Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for "Mechanisms of temperature-dependent oxygen absorption/release and appearance of intermediate phase in κ-$Ce_2Zr_2O_8$: study based on oxygen vacancy formation energy computations"

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Figure S1 shows the total energies of the $Ce_{16}Ti_2Zr_{14}O_{64}$ systems for the symmetrically independent combinations of Ti substitutions. This figure indicates that the two substituted Ti atoms are adjacent to each other in the most stable state.

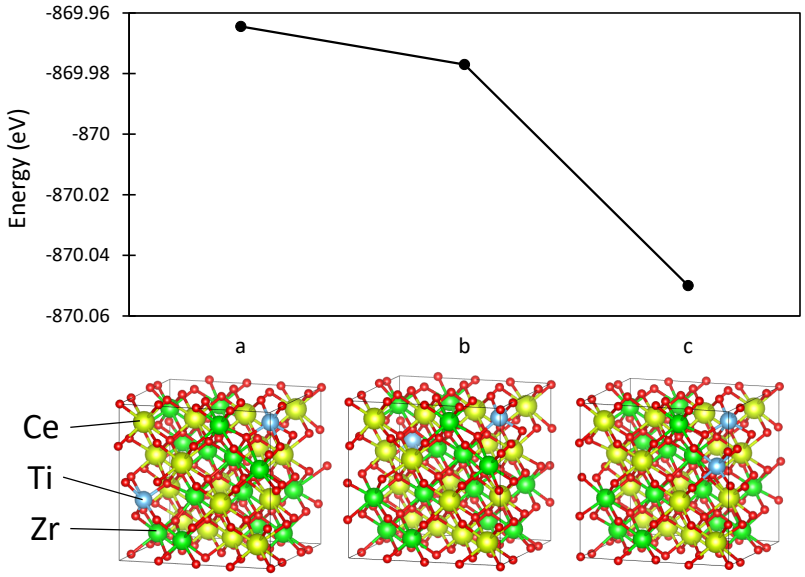

Figure S1: The total energies of the $Ce_{16}Ti_2Zr_{14}O_{64}$ systems for the symmetrically independent combinations of Ti substitutions.

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