Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Understanding the Blue-Emitting Orthoborate Phosphor $NaBaBO_3:Ce^{3+}$ through Experiment and Computation

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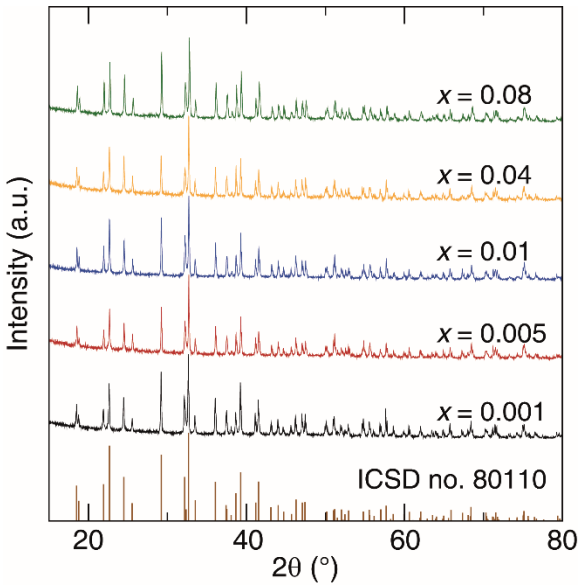

Figure S1 The X-ray powder diffraction patterns of $Na(Ba_{1-x}Ce_x)BO_3$ (x = 0.001, 0.005, 0.01, 0.04, and 0.08).

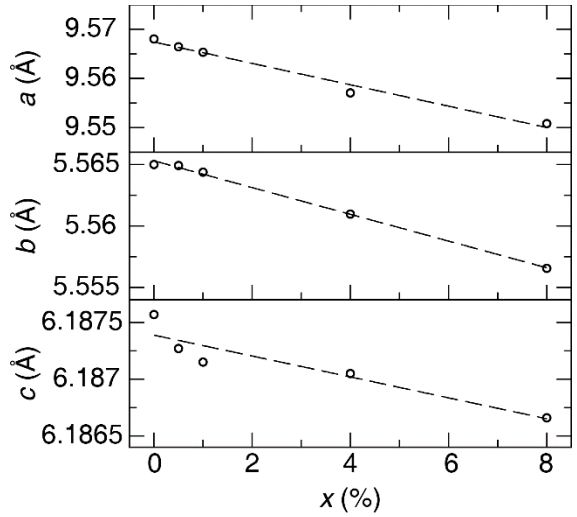

Figure S2 Unit cell lattice parameters as a function of Ce^{3+} concentration.

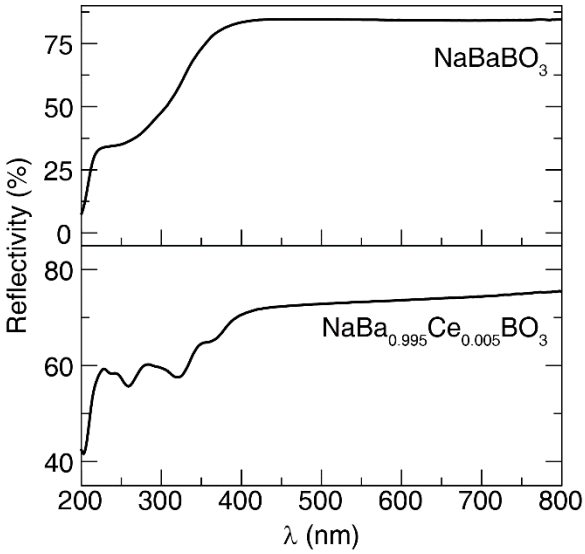

Figure S3 The diffuse reflection spectrum of $NaBaBO_3$ and $Na(Ba_{0.995}Ce_{0.005})BO_3$.

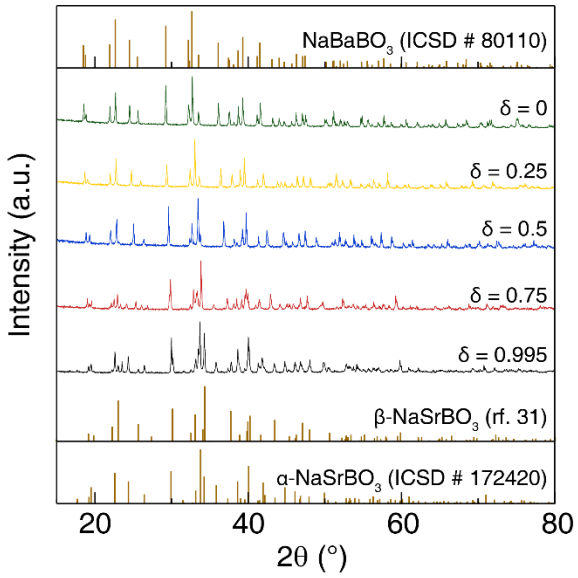

Figure S4 The X-ray powder diffraction patterns of $Na(Ba_{0.995-\delta}Sr_{\delta})Ce_{0.005}BO_3$ (δ = 0, 0.25, 0.5, 0.75, and 1).

