Supporting information for
Tailoring Lanthanide Doping in Perovskite CaTiO$_3$
for Luminescence Applications

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We investigate doping of 11 rare-earth elements and determine the formation energies for various doping configurations. The results for Pr and Yb are discussed in the main text. Here we show the results for the remaining elements.
FIG. S1. Formation energies for (a) Tm, (b) Er, (c) Ho, (d) Dy, (e) Tb, (f) Eu, (g) Sm, (h) Nd and (i) Ce. Here A and B denote the “A point” (O-poor condition) and “B point” (O-rich condition) respectively. The red, green and blue line corresponds to different doping sites $X_{Ca}$, $X_{Ti}$ and $X_{i}$, respectively ($X=$Tm, Er, Ho, Dy, Tb, Eu, Sm, Nd, Ce).