$Ba_3YB_3O_9$ based phosphor ceramic plates with excellent thermal stability for wLEDs applications

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Supporting Information

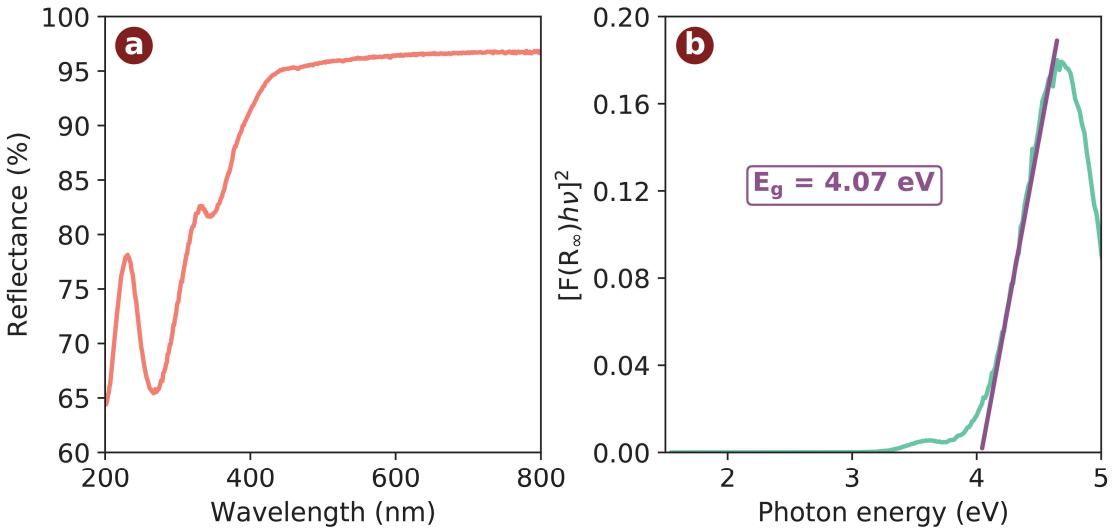

Fig. S1 (a) Diffuse reflectance spectra of undoped $Ba_3YB_3O_9$ phosphor. (b) The dependence of $[F(R_\infty)h\nu]^2$ on the photon energy $h\nu$.

The energy gap (E_g) of $Ba_3YB_3O_9$ phosphor can be evaluated by the following equation:

$$[F(R_\infty)h\nu]^n = A(h\nu - E_g)$$

Where $h\nu$ denotes photon energy, A is a proportional constant, n equals to 2 for direct allowed transition. $F(R_\infty)$ is the Kubelka-Munk function, which can be expressed as:

$$[F(R_\infty)] = (1-R)^2/2R$$

where R is the reflectance coefficient. $[F(R_\infty)h\nu]^2$ is plotted against $h\nu$ according to the Tauc method, from which the energy bandgap is determined to be ~ 4.07 eV.

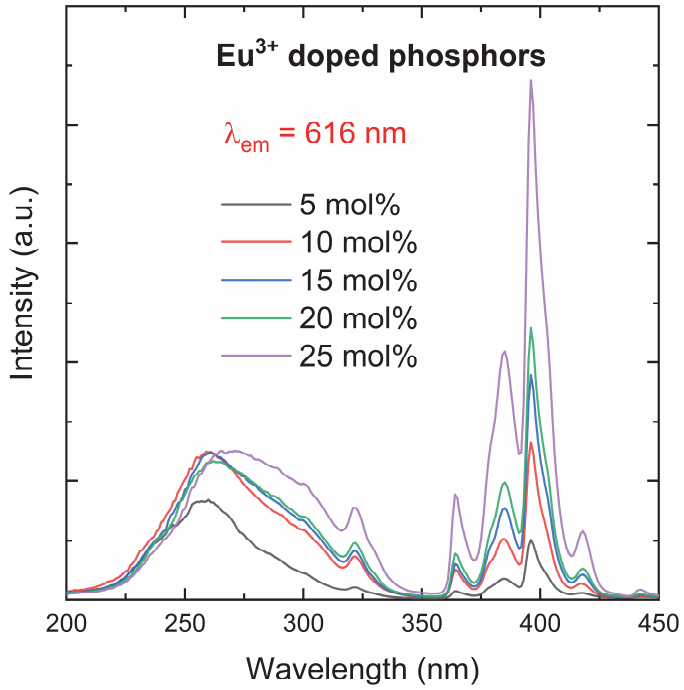

Fig. S2 Excitation spectra of Eu^{3+} doped $Ba_3YB_3O_9$ phosphors monitored at 616 nm.

