

Table S1. Interatomic potential parameters of Morse function used in the calculations. [13].

Pair of Atoms	D_M, eB	$\alpha, \text{\AA}^{-2}$	$r_0, \text{\AA}$	$R_{\max}, \text{\AA}$
O–O	0.018716	1.374805	3.645169	15.0
P–O	0.446152	3.263861	1.609157	15.0
La–O	0.099973	3.456018	2.662300	15.0
Ce–O	0.117341	3.335213	2.631052	15.0
Pr–O	0.133622	3.278962	2.607182	15.0
Nd–O	0.173034	3.563096	2.562213	15.0
Sm–O	0.190876	3.737843	2.518803	15.0
Eu–O	0.193661	3.399594	2.518195	15.0
Gd–O	0.198682	3.172605	2.515892	15.0
Pu–O	0.119590	3.701095	2.596788	15.0
Y–O	0.318939	1.908249	2.540487	15.0
Tb–O	0.231571	2.008679	2.572061	15.0
Dy–O	0.306464	1.898378	2.552877	15.0
Ho–O	0.356088	1.837013	2.539438	15.0
Er–O	0.402338	1.792183	2.526532	15.0
Tm–O	0.441546	1.758439	2.517015	15.0
Yb–O	0.472769	1.729378	2.509278	15.0
Lu–O	0.505421	1.700125	2.501459	15.0

Table S2. Enthalpy of solid solutions of CaSiO₃ and MgSiO₃ with hypothetical REE perovskites with a Ca/Mg site occupation of 0.5.

	0 GPa		24 GPa	
	$\Delta H \text{MgSiO}_3 \text{ eV}$	$\Delta H \text{CaSiO}_3 \text{ eV}$	$\Delta H \text{MgSiO}_3 \text{ eV}$	$\Delta H \text{CaSiO}_3 \text{ eV}$
La	0.816	0.025	3.896	0.037
Ce	0.702	0.031	1.096	0.037
Pr	0.655	0.037	1.029	0.040
Nd	0.625	0.049	1.077	0.045
Sm	0.595	0.072	0.986	0.062
Eu	0.530	0.072	0.876	0.067
Gd	0.466	0.073	0.791	0.072
Tb	0.139	0.072	0.193	0.086
Dy	0.146	0.091	0.196	0.105
Ho	0.141	0.107	0.186	0.121
Er	0.137	0.124	0.177	0.137
Tm	0.138	0.140	0.172	0.153
Yb	0.133	0.158	0.164	0.167
Lu	0.130	0.172	0.154	0.182