Supplementary Information

Details of Convergence Testing for DFT Calculations Using the 4*a*×4*a*×4*a* BCC-Fe Supercell

As shown in Table S1, the formation energies of substitutional rare-earth atoms and the solution energies of oxygen at both tetrahedral and octahedral interstitial sites were compared using 3***a***×3***a***×3***a***, 4***a***×4***a***×4***a***, and 5***a***×5***a***×5*a* BCC-Fe supercells (the lattice constant ***a*** = 2.834 Å). To ensure consistency, . The same k-point sampling density $2\pi \times 0.04$ /Å as used in the main calculations (3×3×3, 2×2×2, and 2×2×2 for the 3***a***×3***a***×3***a***, 4***a***×4***a***×4***a***, and 5***a***×5***a***×5***a*** BCC-Fe supercells, respectively) was applied. The results show that, relative to the 5×5×5 supercell, the 4×4×4 supercell produces converged formation energies of substitutional rare-earth atoms and solution energies of interstitial oxygen within 0.002 eV, confirming the reliability of this supercell size for subsequent calculations. Considering computational efficiency, most density functional theory (DFT) studies, such as those reported in Computational Materials Science (2016, 124, 249–258) and Vacuum (2023, 212, 112005), have also adopted a 4*a*×4*a*×4*a* BCC-Fe supercell for similar systems. This approach was implemented following convergence verification, and the relevant references have been included in the Methods section describing the supercell model.

Table S1. Calculated formation energies of substitutional rare-earth atoms REA (Y, La, and Ce) E_{sub} and solution energies of interstitial O at tetrahedral and octahedral sites (E_{int}^{T} and E_{int}^{O}) in 3*a*×3*a*×3*a* (Fe_{54}), 4*a*×4*a*×4*a* (Fe_{128}), and 5*a*×5*a*×5*a* (Fe_{250}) BCC-Fe supercells.

Calculation Systems	E_{sub} (eV)	E_{int}^{T} (eV)	E_{int}^{O} (eV)
Fe_{54}		-0.621	-0.621
Fe_{128}		-0.626	-0.627
Fe_{250}		-0.627	-0.627
$Fe_{53}Y$	1.796	-1.413	-0.453
$Fe_{127}Y$	1.760	-1.450	-0.459
$Fe_{249}Y$	1.759	-1.451	-0.460
$Fe_{53}La$	7.297	-1.012	-0.392
$Fe_{127}La$	7.290	-1.075	-0.409
$Fe_{249}La$	7.288	-1.077	-0.409
$Fe_{53}Ce$	0.826	-0.908	-0.213
$Fe_{127}Ce$	0.821	-0.959	-0.248

$Fe_{249}Ce$	0.821	-0.960	-0.248