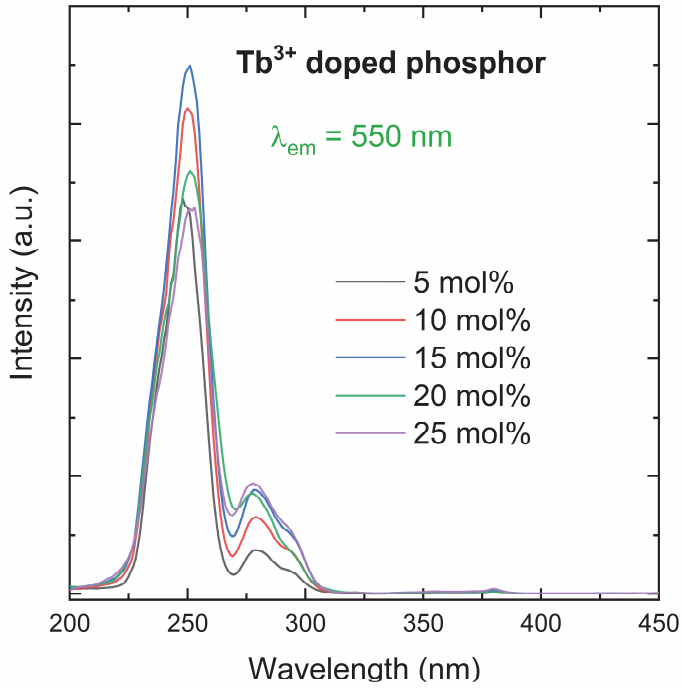

Fig. S3 Excitation spectra of Tb^{3+} doped $Ba_3YB_3O_9$ phosphors monitored at 550 nm.

