

## Electronic Supplementary Information

### Shape-selective synthesis of nanoceria for degradation of paraoxon as chemical warfare simulant

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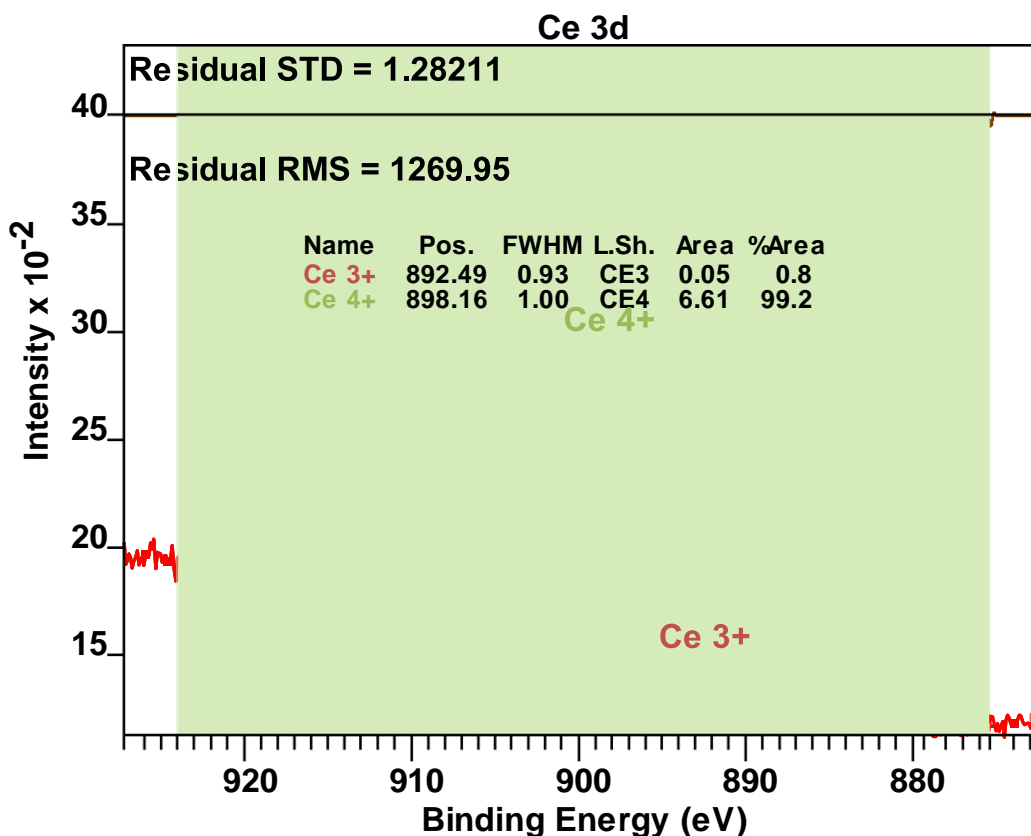