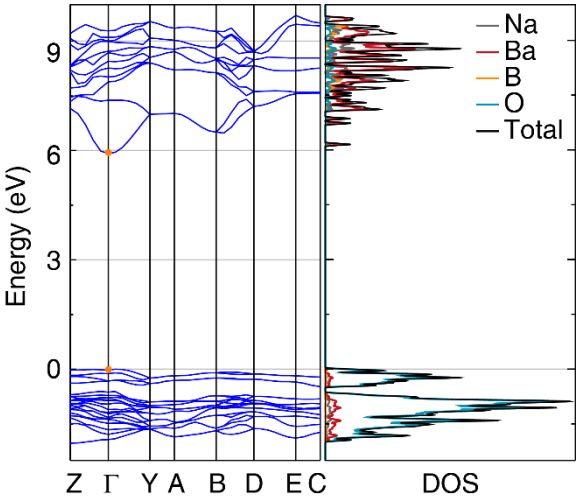

Figure S5 The band structure and density of states DOSs of $NaBaBO_3$ with the PBE0 hybrid functional.

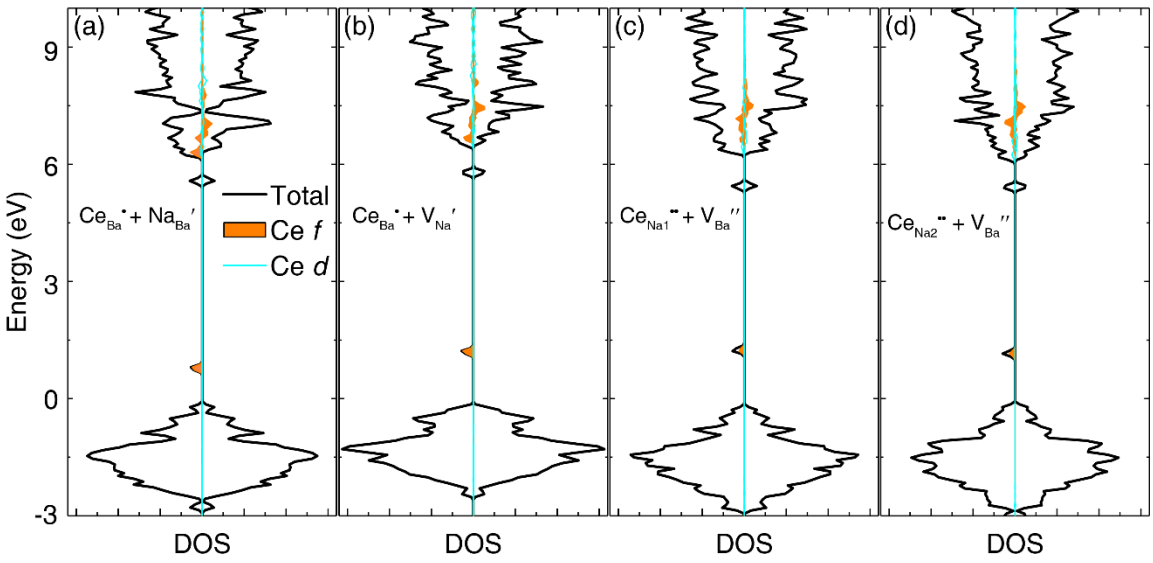

Figure S6 Total and orbital-projected DOSs for a) $Ce_{Ba}^{\bullet}$+ Na_{Ba}', b) $Ce_{Ba}^{\bullet}$+ V_{Na}', c) $Ce_{Na1}^{\bullet}$+V_{Ba}', d) $Ce_{Na2}^{\bullet}$+V_{Ba}' in the $NaBaBO_3$ obtained from the standard DFT-PBE0 method.

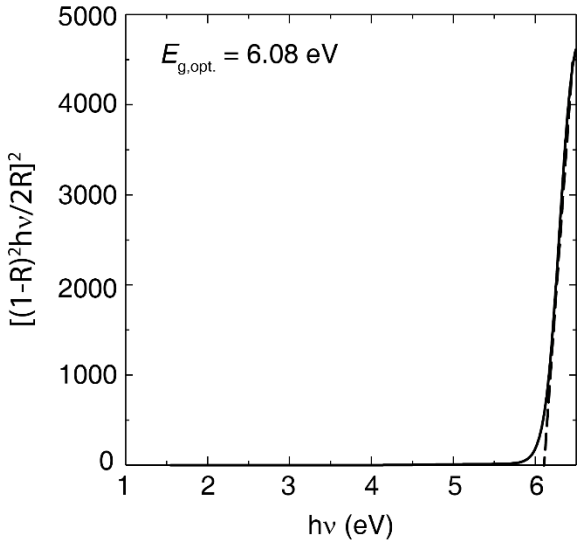

Figure S7 The calculated optical band gap.