Electronic Supplementary Material (ESI) for RSC Advances.

Crystal structure, optical spectroscopy and energy transfer properties in $NaZnPO_4:Ce^{3+}$, Tb^{3+} phosphors for UV- based LEDs

K. Saidi, M. Dammak

(a) Université de Sfax, Laboratoire de Physique Appliquée, Groupe de Physique des matériaux luminescents, Faculté des Sciences de Sfax, Département de Physique, 3018 Sfax, Tunisie.

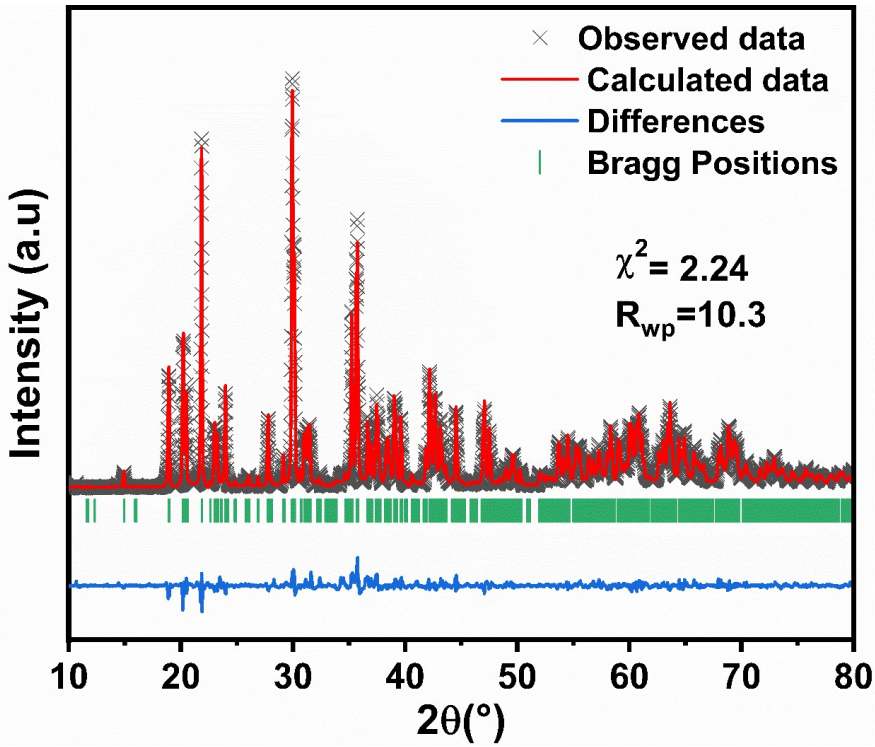

Fig. S1. Rietveld refinement of the XRD structure of NZPO.

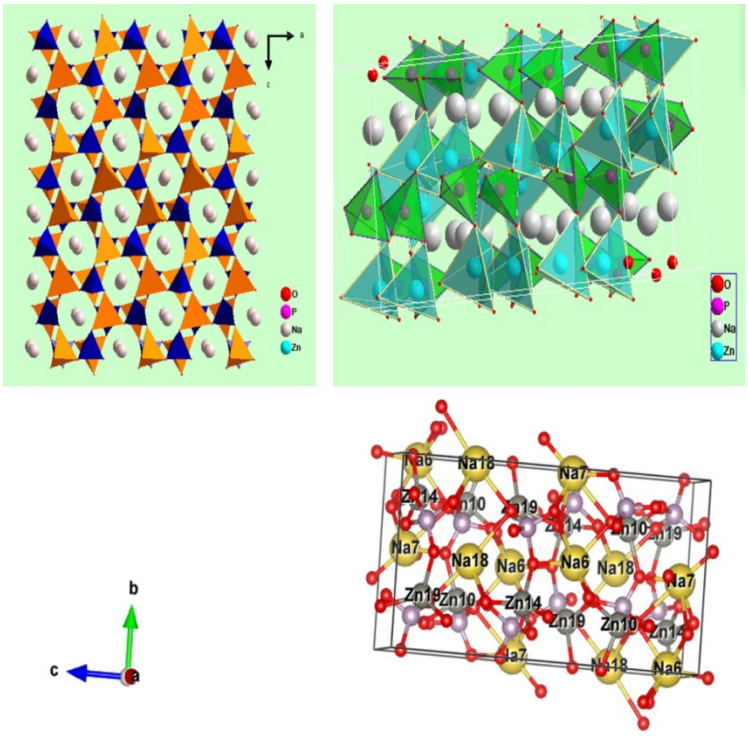

Fig.S2. Schematic illustration of the crystal structure of NZPO.