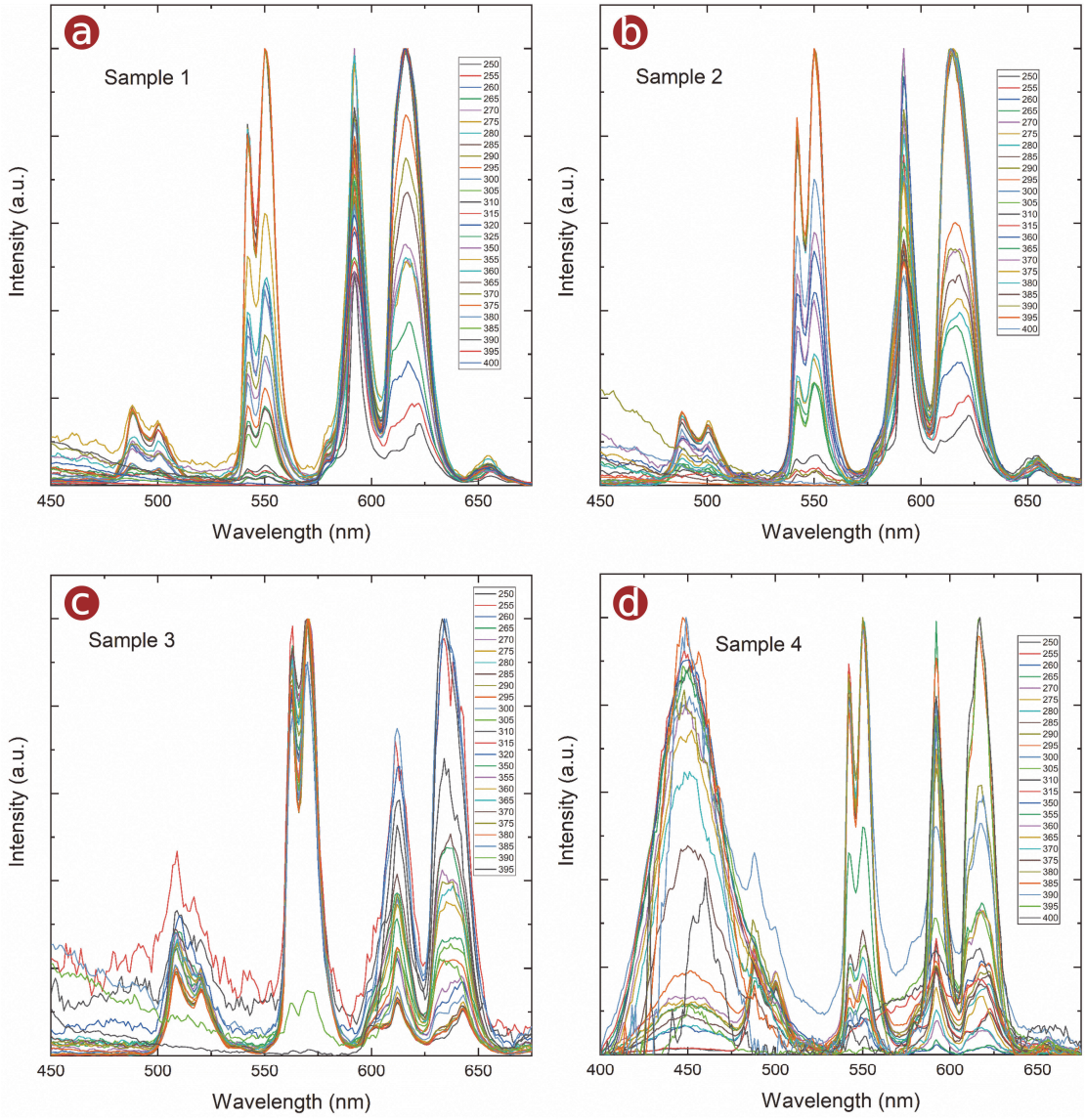

Fig. S4 (a)-(d) Emission spectra of prepared PCPs under various excitation wavelengths.

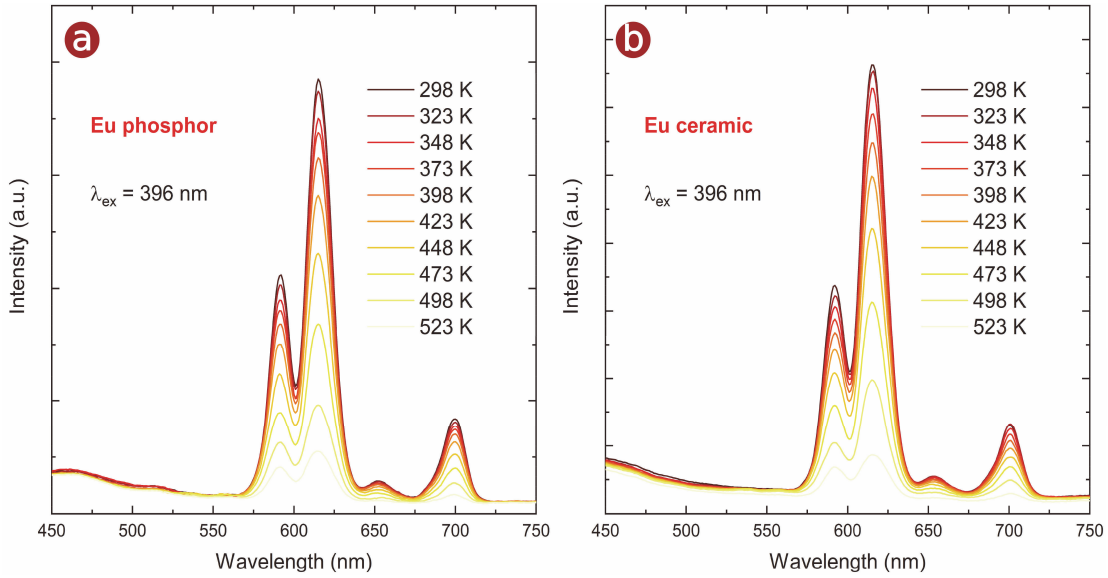

Fig. S5 (a) Emission spectra of Eu^{3+} doped $Ba_3YB_3O_9$ phosphor and (b) PCP measured from 298 to 523 K.