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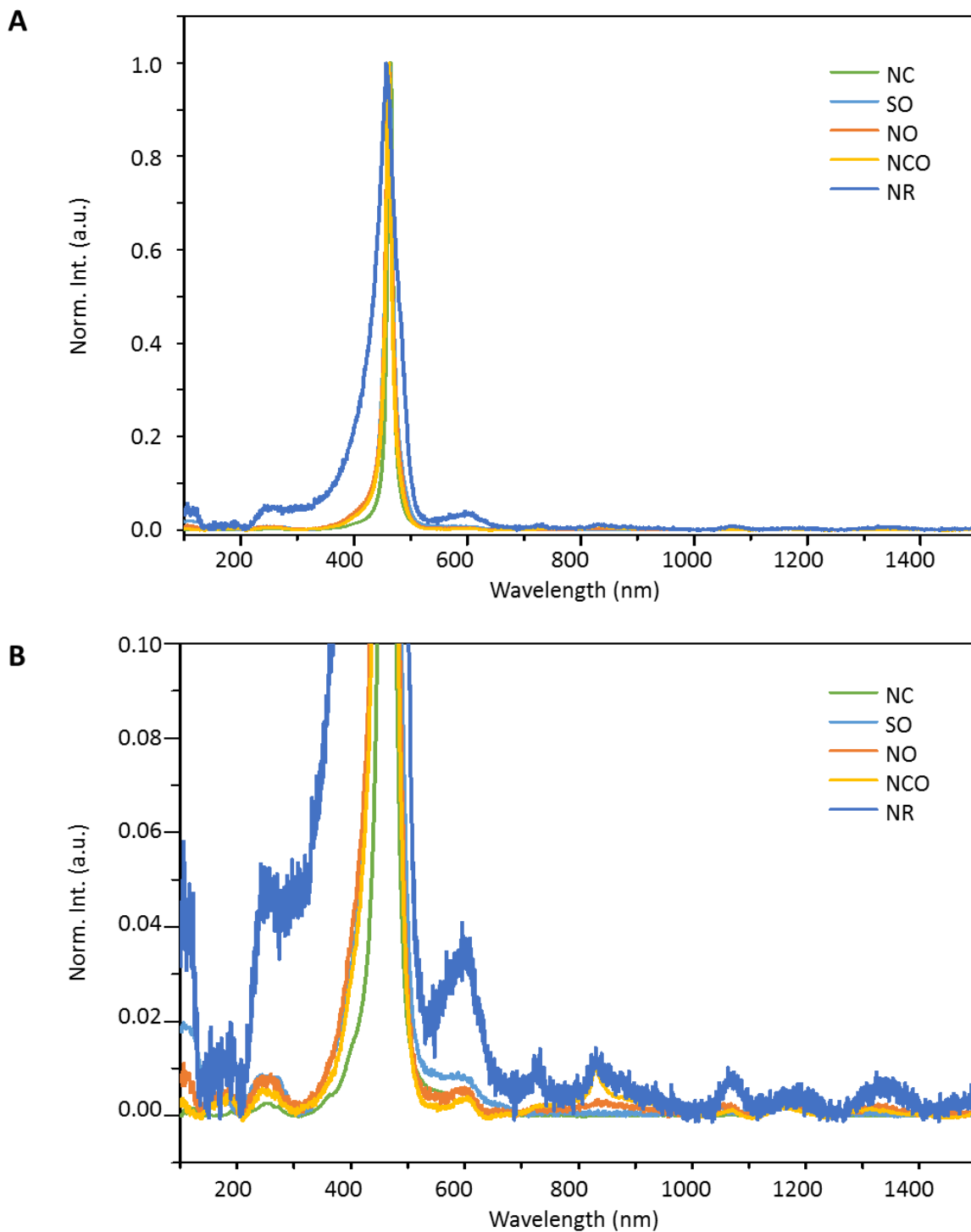
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† contributed equally to the experiment