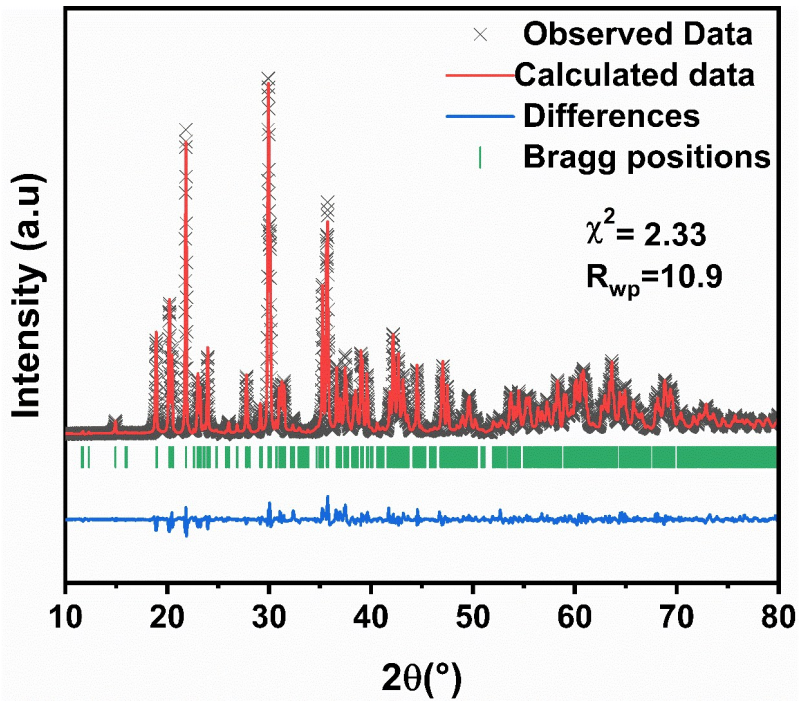

Fig S3: Rietveld refinement of XRD data for NZPO 0.05 Ce^{3+}.

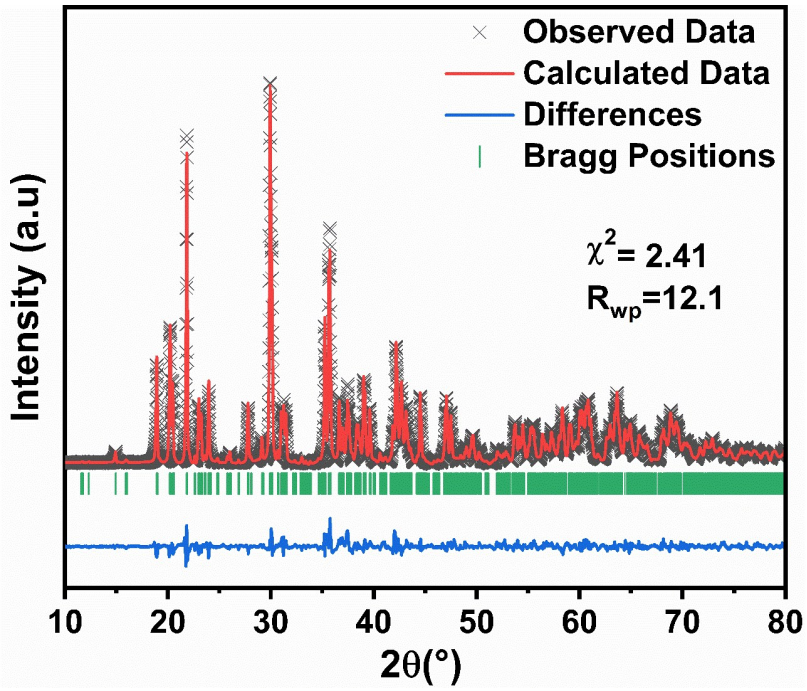

Fig S4: Rietveld refinement of XRD data for NZPO 0.08 Tb^{3+}.

