Structure-activity relationship of nanostructured ceria for the catalytic generation of hydroxyl radicals

Tamra J. Fisher,^a Yunyun Zhou,^{a, †} Tai-Sing Wu,^b Meiyu Wang,^c Yun-Liang Soo,^{b, d} and Chin Li Cheung^{*, a}

a. Department of Chemistry, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, United States

b. Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, R.O.C.

c. Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, Lincoln, Nebraska 68588, United States

d. National Synchrotron Radiation Research Centre, Hsinchu 30076, Taiwan, R.O.C.

† Present Address: National Energy Technology Laboratory, Pittsburgh, PA, 15236, United States



ELECTRONIC SUPPLEMENTARY INFORMATION

Figure S1. TEM image of commercial ceria particles.

[†] Present Address: National Energy Technology Laboratory, Pittsburgh, PA, 15236, United States.

^{*} Corresponding Author. Dr. Chin Li Cheung; Email: ccheung2@unl.edu



Figure S2. Ce 3d XPS spectra of ceria nanorods (NR), ceria nanocubes (NC), ceria nanocutahedra (NO), and commercial ceria. The spectra were normalized at 882.15 eV. The locations of the Ce^{3+} 3d peaks are indicated by the dashed lines. Note: the similarities between the spectra suggests that these ceria samples have similar % of surface Ce^{3+} .



Figure S3. Reaction kinetics of catalytic generation of hydroxyl radicals with and without *t*-butanol as the hydroxyl radical scavenger. Reaction conditions: Reaction temperature: 21.8 °C; $[H_2O_2] = 3 \text{ mM}$; [Ceria NR] = 0.1 g/L; [*t*-butanol] = 2 M.



Figure S4. Determination of optimum $[H_2O_2]$ from reaction kinetics for the catalytic generation of hydroxyl radicals from disproportionation of hydrogen peroxide using ceria nanorods. Reaction conditions: 21.8 °C, $[H_2O_2] = 0.1 - 6$ mM, [Ceria NR] = 0.1 g/L. The solid line was drawn to guide the eye on the trend line of the apparent reaction rate at higher $[H_2O_2]$.



Figure S5. Reaction kinetics for the catalytic generation of hydroxyl radicals from disproportionation of hydrogen peroxide using ceria nanorods. (inset) Log-Log plot of the kinetics data for determining the reaction order with respect to the concentration of ceria nanorod catalysts. Reaction conditions: Reaction temperature: 21.8 °C; $[H_2O_2] = 3 \text{ mM}$; [Ceria NR] = 0.1, 0.5, and 1.0 g/L.