Supplementary Materials

Probing into the In-Situ Exsolution Mechanism of Metal Nanoparticles from Doped Ceria Host

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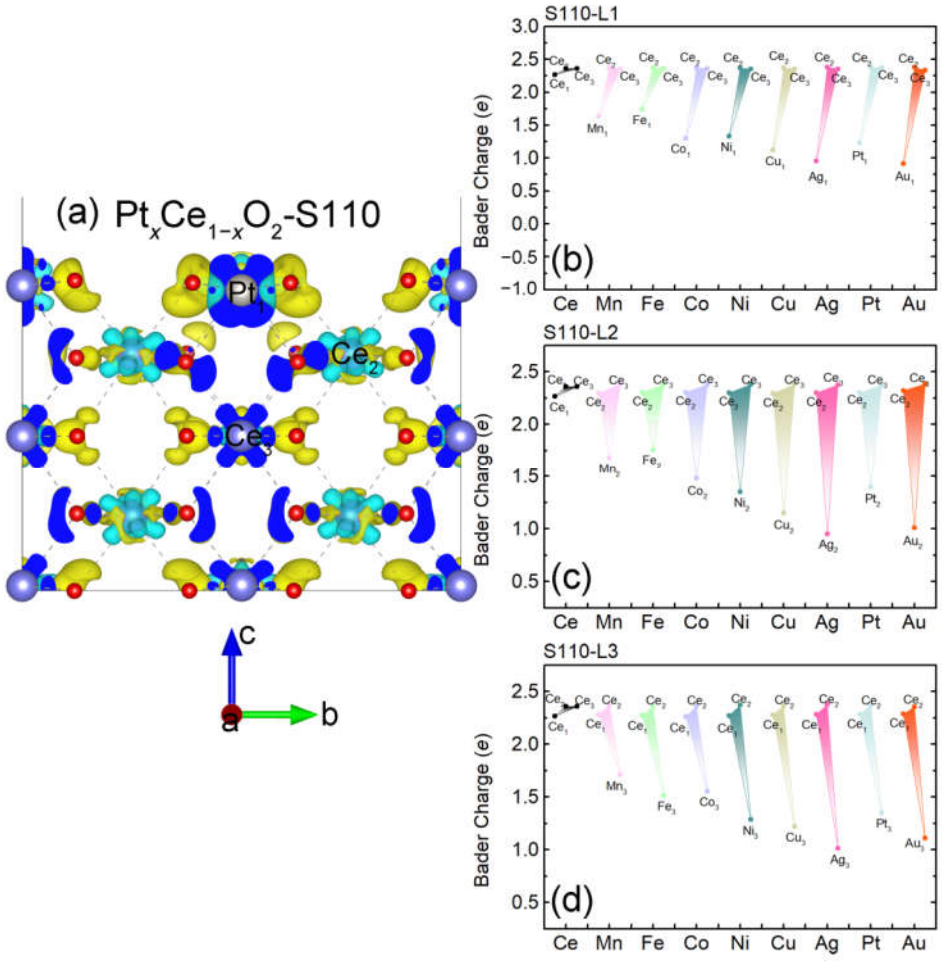

Figure S1. (**a**) The 3D-plot of charge density difference with an isosurface value of 0.02 *e*/Bohr^3 for $Pt_xCe_{1-x}O_2$-S110 with Pt at L1. (**b**–**d**) Evolution of Bader charge for $M_xCe_{1-x}O_2$-S110 with the dependence of Mn, Fe, Co, Ni, Cu, Ag, Pt and Au: (**b**) M in L1, (**c**) M in L2 and (**d**) M in L3.