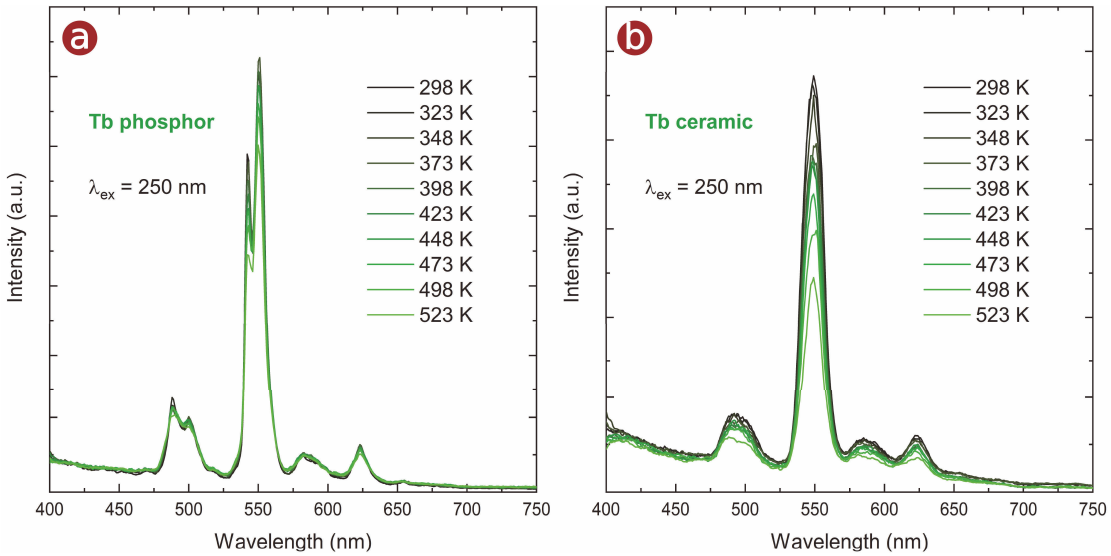

Fig. S6 (a) Emission spectra of Tb^{3+} doped $Ba_3YB_3O_9$ phosphor and (b) PCP measured from 298 to 523 K.