#### A) Supplementary Figures

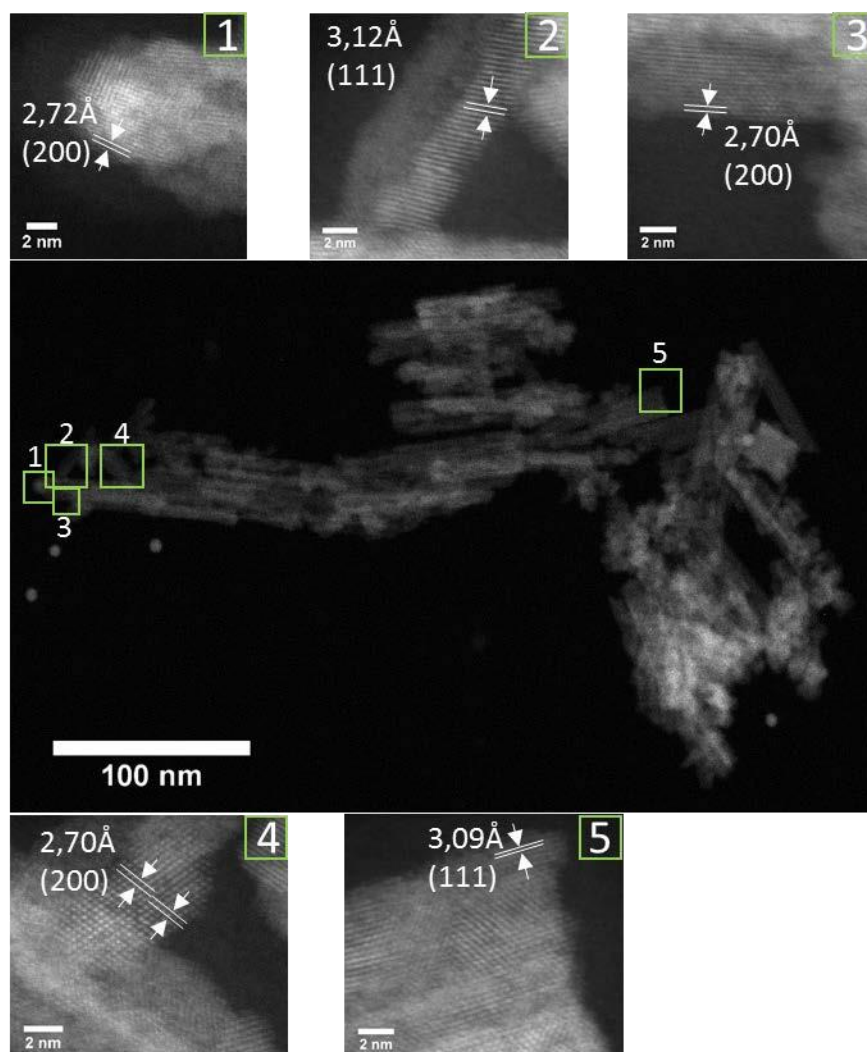


**Fig. S1** - Ce 3d<sub>3/2,5/2</sub> XPS spectrum collected for the CeO<sub>2</sub> nanorods NR. The Ce<sup>3+</sup>/Ce<sup>4+</sup> ratio was calculated by modelling the area of the experimental spectrum with a linear combination of the areas of two experimental spectra of 100% Ce<sup>3+</sup> and 100% Ce<sup>4+</sup>. The experimental spectrum of NR is plotted in bright red. The area of the modelling spectrum is represented in blue. XPS measurements were performed with an AXIS Ultra DLD instrument from Kratos Analytical using monochromatic Al K $\alpha$  X-rays. Ceria powders were imbedded in indium foil and on stainless steel sample holder. Sample charging was minimized using a charge compensator system.

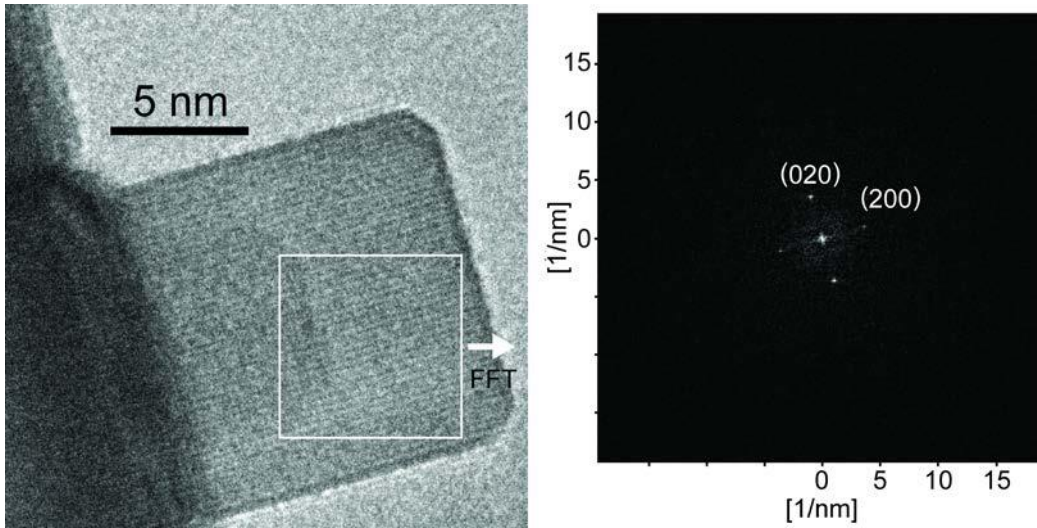


**Fig. S2** – A) Raman spectra of the CeO<sub>2</sub> nanoparticles in the 100-1500cm<sup>-1</sup> range and B) enlarging below the 0.1 intensity ( $\lambda_{\text{exc}} = 633$  nm). All spectra are normalized relative to the maximum intensity of the F<sub>2g</sub> mode of the CeO<sub>2</sub> fluorite phase. For all samples, the Raman spectrum is dominated by a strong peak  $\sim 460$  cm<sup>-1</sup> with weak bands at  $\sim 250$ ,  $\sim 600$  and  $\sim 1175$  cm<sup>-1</sup>. The peaks at  $\sim 250$  and  $\sim 1175$  cm<sup>-1</sup> are assigned to a second-order transverse optic (2TO) and a second-order longitudinal optical (2LO) modes respectively.<sup>1</sup> The peak at  $\sim 460$  cm<sup>-1</sup> (labelled F<sub>2g</sub>) is typical of the CeO<sub>2</sub> fluorite phase, and corresponds to a symmetric breathing