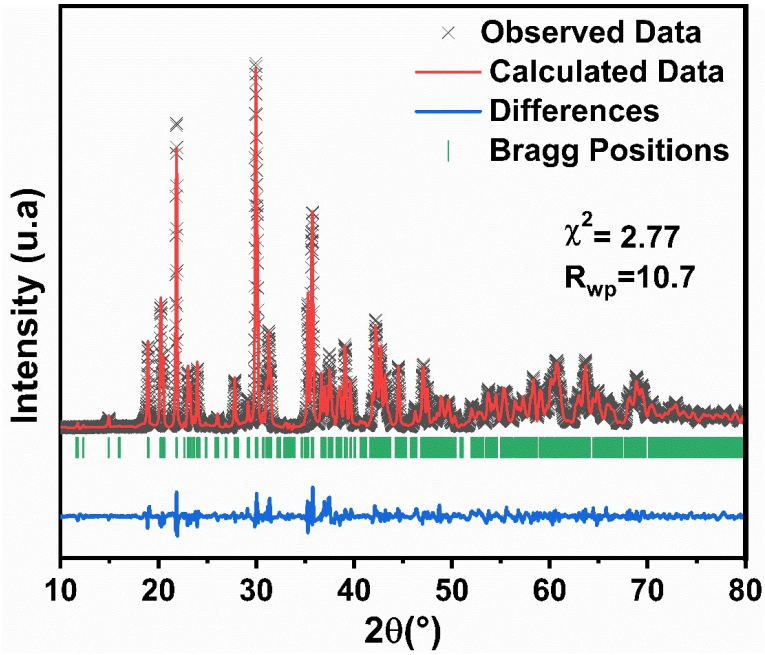

Fig S5: Rietveld refinement of XRD data for NZPO 0.05 Ce^{3+} 0.01Tb^{3+}.

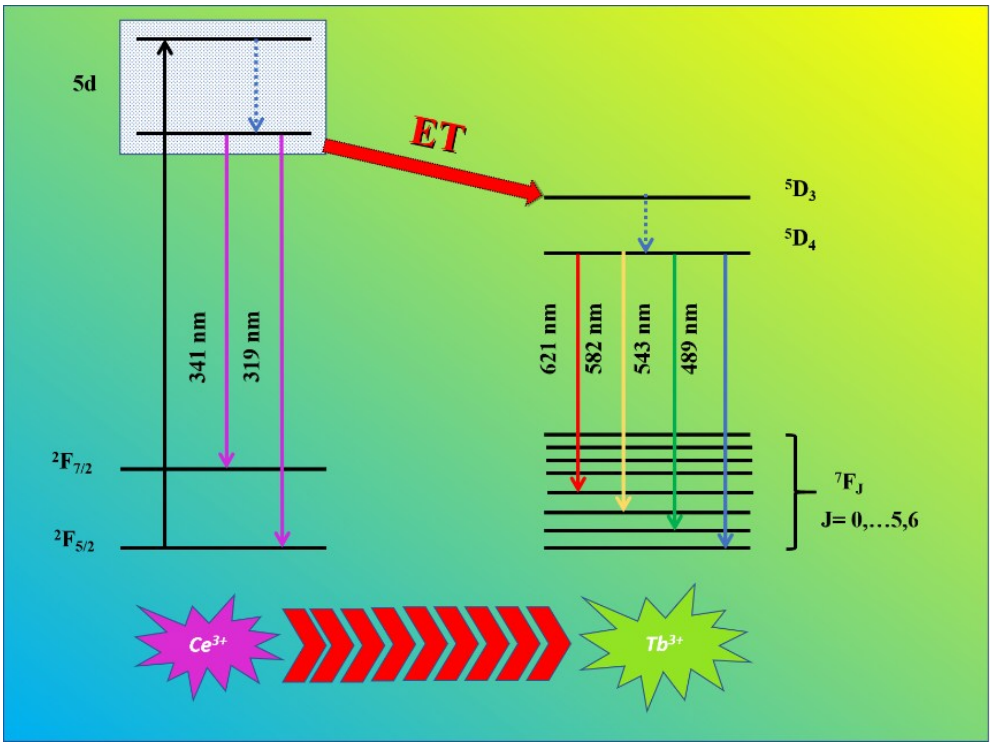

Fig.S6. Energy transfer processes between Ce^{3+} and Tb^{3+} ions.

Table S1. Structural Data of $NaZnPO_4$ from the Rietveld Refinement.

Cryst syst : monoclinic
Z=4
Space group $P2_1/n$
a =8.6681 Å
b= 8.1316 Å
c= 15.2591 Å
α=90°
β =89.8007°
γ=90°
V=1075.548 $Å^3$
R_{wp}= 10.3 %

Table S2. Atom Coordinates of $NaZnPO_4$

No.	Elem.	Symbol	Mult.	Wyck.	Symm.	x/a	y/b	z/c	Uiso/eq
1	O	O1	4	e	1	0.0073	0.5080	0.8825	0.0127
2	P	P2	4	e	1	0.4399	0.8334	0.4075	0.0127
3	O	O3	4	e	1	0.4310	0.2236	0.2011	0.0127
4	O	O4	4	e	1	0.9413	0.3485	0.3688	0.0127
5	O	O5	4	e	1	0.0851	0.2274	0.1751	0.0127
6	Na	Na6	4	e	1	0.7404	0.5206	0.4100	0.0127
7	Na	Na7	4	e	1	0.7203	0.4746	0.0639	0.0127
8	P	P8	4	e	1	0.1013	0.3222	0.4210	0.0127
9	O	O9	4	e	1	0.5740	0.4842	0.1878	0.0127
10	Zn	Zn10	4	e	1	0.9166	0.2201	0.2657	0.0127
11	O	O11	4	e	1	0.9430	0.2070	0.0400	0.0127
12	P	P12	4	e	1	0.9290	0.8221	0.2648	0.0127
13	O	O13	4	e	1	0.0678	0.2279	0.5031	0.0127
14	Zn	Zn14	4	e	1	0.1091	0.7145	0.4212	0.0127
15	O	O15	4	e	1	0.5700	0.3398	0.3306	0.0127
16	O	O16	4	e	1	0.2073	0.2429	0.3708	0.0127
17	O	O17	4	e	1	0.2241	0.3587	0.0335	0.0127
18	Na	Na18	4	e	1	0.2514	0.5195	0.2498	0.0127
19	Zn	Zn19	4	e	1	0.4374	0.2218	0.4078	0.0127
20	O	O20	4	e	1	0.1960	0.5040	0.4521	0.0127
21	O	O21	4	e	1	0.7212	0.2450	0.1974	0.0127

