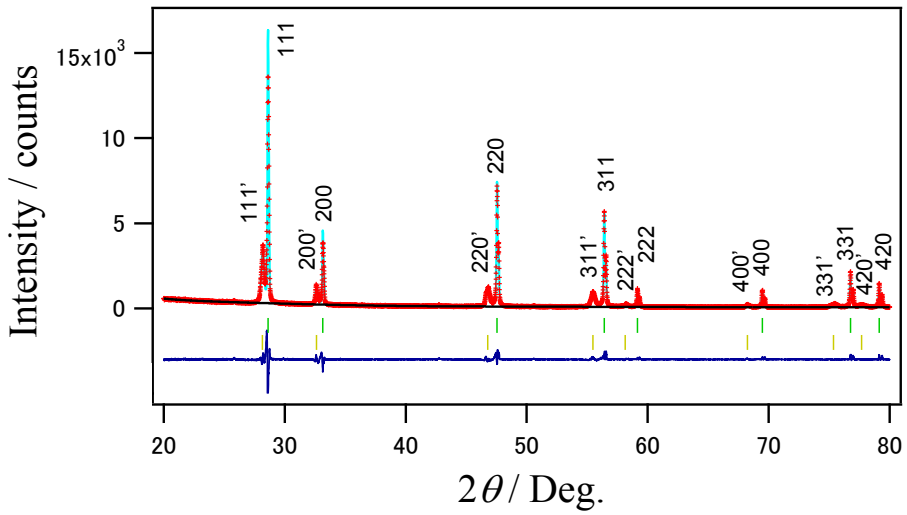


Figure S1. Rietveld refinement patterns of crystalline ceria powder (the holding time is 30 min at 800 ºC). The red "+" marks, the solid light-blue line, the green tick marks, yellow tick marks, and the lower solid blue line stand for experimental data, calculated data, Bragg-peak positions of $CeO_2$, Bragg-peak positions of $HCeO_2$, and the difference between the experimental and calculated intensities, respectively. $R_{wp}$ = 11.5% ($S^2$ = 4.15).

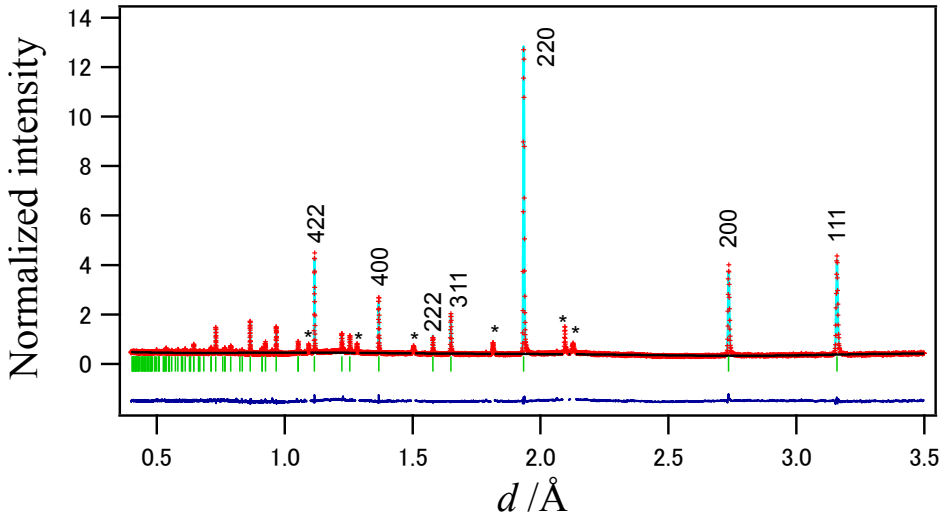


Figure S2. Rietveld refinement patterns of crystalline oxihydroxide ceria ($CeO_2H_{0.04}$) powder at 800 ºC. The red "+" marks, the solid light-blue line, the green tick marks, and the lower solid blue line indicate experimental data, calculated data, Bragg-peak positions, and the difference between the experimental and calculated intensities, respectively. The asterisk denotes the peaks of thermocouple, which are deselected in the refinement. Space group *Fm-3m*, $a$ = 5.470552(7) Å, and $R_{wp}$ = 4.67% ($S^2$ = 2.43).

Table S1. Crystal structure parameters of $CeO_2H_{0.04\text{-}0.06}$ and $CeO_2H$ at 800°C and 600°C.

| Sample | $CeO_2H_{0.04}$ | $CeO_2H_{0.06}$ | $CeO_2H$ |
|---|---|---|---|
| Chemical formula | $CeO_2H_{0.04}$ | $CeO_2H_{0.06}$ | $CeO_2H$ |
| Molecular weight | 172.1 | 172.1 | 173.1 |
| Crystal system | Cubic | Cubic | Cubic |
| Space group | *Fm*-3*m* | *Fm*-3*m* | *Fm*-3*m* |
| *a* (Å) | 5.470552(7) | 5.448319(5) | 5.518012(8) |
| *V* (Å$^3$) | 163.717 | 161.729 | 168.015 |
| *Z* | 4 | 4 | 4 |

| | | site | *g* | *x* | *y* | *z* | $B_{iso}$ (Å$^2$) |
|---|---|---|---|---|---|---|---|
| $CeO_2H_{0.04}$ | Ce | 4*a* | 1 | 0 | 0 | 0 | 1.056(9) |
| | O | 8*c* | 1 | 1/4 | 1/4 | 1/4 | 1.802(8) |
| | H | 32*f* | 0.005 | 0.363(8) | 0.363(8) | 0.363(8) | 0.87 |
| $CeO_2H_{0.06}$ | Ce | 4*a* | 1 | 0 | 0 | 0 | 0.854(8) |
| | O | 8*c* | 1 | 1/4 | 1/4 | 1/4 | 1.224(8) |
| | H | 32*f* | 0.008 | 0.362(3) | 0.362(3) | 0.362(3) | 1.08(6) |
| $CeO_2H$ | Ce | 4*a* | 1 | 0 | 0 | 0 | 1.9(1) |
| | O | 8*c* | 1 | 1/4 | 1/4 | 1/4 | 0.73(9) |
| | H | 32*f* | 0.125 | 0.354(2) | 0.354(2) | 0.354(2) | 1.1(9) |