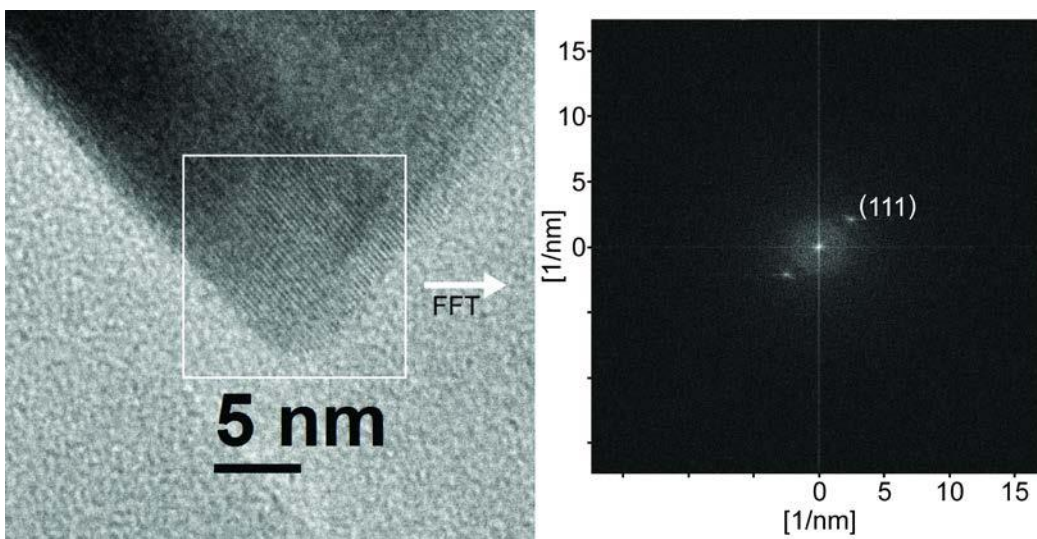
mode of the oxygen atoms around cerium ions. Other weak bands are visible at around 730, 830, 1060 and 1340  $\text{cm}^{-1}$ . They can be the manifestation of the carbonate species adsorbed at the surface of the  $\text{CeO}_2$  nanoparticles from the ambient air.<sup>2</sup>



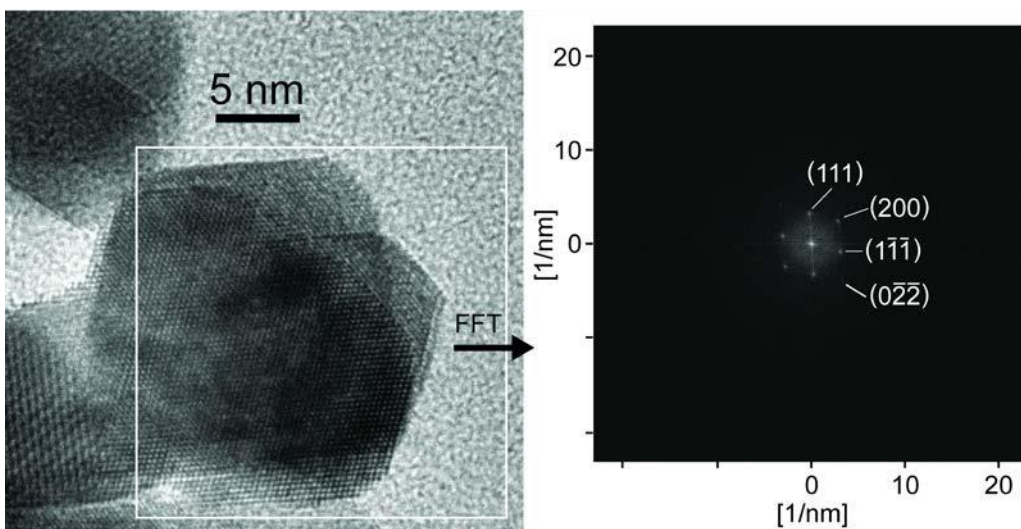
**Fig. S3** – STEM-HAADF projection at  $0^\circ$  extracted from the tilted series used for the volume reconstruction. The green rectangles show HR-STEM images made on different places on the sample.



