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Electronic Supplementary Information

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

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A) Supplementary Figures

Fig. S1 - Ce 3d_{3/2,5/2} XPS spectrum collected for the CeO$_2$ nanorods NR. The Ce$^{3+}$/Ce$^{4+}$ 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$^{3+}$ and 100% Ce$^{4+}$. 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 Kα 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$_2$ nanoparticles in the 100-1500 cm$^{-1}$ range and B) enlarging below the 0.1 intensity ($\lambda_{ex} = 633$ nm). All spectra are normalized relative to the maximum intensity of the $F_{2g}$ mode of the CeO$_2$ fluorite phase. For all samples, the Raman spectrum is dominated by a strong peak ~460 cm$^{-1}$ with weak bands at ~250, ~600 and ~1175 cm$^{-1}$. The peaks at ~250 and ~1175 cm$^{-1}$ are assigned to a second-order transverse optic (2TO) and a second-order longitudinal optical (2LO) modes respectively. The peak at ~460 cm$^{-1}$ (labelled $F_{2g}$) is typical of the CeO$_2$ 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 cm\(^{-1}\). They can be the manifestation of the carbonate species adsorbed at the surface of the CeO\(_2\) nanoparticles from the ambient air.\(^2\)

**Fig. S3** – STEM-HAADF projection at 0° 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).

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

Notes and References