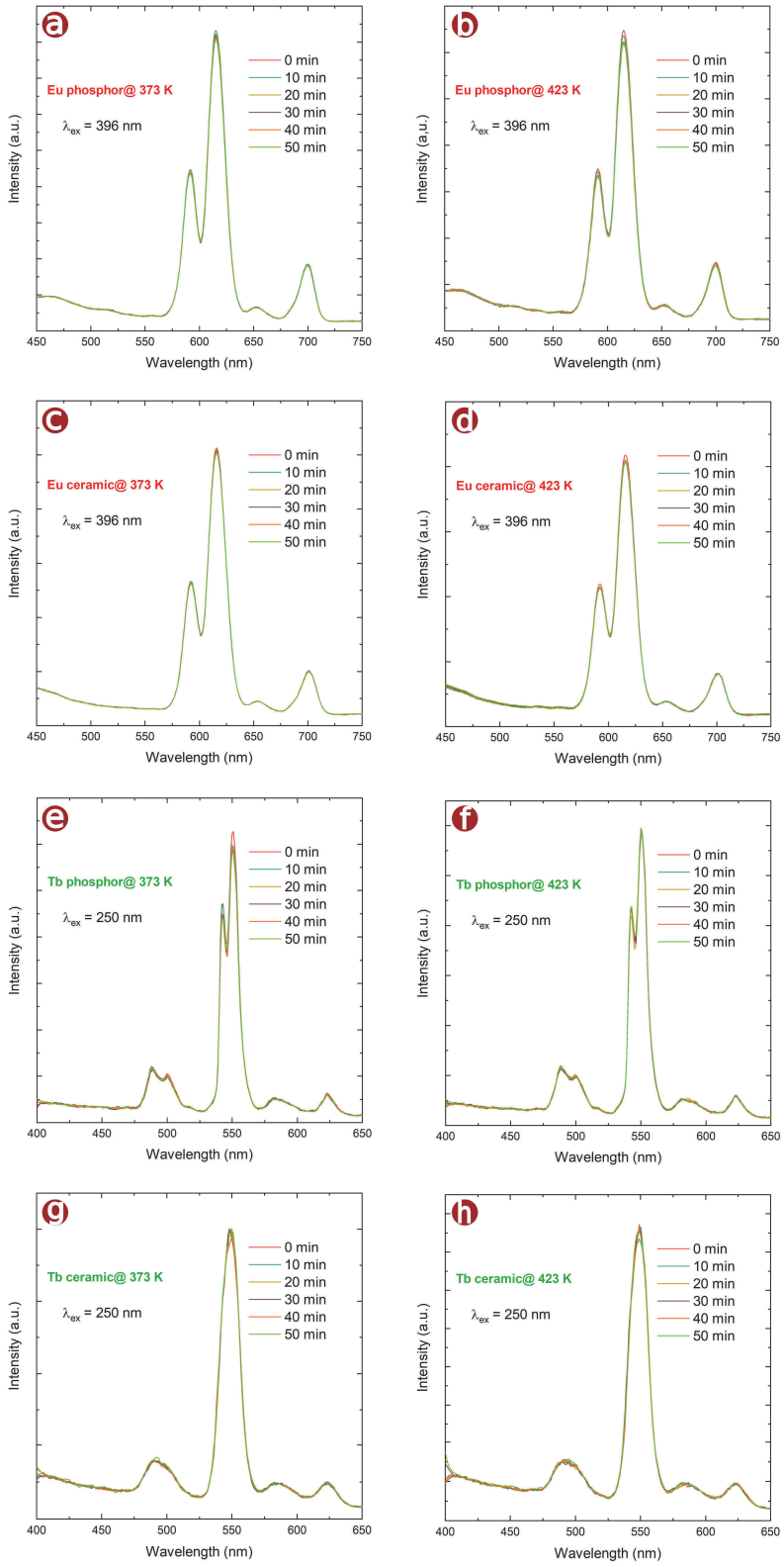

Fig. S7 (a)-(d) Emission spectra of Eu^{3+} doped $Ba_3YB_3O_9$ phosphor and PCP heated at 373 and 423 K in a time period of 0-50 mins. (e)-(h) Emission spectra of Tb^{3+} doped $Ba_3YB_3O_9$ phosphor and PCP heated at 373 and 423 K in a time period of 0-50 mins.

Table. S1 Atomic parameters for $Ba_3YB_3O_9$: 0.05 Eu^{3+}

Atom	Wyck.	x/a	y/b	z/c	S.O.F	U_{iso}
Ba1	6c	0.34808	0	0.44010	1	0.00179
Ba2	6c	0.32900	0	0.20013	1	0.00584
Ba3	2a	0	0	0.34264	1	0.00126
Ba4	4b	0.66670	0.3333	0.29915	1	0.00242
Y1	4b	0.33330	0.6667	0.56838	0.873	0.00192
Eu1	4b	0.33330	0.6667	0.56838	0.127	0.00192
Y2	2a	0	0	0.56316	0.632	0.00141
Eu2	2a	0	0	0.56316	0.368	0.00141
B1	6c	0	0.60842	0.48516	1	0.00651
B2	6c	0.64228	0.64228	0.64889	1	-0.00932
B3	6c	0	0.70095	0.32352	1	-0.00282
O1	12d	0.30936	0.47134	0.50209	1	0.00312
O2	12d	0.53795	0.6924	0.66200	1	0.00182
O3	6c	0	0.79856	0.49551	1	0.00245
O4	6c	0	0.1945	0.65813	1	0.00111
O5	12d	0.12952	0.8352	0.31869	1	0.00213
O6	6c	0.52824	0	0.30847	1	0.00328

Table. S2 Atomic parameters for $Ba_3YB_3O_9$: 0.25 Eu^{3+}

Atom	Wyck.	x/a	y/b	z/c	S.O.F	U_{iso}
Ba1	6c	0.36095	0	0.47027	1	0.00212
Ba2	6c	0.33223	0	0.22814	1	0.00176
Ba3	2a	0	0	0.37201	1	0.00176
Ba4	4b	0.66670	0.33330	0.32818	1	0.00176
Y1	4b	0.33330	0.66670	0.58813	0.615	0.00182
Eu1	4b	0.33330	0.66670	0.58813	0.385	0.00182
Y2	2a	0	0	0.57569	0.574	0.00174
Eu2	2a	0	0	0.57569	0.426	0.00174
B1	6c	0	0.68365	0.47645	1	0.00492
B2	6c	0.65835	0.65835	0.61818	1	0.01308
B3	6c	0	0.67814	0.35418	1	-0.00155
O1	12d	0.31450	0.47841	0.44318	1	0.00173
O2	12d	0.57847	0.65603	0.67974	1	0.00176
O3	6c	0	0.86732	0.51979	1	0.00176
O4	6c	0	0.15358	0.68996	1	0.00176
O5	12d	0.15576	0.87588	0.32314	1	0.01825
O6	6c	0.52775	0	0.33424	1	-0.00206

Table. S3 The bond length (d_{av}) for Y/Eu-O and lattice distortion index (D) for the undoped $Ba_3YB_3O_9$ sample.

