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Density-functional theory calculations, luminescence properties and fluorescence ratiometric thermo-sensitive for a novel borate based red phosphor: $NaBaSc(BO_3)_2:Ce^{3+},Mn^{2+}$

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The formation energies as a function of E_f for point defects in NBS

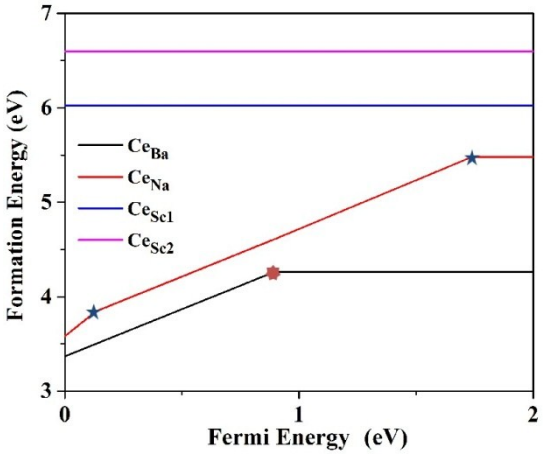

Figure S1. Formation energies as a function of E_f for point defects in NBS.

The formation energies as a function of E_f for each point defect in NBS are shown in Figure S1. The highlight points in the curves for Ce_{Ba} and Ce_{Na} demonstrate the transitions between different charge states. As shown in the Figure S1, the Ce_{Ba} and Ce_{Na} always have lower formation energy in NBS. When fermi energy is higher than 0.892 or 1.736 eV, the neutral Ce_{Ba} and Ce_{Na} shows lower formation, while Ce_{Na}^{2+} becomes more stable when the Fermi level is below 0.133 eV. Because the band gap value of NBS is 5.90 eV, the Fermi energy at 0.133, 0.892 or 1.736 all close to VBM than to CBM. Thus, the +2, +1 charged Ce_{Na} and +1 charged Ce_{Ba} are stable at the hole doping compound, while the neutral Ce_{Na} and Ce_{Ba} are stable in the electron doping cases. [1-2]

References

1. H. Chen, C. Y. Wang, J. T.Wang, X. P. Hu and S. X. Zhou, *J. Appl. Phys.*, 2012, **112**, 084513.

2. B. Qu, B. Zhang, L.Wang, R. Zhou and X. C. Zeng, *Chem. Mater.*, 2015, **27**, 2195

Morphology of NBS:0.02Ce^{3+},0.03Mn^{2+}

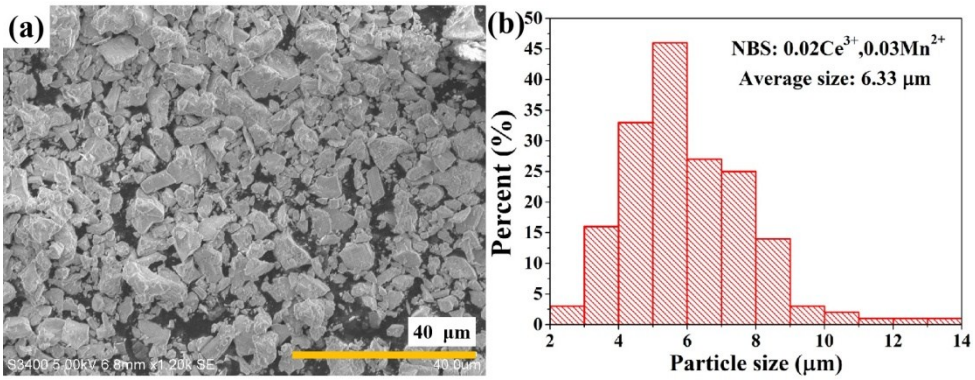

Figure S2. (a) SEM micrograph and (b) the particle size distribution of NBS:0.02Ce^{3+},0.03Mn^{2+}.

The irregular morphology of NBS:0.02Ce^{3+},0.03Mn^{2+} has been observed by the SEM micrograph (as shown in Figure S2(a)) and the sample shows good dispersion. The particle size distribution of the NBS:0.02Ce^{3+},0.03Mn^{2+} has also been investigated by using the Nano Measurer program (as shown in Figure 1(b)). The results indicate that the particle size of the sample ranges from 2 μm to 14 μm and the average diameter is 6.33 μm.