Supplementary Information of

Advanced Thermal/Environmental Barrier Coatings of High-Entropy Rare Earth Disilicates Tuned by Strong Anharmonicity of $Eu_2Si_2O_7$

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The C_{11} and C_{66} type lattice distortions denoted as LD_{C11} and LD_{C66} alter the lattice parameters according to the following matrices:

$$LD_{C11} = \begin{pmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; LD_{C66} = \begin{pmatrix} 1 & \delta & 0 \\ \delta & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

where δ values are set to $\pm 0.007,\ \pm 0.014, and\ \pm 0.021$ in percentage. The resulting energy deviation ($\Delta E = E(\delta) - E(\delta=0)$) versus δ for $Eu_2Si_2O_7$, $Er_2Si_2O_7$, and $Gd_2Si_2O_7$ are shown in Figure S1.

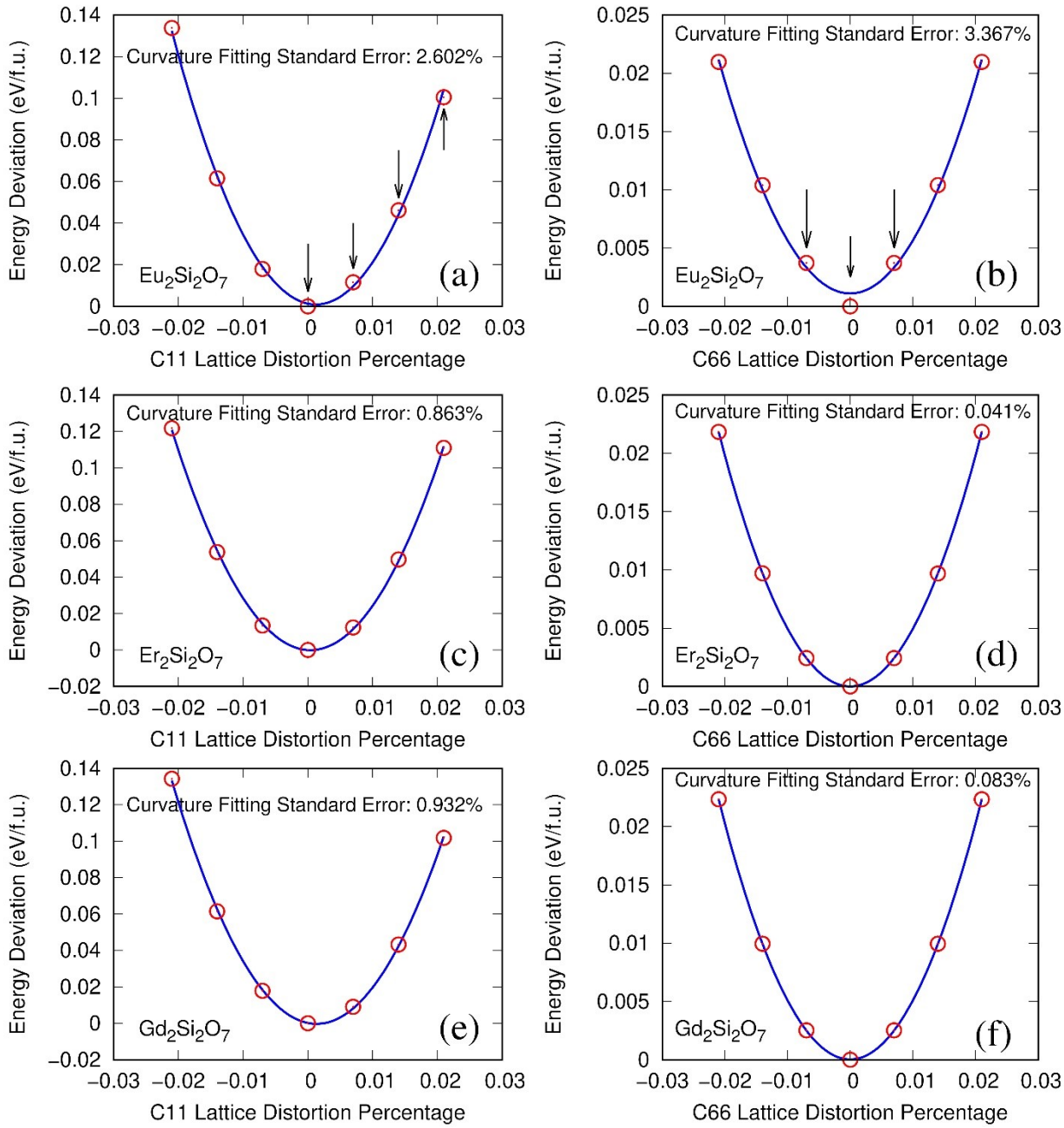

Fig. S1 The potential energy deviation relative to the fully relaxed equilibrium states as the lattice undergoes a series of C_{11} and C_{66} type lattice distortions for (a-b) $Eu_2Si_2O_7$, (c-d) $Er_2Si_2O_7$, and (e-f) $Gd_2Si_2O_7$. The much larger energy deviation points from the fitted parabolic lines are highlighted in (a) and (b) by arrows. The much larger curvature fitting standard errors of $Eu_2Si_2O_7$ than $Er_2Si_2O_7$ and $Gd_2Si_2O_7$ suggest that $Eu_2Si_2O_7$ lattice exhibits much stronger lattice anharmonicity.