Bond	d_{av}	D
Y1-O	2.21091	0.01716
Y2-O	2.24067	0.002

Table. S4 The bond length (d_{av}) for Y/Eu-O and lattice distortion index (D) for the $Ba_3YB_3O_9$: 0.05 Eu^{3+} sample.

Bond	d_{av}	D
Y1-O	2.24066	0.01765
Y2-O	2.24993	0.01203

Table. S5 The bond length (d_{av}) for Y/Eu-O and lattice distortion index (D) for the $Ba_3YB_3O_9$: 0.25 Eu^{3+} sample.

Bond	d_{av}	D
Y1-O	2.32374	0.03497
Y2-O	2.36638	0.03323

Table. S6 Comparison of thermal stability for the reported Eu^{3+} and Tb^{3+} doped materials and the synthesized Eu^{3+} and Tb^{3+} doped $Ba_3YB_3O_9$ samples.

Host	Activated ions	Heating temperature	Residual intensity	Literature
$Sr_{1.7}Zn_{0.3}CeO_4$	Eu^{3+}	423 K	~ 36%	1
$MgY_4Si_3O_{13}$	Eu^{3+}	423 K	~ 45%	2
$LaBWO_6$	Eu^{3+}	423 K	~ 57%	3
$Na_3Sc_2(PO)_4$	Eu^{3+}	423 K	~ 73%	4
$Ba_3YB_3O_9$ phosphor	Eu^{3+}	423 K	~ 81%	This work
$Ba_3YB_3O_9$ PCP	Eu^{3+}	423 K	~ 81%	This work
$LaAl_{2.03}B_4O_{10.54}$	Tb^{3+}	423 K	~ 28%	5
$Li_3Sc_2(PO_4)_3$	Tb^{3+}	423 K	~ 47%	6
$Ca(Mg0.8Al_{0.2})(Si_{1.8}Al_{0.2})O_6$	Tb^{3+}	423 K	~ 64%	7
$Ca_3Gd(GaO)_3(BO_3)_4$	Tb^{3+}	423 K	~ 70%	8
$Ba_3YB_3O_9$ phosphor	Tb^{3+}	423 K	~ 97%	This work
$Ba_3YB_3O_9$ PCP	Tb^{3+}	423 K	~ 83%	This work

References

1 H. Li, R. Zhao, Y. Jia, W. Sun, J. Fu, L. Jiang, S. Zhang, R. Pang and C. Li, *ACS Appl. Mater. Interfaces*, 2014, **6**, 3163-3169.

2 Z. Ci, R. Guan, K. Nie, L. Liu, L. Han, J. Zhang and Y. Wang, *J. Am. Ceram. Soc.*, 2015, **98**, 2488-2492.

3 B. Li, X. Huang, H. Guo and Y. Zeng, *Dyes Pigm.*, 2018, **150**, 67-72.

4 H. Guo, X. Huang and Y. Zeng, *J. Alloys Compd.*, 2018, **741**, 300-306.

5 F. Junqin, J. Cao, Z. Li, Z. Li, J. Li, J. Lin, W. Li, Z. Mu and F. Wu, *Ceram. Int.*, 2019, **45**, 20316-20322.

6 M. Jiao, Q. Xu, M. Liu, C. Yang and Y. Yu, *Phys. Chem. Chem. Phys.*, 2018, **20**, 26995-27002.

7 Z. An, S. Che, Y. Song, X. Zhang, R. Dong, D. Zhang, X. Zhou, Z. Shi and H. Zou, *Inorg. Chem.*, 2020, **59**, 4790-4799.

8 B. Li and X. Huang, *Ceram. Int.*, 2018, **44**, 4915-4923.