Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2020

(Supplementary Information)

Down Converting Serine-functionalised NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺@NaGdF₄:Tb³⁺

Photoluminescent Probe for Chemical Sensing of Explosive Nitroaromatic Compounds

Table of Contents



Fig. S1 Rietveld refinement plots of NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺ nanostructure with different Eu³⁺ contents; (a) 10% (b) 15% (c) 20% (d) 25%



Fig. S2 (a) HR-TEM image of Serine-functionalised core shell nanocrystal and (b) TEM image of Core shell nanostructure.



Fig. S3 EDS spectra of NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺ nanophosphors with different Eu³⁺ contents: (a) 3% (b) 5% (c) 7% (d) 10%



Fig. S4 EDS spectra of as synthesized NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺ nanocrystals with different Eu³⁺ contents: (a) 15 % (b) 20 % (c) 25%



Fig. S5 EDS spectra of nanophosphors: (a) NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺@NaGdF₄:Tb³⁺ core shell
(b) Serine functionalised NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺@NaGdF₄:Tb³⁺ core shell



Fig. S6 FTIR spectra of NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺ with different Eu³⁺ contents; (a) 3% (b) 5% (c) 7% (d) 10% (e) 15% (f) 20% (g) 25%



Fig. S7 FTIR spectra of synthesized nanostructure; (a) core shell (b) Serine-functionalized core shell



Fig. S8 Photoluminescence decay curves of NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺ with different Eu³⁺ contents; (a) 3% (b) 5% (c) 7% (d) 10% (e) 15% (f) 20% (g) 20%



Fig. S9 Photoluminescence decay curves of nanophosphors; (a) Core shell (b) serine-functionalized core shell nanomaterials.



NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺@NaGdF₄:Tb³⁺ core shell and different nitro-compounds (100 ppm) in aqueous sol

Sample	3 %	5 %	7 %	10 %	15 %	20 %	25 %
Space Group	P -6						
Symmetry	Hexagonal						
2θ interval (°)	20-80	20-80	20-80	20-80	20-80	20-80	20-80
Lattice parameters							
a (Å)	5.96236	5.87754	6.40764	11.14293	6.09353	5.88150	9.38186
b (Å)	5.96236	5.87754	6.40764	11.14293	6.09353	5.88150	9.38186
c (Å)	3.06273	3.70879	3.59470	2.95871	3.50211	3.15020	3.25801
V (Å ³)	94.292	110.957	127.817	318.150	112.615	94.372	248.348
R _w	4.98%	4.59%	4.62%	5.01%	4.23%	5.00%	4.49%

Table S1. Crystallographic data of hexagonal NaYF₄:Ce³⁺/Gd³⁺/Eu³⁺ nanostructures synthesized with different Eu³⁺ contents; 3%, 5%, 7%, 10%, 15%, 20% and 25%.

Elements	Eu ³⁺ 3 %		Eu ³⁺ 5 %		Eu ³⁺ 7 %		Eu ³⁺ 10 %		Eu ³⁺ 15 %		Eu ³⁺ 20 %		Eu ³⁺ 25 %	
	W%	At%	Wt	At%	Wt	At	Wt	At	Wt	At	Wt	At	Wt	At
			%		%	%	%	%	%	%	%	%	%	%
Yttrium	55.7	48.94	55.02	49.83	58.6	53.1	52.74	55.9	42.49	49.9	42.37	42.6	25.98	28.3
	7				9	2		9		5		4		3
Gadolinium	16.2	8.08	19.74	10.11	11.8	6.04	22.14	13.2	21.49	14.2	15.84	9.01	17.91	11.0
	8				0			9		8				4
Europium	4.87	2.50	7.83	4.15	11.1	5.92	10.12	6.28	21.14	14.5	27.53	16.2	38.24	24.3
					8					4		0		9
Cerium	2.50	8.14	9.96	5.72	11.2	6.46	11.39	7.67	12.60	9.40	8.15	5.20	12.01	8.31
					5									
Sodium	3.40	11.53	1.91	6.68	2.10	7.36	1.37	5.61	0.75	3.40	2.21	8.60	2.25	9.50
Fluorine	5.07	20.82	5.55	23.51	4.98	21.1	2.25	11.1	1.53	8.43	3.90	18.3	3.61	18.4
						0		6				4		3

Table S2 Atomic and Weight % of elements present in NaYF4: $Ce^{3+}/Gd^{3+}/Eu^{3+}$ with different Eu^{3+} contents

Table S3 Atomic and Weight (%) of elements present in core shell and Serine functionalised core shell nanostructure

Elements	Core shell		Serine functionalized				
			core shell				
	Wt%	At%	Wt%	At%			
Yttrium	48.53	49.30	12.07	3.56			
Gadolinium	27.99	16.08	29.98	5.00			
Europium	7.96	4.73	2.04	0.35			
Terbium	1.29	0.73	4.71	0.78			
Cerium	9.08	5.86	3.02	0.56			
Sodium	1.38	5.44	0.22	0.25			
Fluorine	3.76	17.86	2.67	3.68			
Carbon			20.65	45.07			
Nitrogen			1.53	2.87			
Oxygen			23.11	37.87			