} = 1541 ν_s = 1407	ν_{as} = 1538 ν_s = 1404

3 Determination of the optimum Ln^{III}/NP ratio



a)



b)

Figure S1. a) Plot of Eu^{III} emission intensity at 615 nm as a function of added NPs and b) the corresponding emission spectra obtained in H_2O at 298 K.

4 Powder XRD of the 3-MPA-NP and 3-MPA-Ln-NP systems

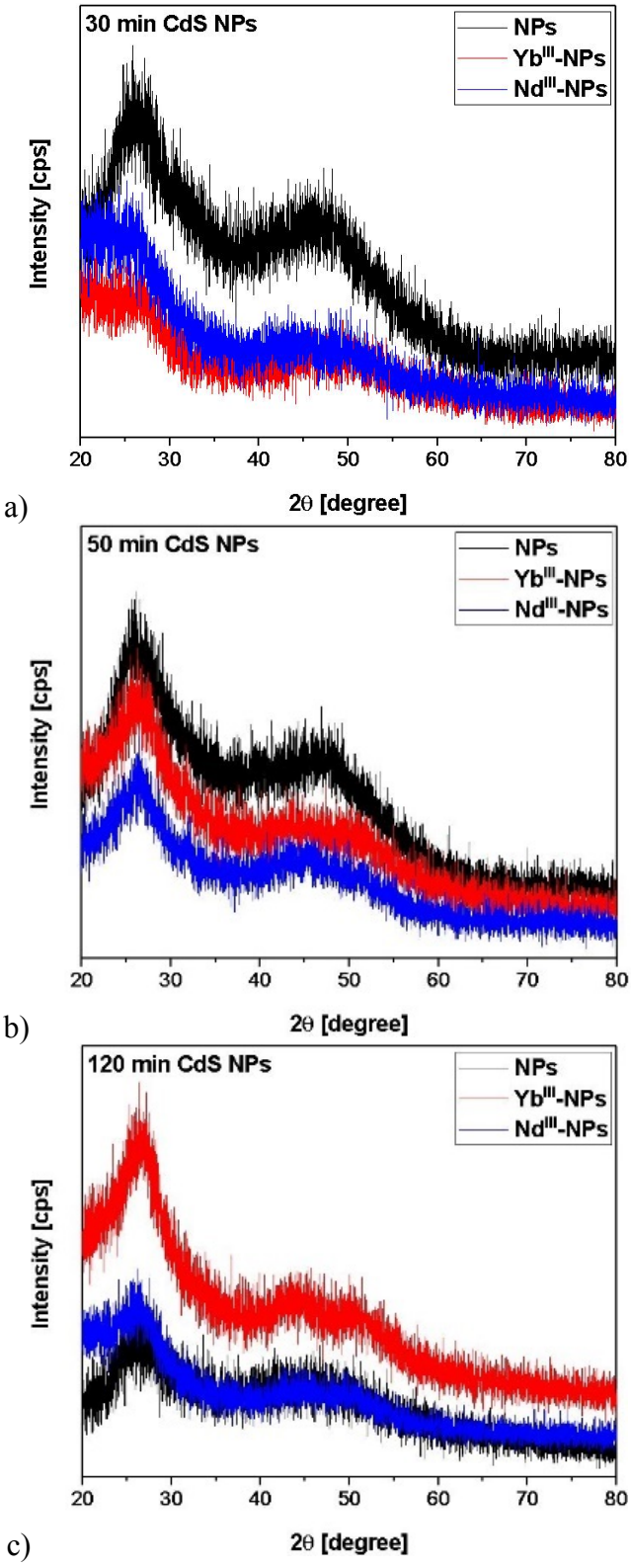


Figure S2. Powder X-ray diffractograms of the a) 30, b) 50 and c) 120 min 3-MPA-NPs and 3-MPA-Ln-NPs.

5 Excitation and emission spectra of the $LnCl_3$ and Ln^{III}-complexes of 3-MPA

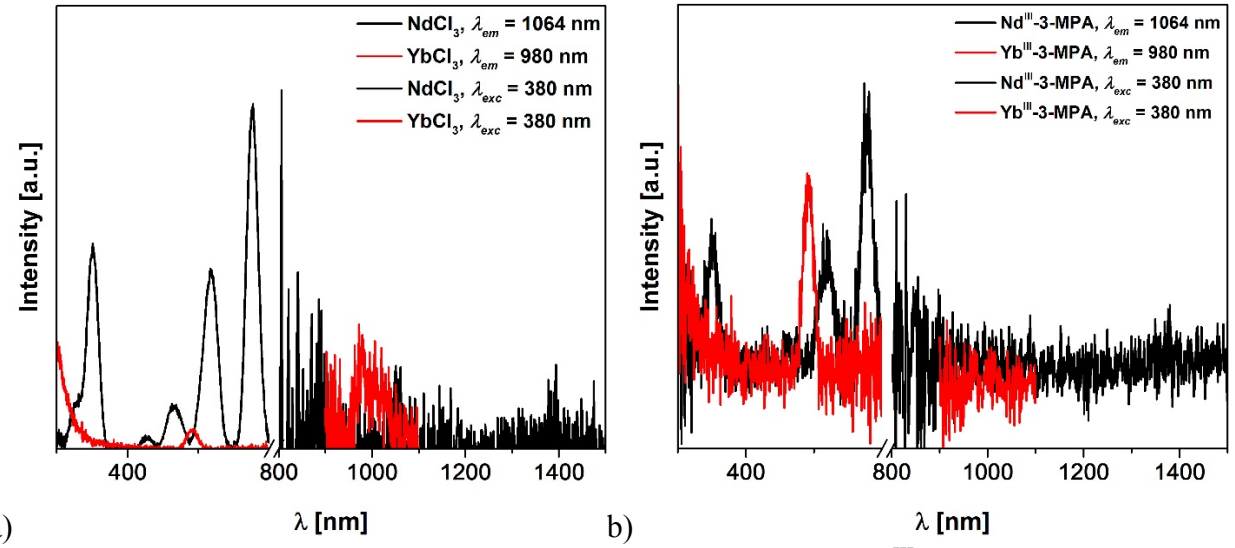


Figure S3. NIR Excitation and emission spectra of a) $LnCl_3$ and b) Ln^{III}-complexes of 3-MPA in D_2O obtained at 298 K. Ln = Nd (black lines) and Yb (red lines).