Supporting Information

Understanding the Blue-Emitting Orthoborate Phosphor NaBaBO₃:Ce³⁺ through Experiment and Computation

Jiyou Zhong†‡, Weiren Zhao*†, Ya Zhuo‡, Chunpei Yan§, Jun Wen†∗, and Jakoah Brgoch‡∗

†School of Physics and Optoelectronic Engineering, Guangdong University of Technology, Guangzhou 510006, China
‡Department of Chemistry, University of Houston, Houston, Texas 77204, United States
§School of Physics and Electronic Engineering, Anqing Normal University, Anqing 246133, China

*E-mail: zwren123@126.com; wenjunkd@mail.ustc.edu.cn; jbrgoch@uh.edu

Figure S1 The X-ray powder diffraction patterns of Na(Ba₁₋ₓCeₓ)BO₃ (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$_3$ ($\delta$ = 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) $\text{Ce}_{\text{Ba}}^+ + \text{Na}_{\text{Ba}}^-$, b) $\text{Ce}_{\text{Ba}}^+ + \text{V}_{\text{Na}}^-$, c) $\text{Ce}_{\text{Na}1}^+ + \text{V}_{\text{Ba}}^-$, d) $\text{Ce}_{\text{Na}2}^+ + \text{V}_{\text{Ba}}^-$ in the NaBaBO$_3$ obtained from the standard DFT-PBE0 method.

Figure S7 The calculated optical band gap.