

Morphology-Dependent Interplay of Reduction Behaviors, Oxygen Vacancies and Hydroxyl Reactivity of CeO₂ Nanocrystals

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Supporting Information

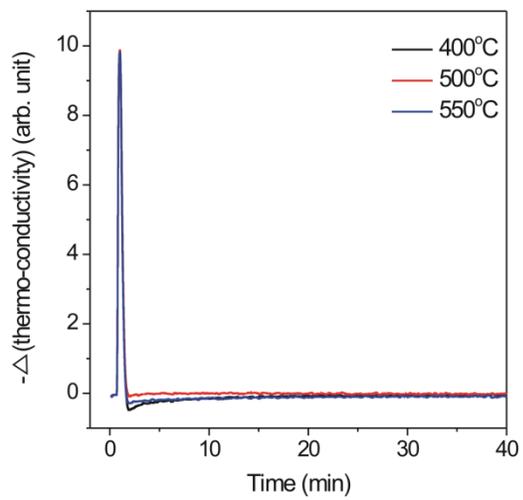


Figure S1. Isothermal H₂ reduction profiles of SiO₂ at indicated temperatures.

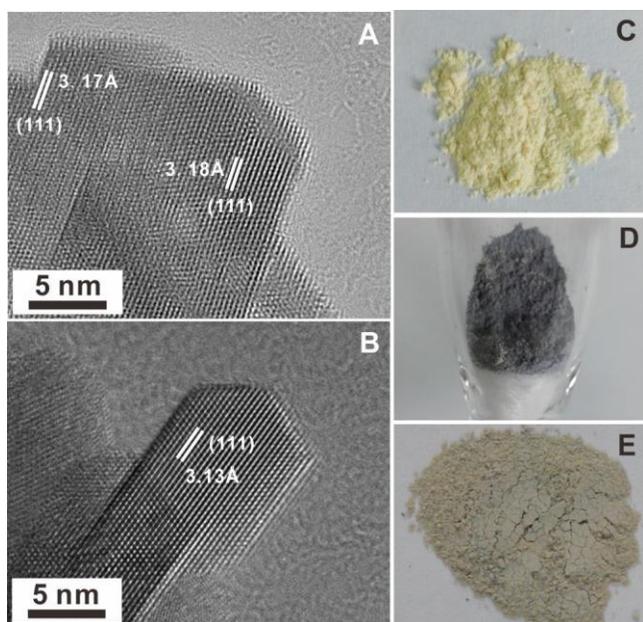


Figure S2. HRTEM images and photographs of of CeO₂ nanorods preferentially exposing {111} and {100} crystal planes prepared by calcination at 700 °C for 4 hours. HRTEM images of samples (A) calcined, (B) 500°C reduced, and photographs of (C) calcined, (D) 500°C reduced, (E) sample in (D) exposed to air.

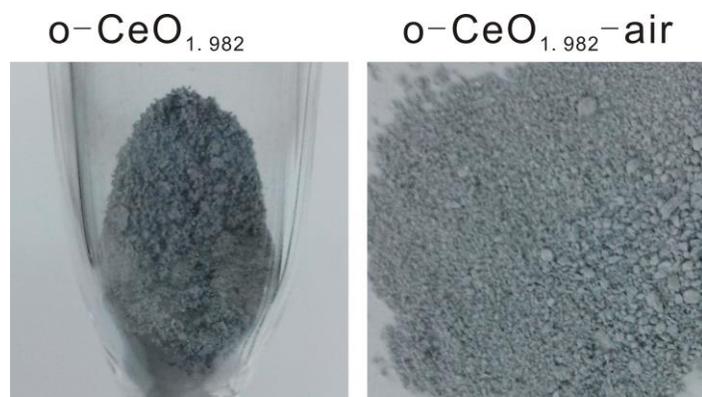


Figure S3. Photographs of $\text{o-CeO}_{1.982}$ nanocrystals prepared by H_2 isothermal reduction at $500\text{ }^\circ\text{C}$ and $\text{o-CeO}_{1.982}$ exposed to air at RT (denoted as $\text{o-CeO}_{1.982}\text{-air}$).