Table S3. Selection Bond Distances of $NaZnPO_4$

Atom 1	Atom 2	Symmetry op.	d 1,2 [Å]
Zn10	O9	3/2-x, -1/2+y, 1/2-z	2.0470
Zn10	O4	x, y, z	1.9007
Zn10	O5	1+x, y, z	2.0099
Zn10	O21	x, y, z	2.0370
Zn14	O3	1/2-x, 1/2+y, 1/2-z	1.9031
Zn14	O17	1/2-x, 1/2+y, 1/2-z	1.9875
Zn14	O13	-x, 1-y, 1-z	1.9737
Zn14	O20	x, y, z	1.9289
Zn19	O16	x, y, z	2.0824
Zn19	O1	1/2+x, 1/2-y, -1/2+z	2.0019
Zn19	O15	x, y, z	1.9032
Zn19	O11	-1/2+x, 1/2-y, 1/2+z	2.1008

Table S3 (continued)

Atom 1	Atom 2	Symmetry op.	d 1,2 [Å]
P2	O5	1/2-x, 1/2+y, 1/2-z	1.5436
P2	O17	1/2-x, 1/2+y, 1/2-z	1.6023
P2	O11	3/2-x, 1/2+y, 1/2-z	1.6545
P2	O1	1/2+x, 3/2-y, -1/2+z	1.4662
P8	O13	x, y, z	1.4978
P8	O20	x, y, z	1.5257
P8	O16	x, y, z	1.5622
P8	O4	-1+x, y, z	1.6025
P12	O15	3/2-x, 1/2+y, 1/2-z	1.4643
P12	O9	3/2-x, 1/2+y, 1/2-z	1.5040
P12	O3	3/2-x, 1/2+y, 1/2-z	1.5459
P12	O21	3/2-x, 1/2+y, 1/2-z	1.5548

Table S3 (continued)

Atom 1	Atom 2	Symmetry op.	d 1,2 [Å]
Na6	O20	1-x, 1-y, 1-z	2.1882
Na6	O4	x, y, z	2.3194
Na6	O11	3/2-x, 1/2+y, 1/2-z	2.3240
Na6	O15	x, y, z	2.4137
Na6	O21	3/2-x, 1/2+y, 1/2-z	2.4752
Na6	O13	1-x, 1-y, 1-z	2.9536
Na7	O9	x, y, z	2.2757
Na7	O17	1-x, 1-y, -z	2.0683
Na7	O13	1/2+x, 1/2-y, -1/2+z	2.3091
Na7	O1	1-x, 1-y, 1-z	2.5056
Na7	O21	x, y, z	2.7643
Na7	O11	x, y, z	2.9314
Na18	O16	1/2-x, 1/2+y, 1/2-z	2.6106
Na18	O3	1/2-x, 1/2+y, 1/2-z	2.4104
Na18	O5	1/2-x, 1/2+y, 1/2-z	2.4892
Na18	O9	x, y, z	2.9634
Na18	O5	x, y, z	3.0053
Na18	O1	-x, 1-y, 1-z	3.0322
Na18	O3	x, y, z	2.9598
Na18	O16	x, y, z	2.9351

Table S4 CIE chromaticity coordinates of NZPO 0.05 Ce^{3+}/ yTb^{3+}:

Samples	CIE (x, y)
NZP O : 0.05Ce^{3+}	**(0.1261,0.0636)**
NZPO : 0.05Ce^{3+}/0.01 Tb^{3+}	**(0.3366,0.5336)**
NZPO : 0.05Ce^{3+}/0.02 Tb^{3+}	**(0.3365,0.5290)**
NZPO : 0.05Ce^{3+}/0.04 Tb^{3+}	**(0.3439,0. 5179)**
NZPO : 0.05Ce^{3+}/0.06 Tb^{3+}	**(0.3399,0.5041**
NZPO : 0.05Ce^{3+}/0.08 Tb^{3+}	**(0.3388,0.5012)**