Supporting information

Insight into Several Factors that Affect the Conversion between Antioxidant and Oxidant Activities of Nanoceria

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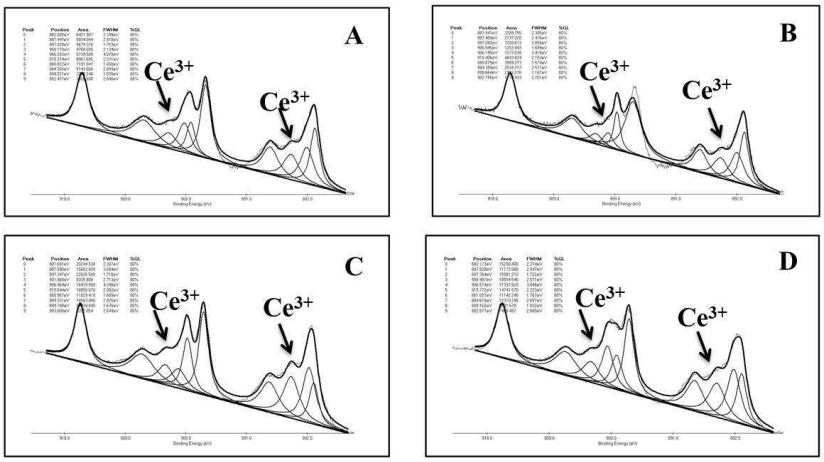

Figure S1 Ce $3d_{3/2,\ 5/2}$ XPS spectra of 20–25 nm nanocubes (A), 30–40 nm nanocubes (B), 5–10 nm nanoparticles (C), 15–20 nm nanoparticles (D).

The contents of Ce^{3+} on the surface of nanoceria: the Ce 3d spectra are composed of two multiplets (v and u) corresponding to the spin-orbit splitting of $3d_{5/2}$ and $3d_{3/2}$ core holes.[1] Each spin-orbit component of Ce^{3+} is dominated by four components: peaks u' and v' are respectively located at 903.1±0.1eV and 884.5±0.1eV; peaks u_0 and v_0 are respectively located at 899.9±0.1eV and 881.8±0.1eV. For Ce^{4+} states, each spin-orbit component is dominated by other six components (v + v'' + v''' + u + u'' + u'''). [2] The peak area can be obtained by the PeakFit 4.0 software, and the ratio of Ce^{3+}/Ce^{4+} can be calculated from the following equations: [3-5]

$$A_{Ce}^{3+} = A_{v0} + A_{v'} + A_{u0} + A_{u'}$$

$$A_{Ce}^{4+} = A_{v} + A_{v''} + A_{v'''} + A_{u} + A_{u''} + A_{u'''}$$

$$C_{Ce^{3+}} = \frac{A_{Ce^{3+}}}{A_{Ce^{4+}} + A_{Ce^{3+}}}$$

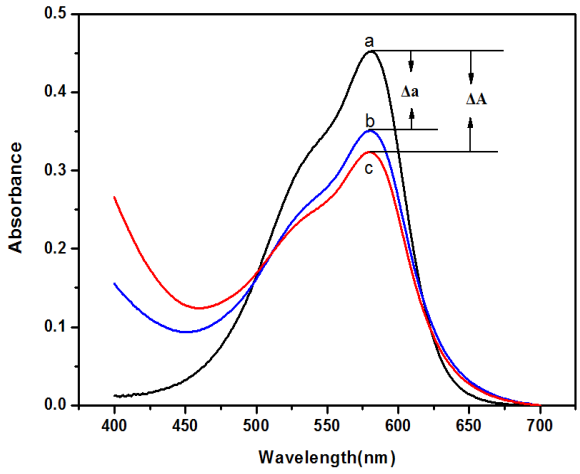

Figure S2 UV-Vis absorption spectra of MV: 10μM 15-20 nm particles add into a certain Fenton reagent (0.1 M H_2O_2, 0.45 mM $FeSO_4$)