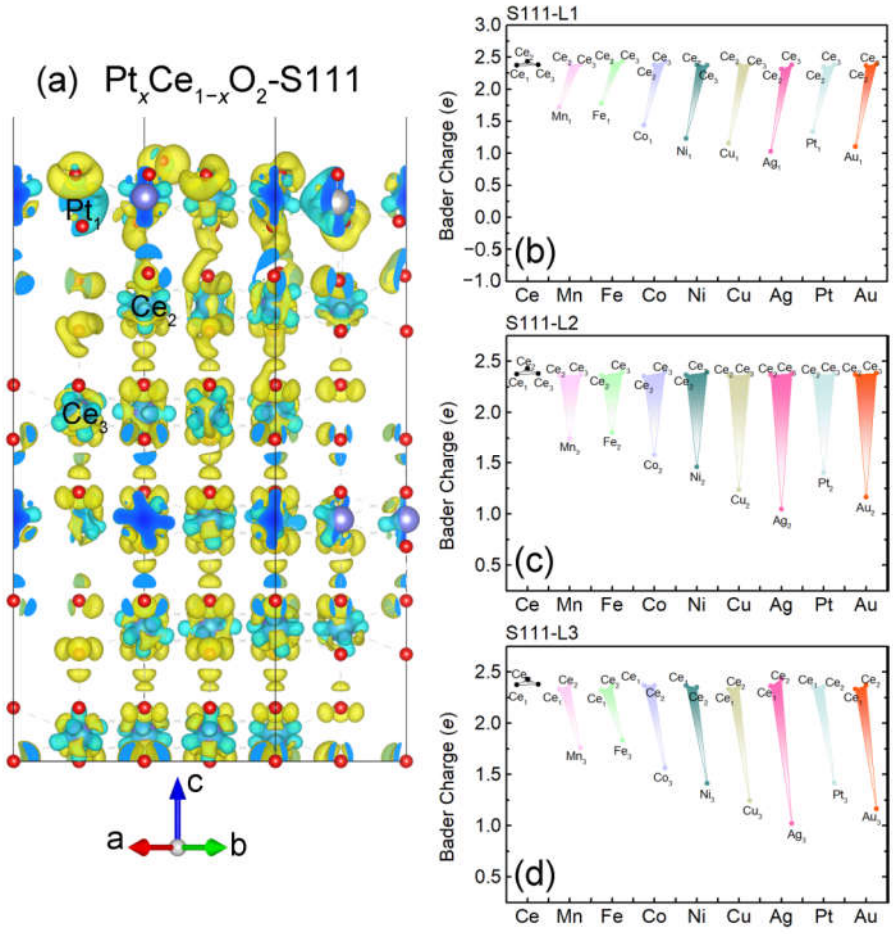

Figure S2. (**a**) The 3D-plot of charge density difference with an isosurface value of 0.02 *e*/Bohr^3 for $Pt_xCe_{1-x}O_2$-S111 with Pt at L1. (**b–d**) Evolution of Bader charge for $M_xCe_{1-x}O_2$-S111 with the dependence of Mn, Fe, Co, Ni, Cu, Ag, Pt and Au: (**b**) M in L1, (**c**) M in L2 and (**d**) M in L3.

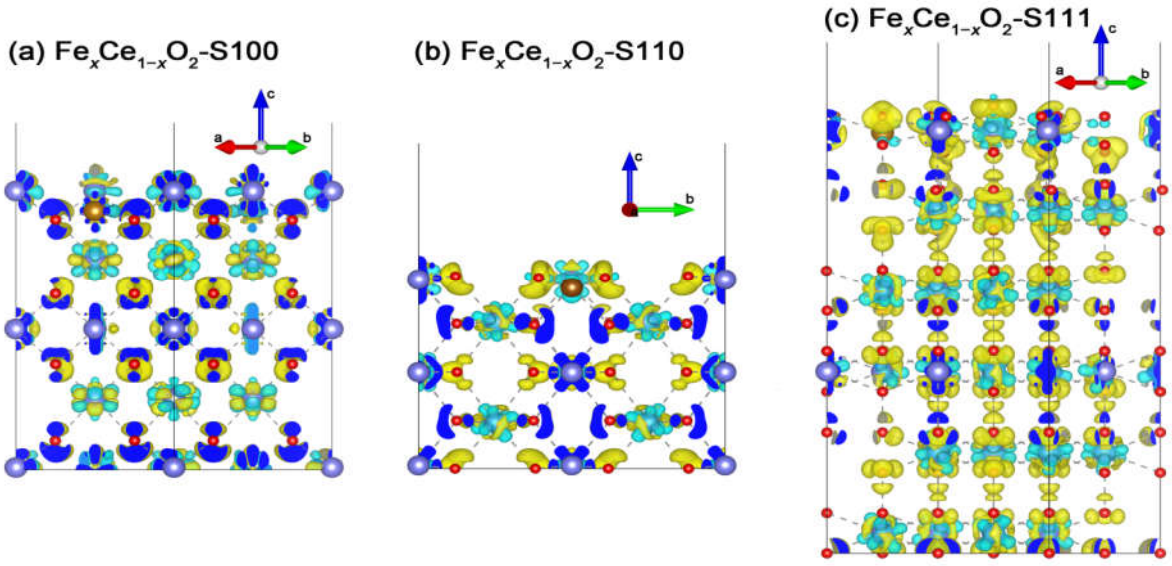

Figure S3. The 3D plots of charge density difference with an isosurface value of 0.02 *e*/Bohr^3 for $Fe_xCe_{1-x}O_2$ with different oriented surfaces: (**a**) $Fe_xCe_{1-x}O_2$-S100, (**b**) for $Fe_xCe_{1-x}O_2$-S110 and (**c**) $Fe_xCe_{1-x}O_2$-S111.

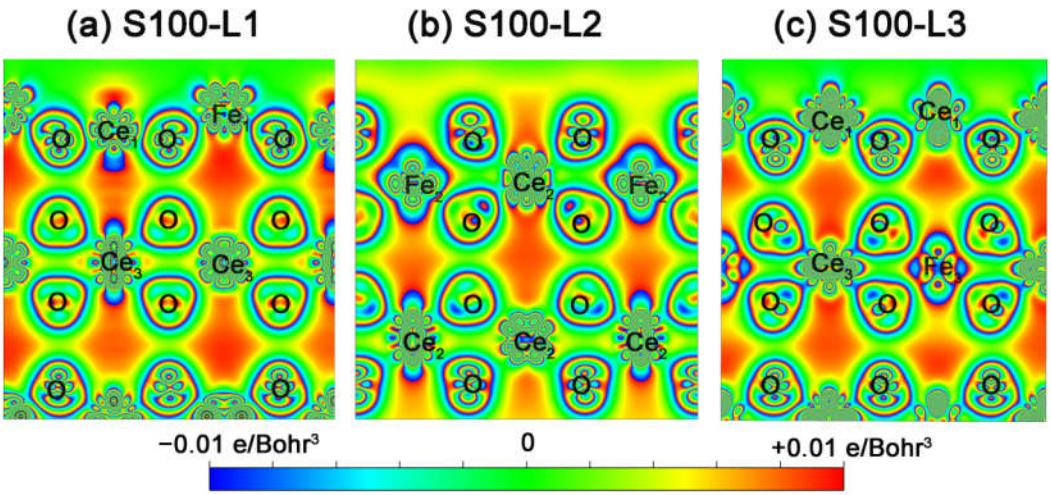

Figure S4. 2-D charge density difference plots along the (001)-direction ($\Delta n(\mathbf{r})$ in units of e/Bohr^3) for 1.5 × 1.5 × 1 $Fe_xCe_{1-x}O_2$-S100, which with Fe (**a**) on surface layer L1, (**b**) in second layer L2 and (**c**) in the 'bulk' layer L3.