

Supporting Information for

Exclusively selective oxidation of toluene to benzaldehyde on ceria nanocubes by molecular oxygen

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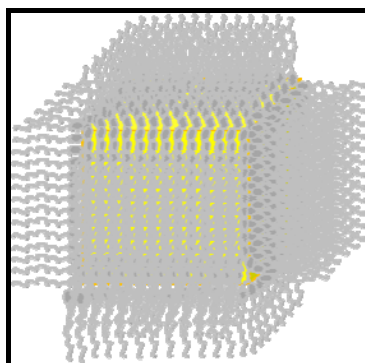


Fig. S1 Schematic representation of the oleic acid molecules adsorbed on a ceria nanocube.

According to the model of the oleic acid adsorbed on the {100} plane of ceria nanocubes (Fig. S1), the highest density of the oleic acid adsorbed on the ceria cubes is figured out as $13.7 \text{ molecules nm}^{-2}$, by the structural analysis. According to the TEM measurement, the average side length of the cubes is $\sim 8 \text{ nm}$ and the density of the CeO_2 is 7.13 g/cm^3 . By these data, the largest amount of densely adsorbed oleic acid of $\sim 41 \text{ wt. \%}$ can be calculated. The weight loss in TGA measurement surpasses the amount of densely adsorbed oleic acid, indicating that some oleic acid molecules are physically blended in the adsorbed layer of oleic acid on the surface. In experiment, the ceria nanocubes are washed using ethanol to remove the blended oleic acid and it is found the blended oleic acid molecules are not so easy to be removed by the washing. We think this is the reason that the weight loss is larger than the largest amount of dense adsorbed oleic acid. The IR spectra (Fig.S2) of the samples show the co-existence of the physically blended and the chemically adsorbed oleic acid with the samples.

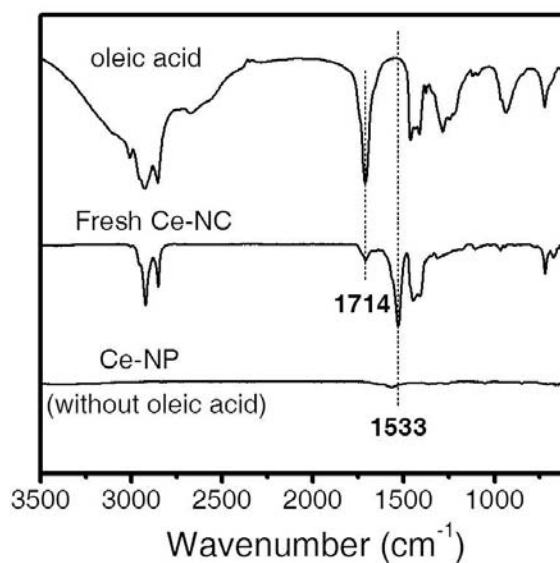


Fig.S2 IR spectra of the oleic acid, ceria nanocubes with adsorbed oleic acid and the ceria nanoparticles without oleic acid.

The Fig.S2 depicts the clear IR spectra of the oleic acid, ceria nanocubes with adsorbed oleic acid and the ceria nanoparticles without oleic acid. The IR spectra of adsorbed oleic acid and the free oleic acid molecules in solution are different. As shown in the Fig. S2, the stretching of carbonyl in the adsorbed oleic acid is observed at 1533 cm⁻¹. Compared with the peak (1714 cm⁻¹) of the carbonyl in free oleic acid, the adsorption of the carboxyl of oleic acid on ceria causes a significant red shift of the stretching of the carbonyl. It is reasonable that the adsorption weakens the stretching of the carbonyl groups. Simultaneously, a peak at 1714 cm⁻¹ is also observed in the IR of the ceria nanocubes with adsorbed oleic acid. The peak refers to the oleic acid molecules physically blended in the sample.