Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Combining experiment and computation to elucidate the optical properties of Ce^{3+} in $Ba_5Si_8O_{21}$

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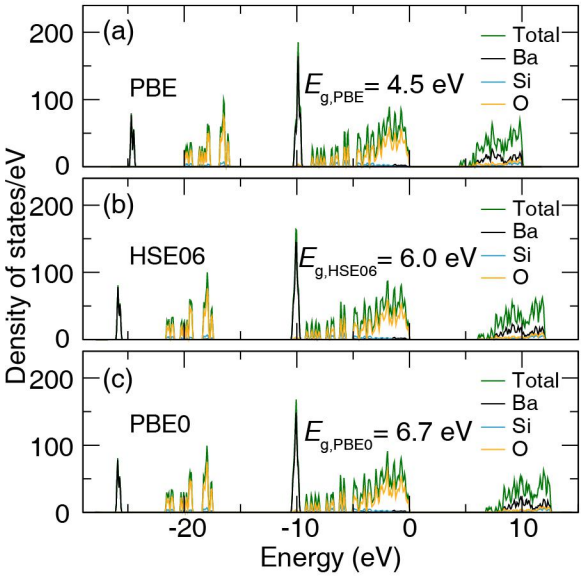

Figure S1 Density of states (DOS) of $Ba_5Si_8O_{21}$ and resulting band gap calculated with the a) PBE functional, b) HSE06 hybrid functional, and c) PBE0 hybrid functional.

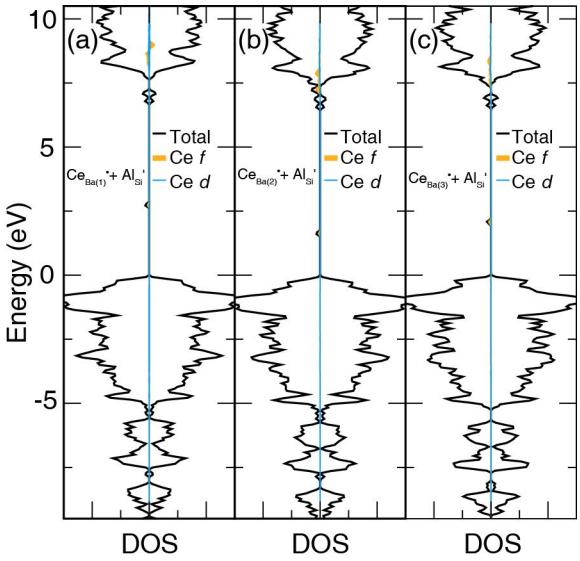

Figure S2 Total and orbital-projected DOSs for a) $Ce_{Ba(1)}^{\bullet}$+ $Al_{Si}^{'}$, b) $Ce_{Ba(2)}^{\bullet}$+ $Al_{Si}^{'}$, c) $Ce_{Ba(3)}^{\bullet}$+ $Al_{Si}^{'}$ in the $Ba_5Si_8O_{21}$ obtained from the standard DFT-PBE0 method.