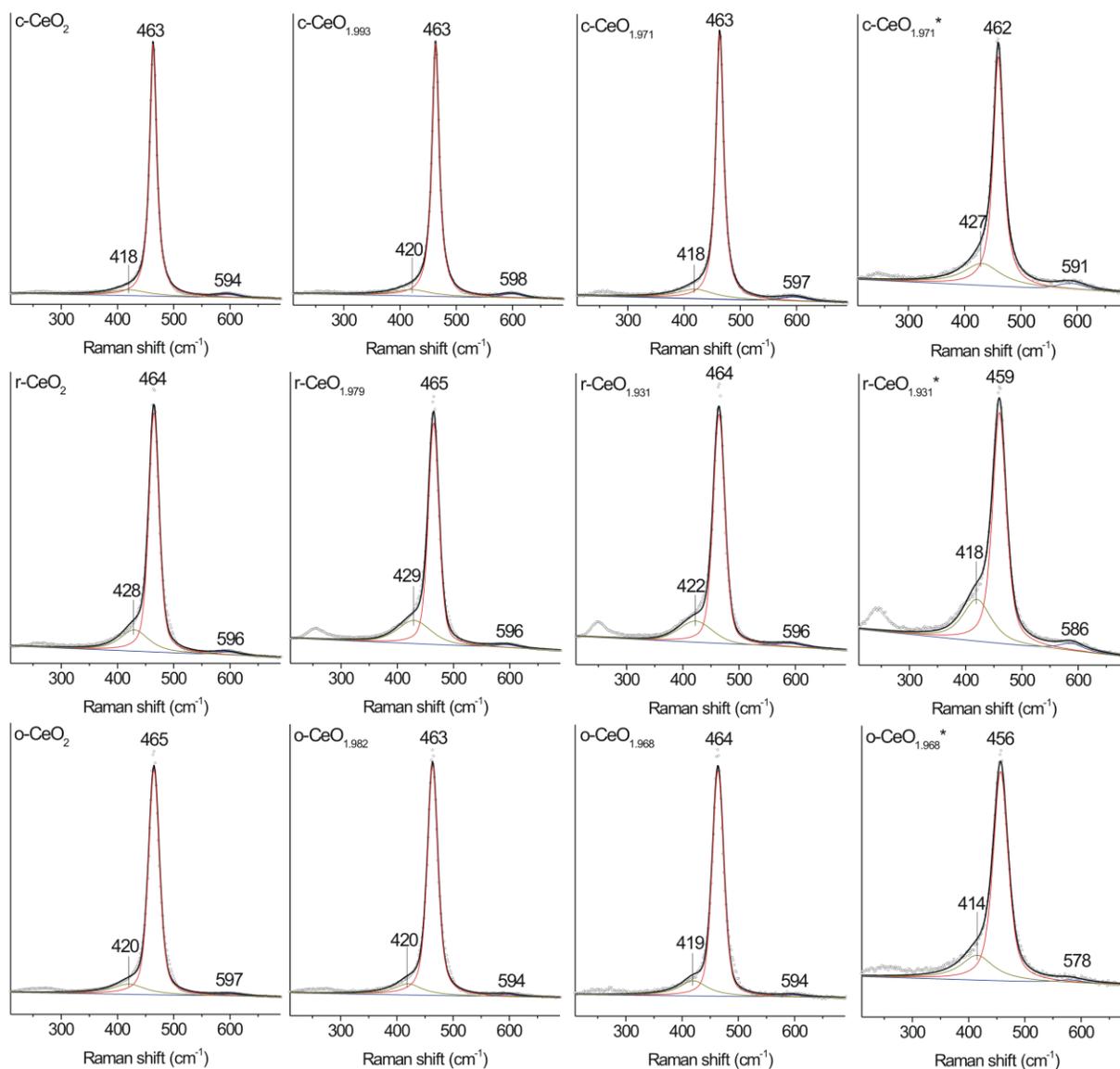


Figure S4. Peak-fitting results of in-situ Raman spectra of various CeO_x nanocrystals recorded at RT. The in-situ Raman spectra of selected CeO_x nanocrystals recorded at the reduction temperature are also presented and denoted as CeO_x^* . The scattered data and solid lines represent original and fitted spectra, respectively. The Raman spectra were fitted employing an XPSPeak software (Version 4.1) with a linear baseline and a Lorentz-Gaussian (50% Lorentz/Gaussian ratio) line-shape. The peak position and full width at half maximum were not fixed during the peak-fitting processes. The peak at 465 cm^{-1} were found to need two

components to acquire satisfying fitting results with the peak maxima at 465 and 420 cm^{-1} . The 465 cm^{-1} feature corresponds to F_{2g} mode, and the 420 cm^{-1} feature was previously observed but its assignment is not identified (Chem. Eur. J. 2011, 17, 4356-4361; Phys. Rev. B 2001, 64, 245407; J. Phys. Chem. C 2007, 111, 11026-11038; J. Catal. 2006, 240, 1-7; Phys. Rev. B 1994, 50, 13297-13307). In the present study the reported $I_D/I_{\text{F}_{2g}}$ was calculated employing the peak areas of the 596 cm^{-1} and 465 cm^{-1} components.