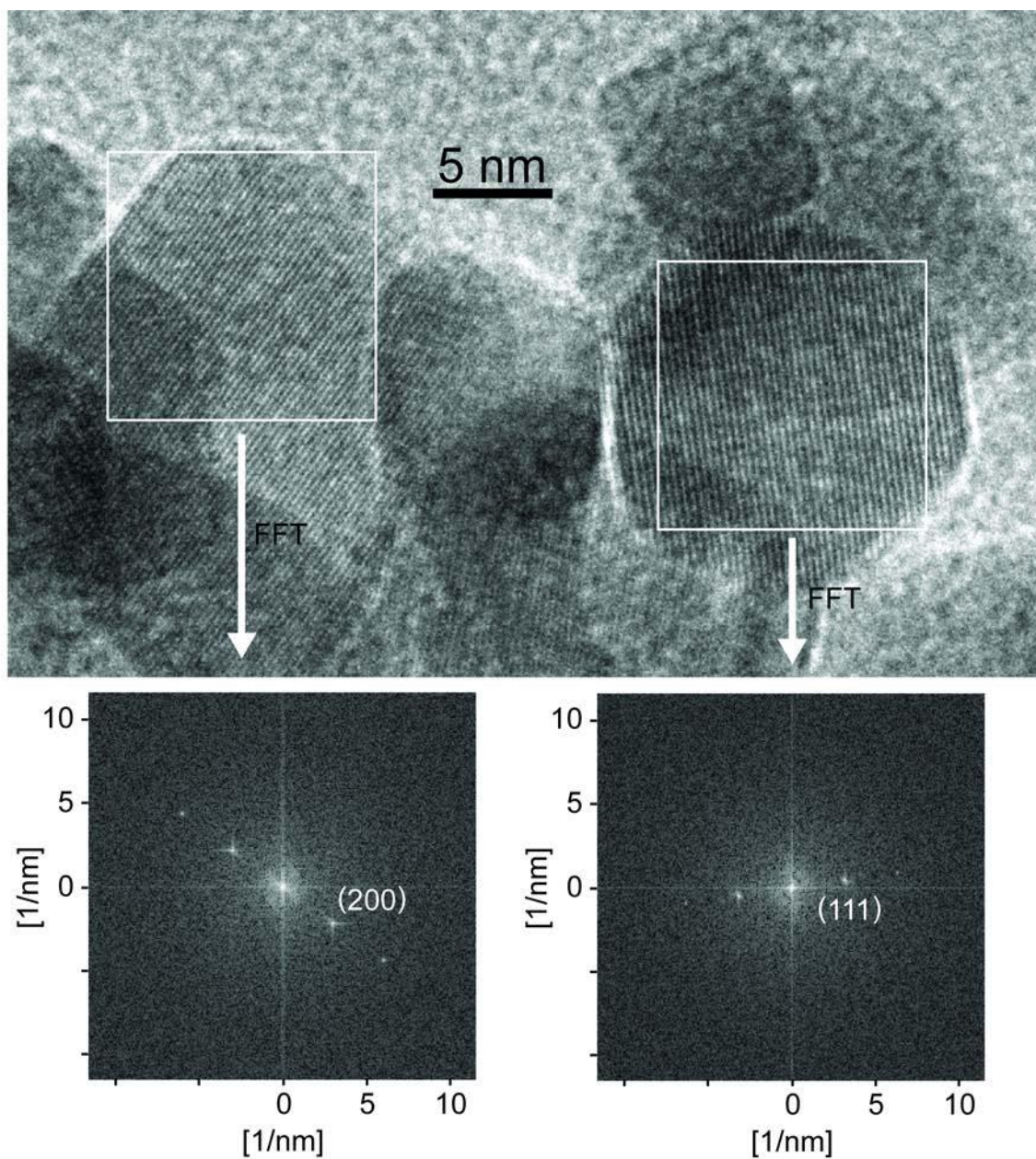
**Fig. S4** – Particle shown in Figure 2B and the fast Fourier transform of the framed area showing the families of lattice planes (200) and (020) (inter-reticular distance 0.271 nm).



**Fig. S5** – Particle shown in Figure 2D and the fast Fourier transform of the framed area showing the family of lattice planes (111) (inter-reticular distance 0.313 nm).



**Fig. S6** – Particles shown in Figure 2F and the fast Fourier transform of the framed area showing the families of lattice planes (111), (200), (1-1-1), and (0-2-2) (inter-reticular distance 0.313 nm, 0.271 nm, 0.313 nm, and 0.192 respectively).



**Fig. S7** – Particles shown in Figure 2H and the fast Fourier transforms of the framed areas showing the families of lattice planes (200) and (111) (inter-reticular distance 0.271 nm and 0.313 nm respectively).

B) Video CeO2\_volume.avi

Tomography performed on the nanorods shown in Fig. S3 and in Fig. 4.

## Notes and References

- 1 W. H. Weber, K. C. Hass and J. R. McBride, *Phys. Rev. B*, 1993, **48**, 178–185.
- 2 G. Busca and V. Lorenzelli, *Mater. Chem.*, 1982, **7**, 89–126.