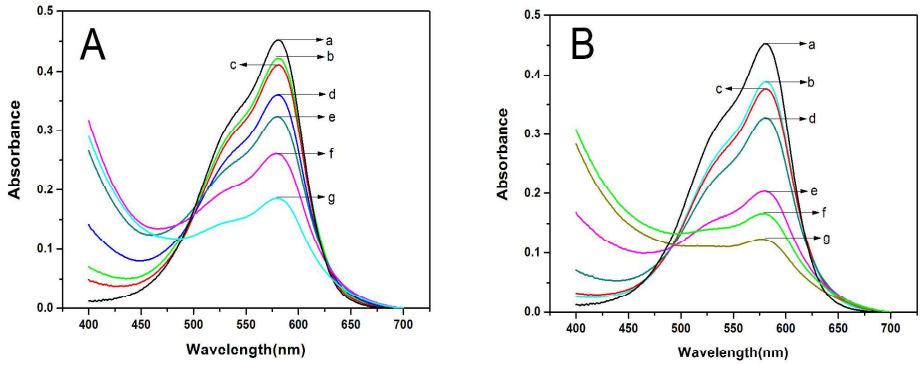

Figure S3 UV-Vis absorption spectra of MV in different Fenton systems: 0.1M H_2O_2 (A) with different concentration of $FeSO_4$ (b-g: 0.075, 0.15, 0.30, 0.45, 0.60 and 0.75 mM $FeSO_4$). 1.0M H_2O_2 (B) with different concentration of $FeSO_4$ (b-g: 0.075, 0.15, 0.30, 0.45, 0.5 and 0.60 mM $FeSO_4$). Curve a in the figures (A, B) is 1.2×10^{-5} M MV's UV-Vis absorption spectra.

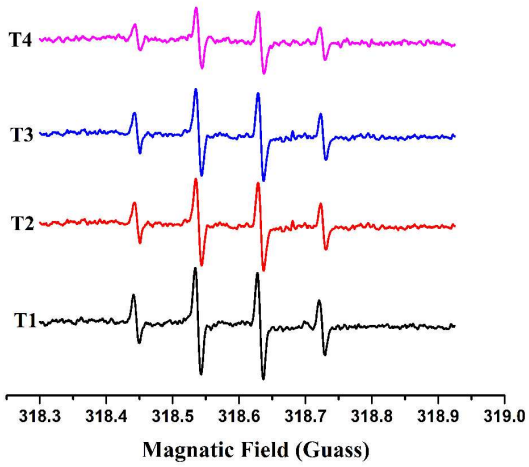

Figure S4 ESR images of four hydroxyl radical systems: 0.1M H_2O_2+0.45mM $FeSO_4$ (T1), 0.1M H_2O_2+0.30mM $FeSO_4$ (T2), 1.0M H_2O_2+0.15mM $FeSO_4$ (T3), 1.0M H_2O_2+0.09mM $FeSO_4$ (T4).

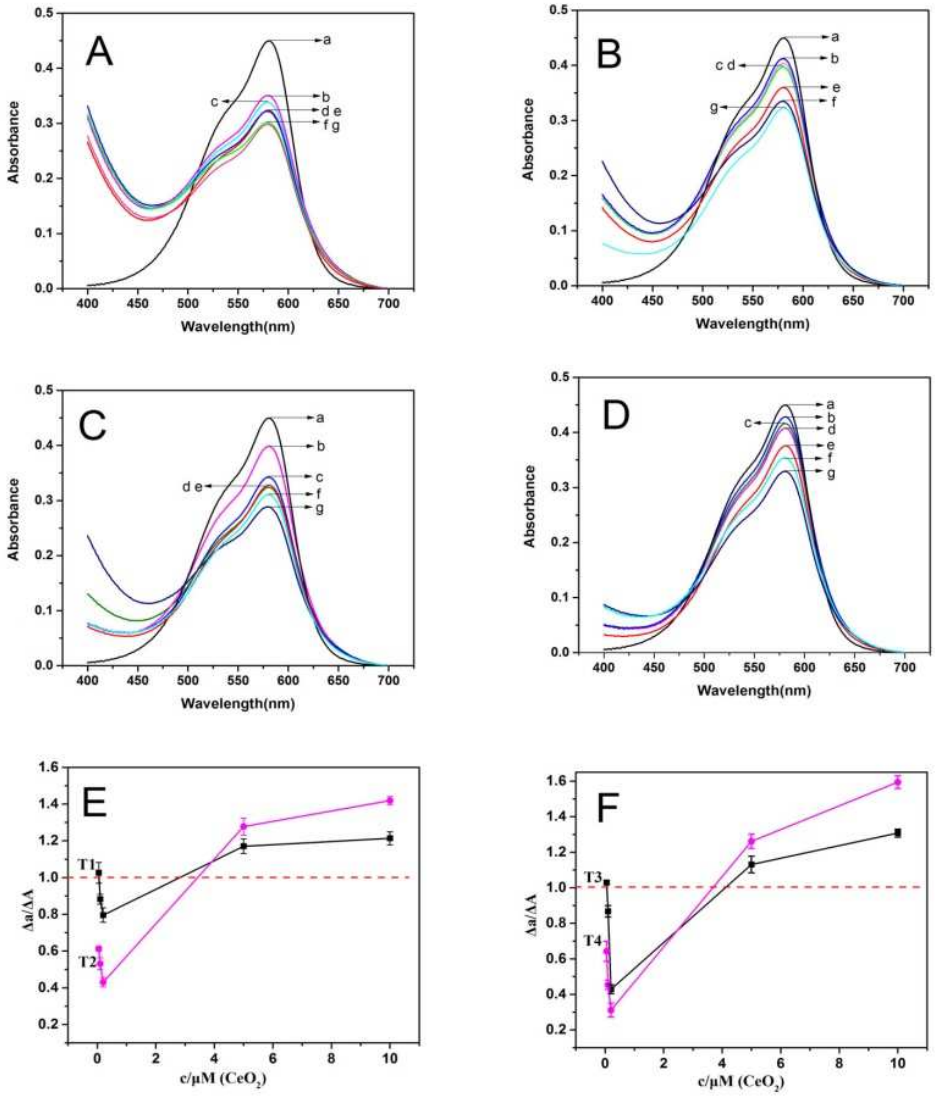

Figure S5 UV-Vis absorption spectra of MV in different Fenton reagent systems: T1 (A) or T2 (B) system with different concentration of 5-10nm nanoparticles (b: 0.20, c: 0.10, d: 0.05, e: 0, f: 5 and g: 10μM). T3 (C) or T4 (D) system with different concentration of CeO_2 (b: 0.20, c: 0.10, d: 0.05, e: 0, f: 5 and g: 10μM). The variation tendency of Δa/ΔA with the increasing concentration of 5-10nm nanoparticles in different Fenton reagents: T1 and T2 systems (E), T3 and T4 systems (F). Curve a in the figures (A-D) is 1.2×10^{-5} M MV's UV-Vis absorption spectra. The relative standard deviations (percentage of RSD) are all less than 5.64% in E and F.

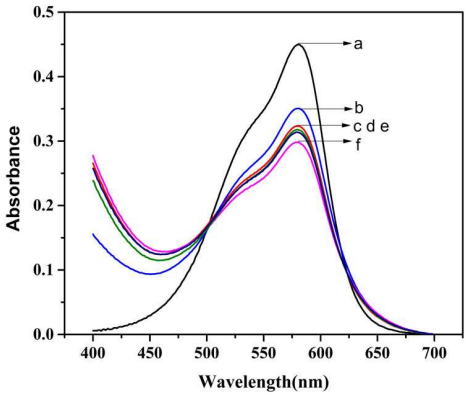

Figure S6 UV-Vis absorption spectra of MV and four kinds of nanoceria in 10 μM (a: 1.2×10^{-5} M MV, b: 15 - 20 nm nanoparticles, c: Fenton of T1system, d: 20 - 25 nm nanocubes, e: 30 - 40 nm nanocubes, f: 5 - 10 nm nanoparticles)

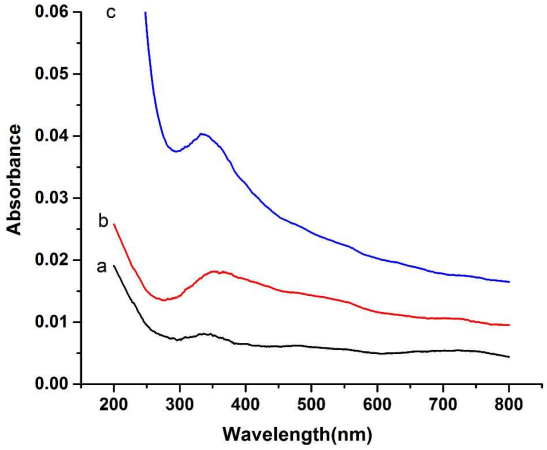

Figure S7 UV-Vis absorption spectra of 15 - 20 nm CeO_2 nanoparticles (a); CeO_2 interacted with 0.75 mM $FeSO_4$ (b); CeO_2 interacted with 0.1 M H_2O_2 (c).

Reference

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[2] Anandan, C.; Bera, P. XPS Studies on the Interaction of CeO_2 with Silicon in Magnetron Sputtered CeO_2 Thin Films on Si and Si_3N_4 Substrates. *Appl. Surf. Sci.*

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