Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information

The enzymatic performance derived from the lattice planes of Ir nanoparticles

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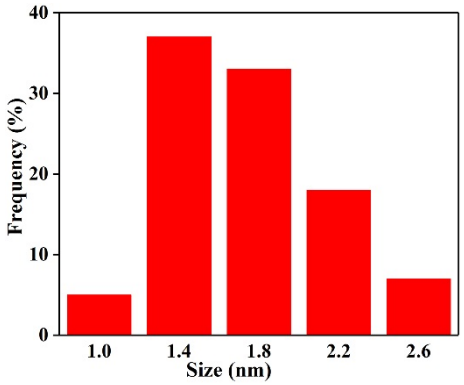

Fig.S1 Particle size distributions of CD-IrNPs

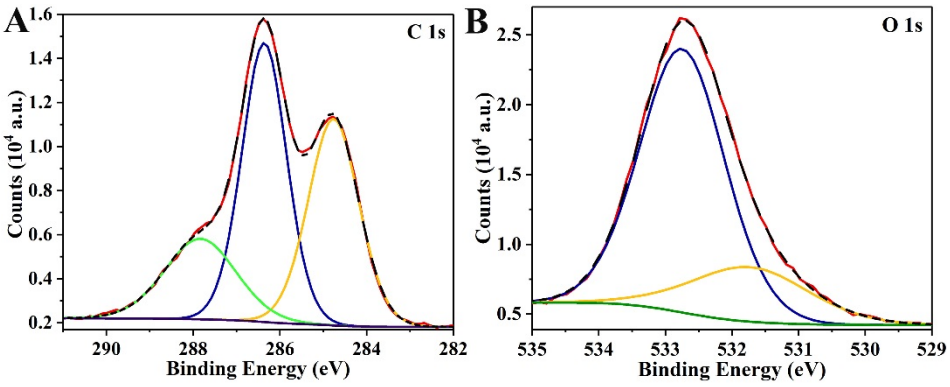

Fig.S2 High-resolution XPS survey scan of C1s (A) and O1s (B) of CD-IrNPs.

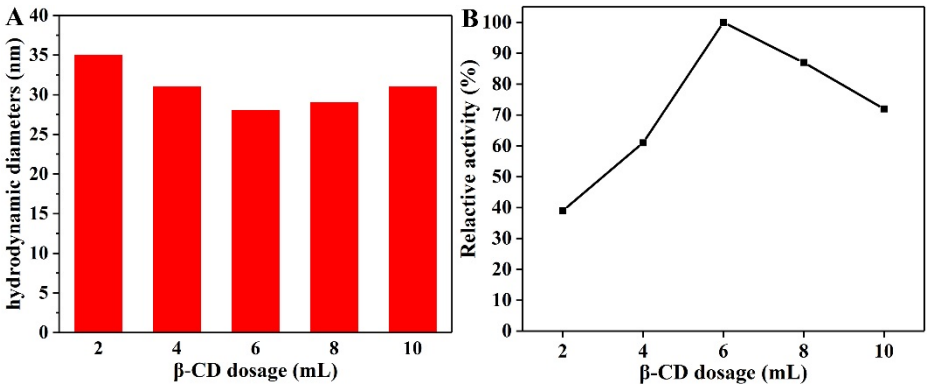

Fig.S3 (A) The average hydrodynamic diameters of the CD-IrNPs prepared from different amount of β-CD. (B) Dependency of the IrNPs oxidase-like activity on the β-CD dosage.

The average hydrodynamic diameters are 35, 31, 28, 29 and 31 nm respectively when the amount of β-CD was varied from 2 mL to 10 mL in the IrNPs preparation process. When the molar ratio of Ir3+ to β-CD was 1:5.1, the catalytic activity of IrNPs was the highest among all the tested ratios. Therefore, the amount of 6 mL 34 mM β-CD was chosen in the synthesis of CD-IrNPs.

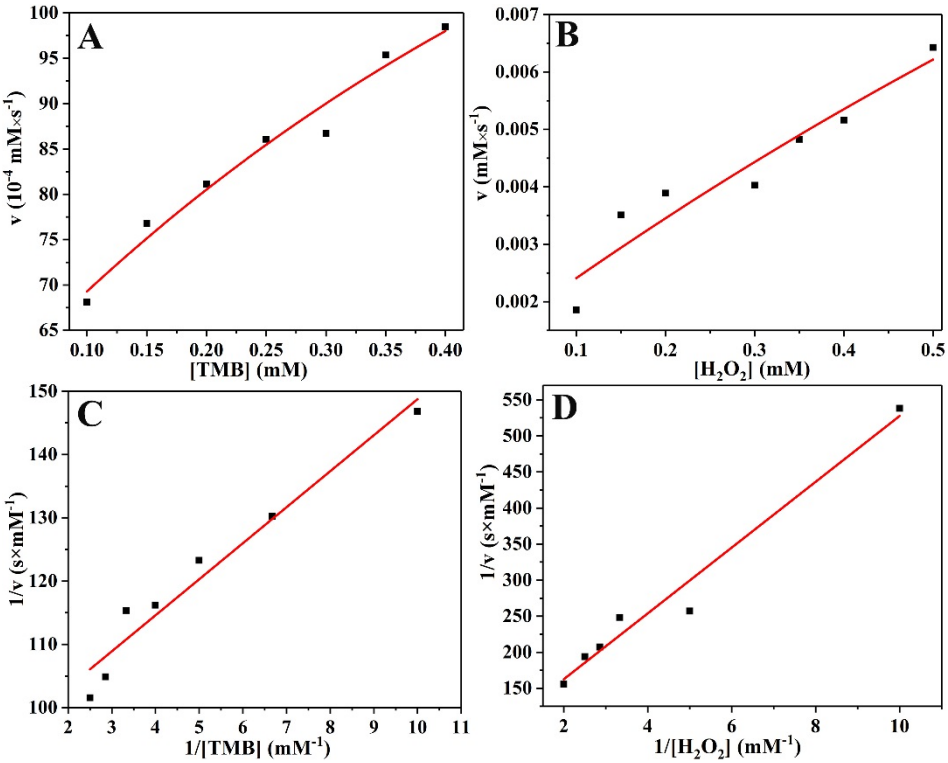

Fig.S4 Steady state kinetic assay of peroxidase-like activity of CD-IrNPs in Hac-HAc buffer (0.01 M, pH 3.86) at room temperature. (A) The H_2O_2 concentration was 0.5 mM and TMB was varied. (B) TMB concentration was fixed at 0.5 mM and H_2O_2 was varied. (C, D) were double-reciprocal plots of activity of CD-IrNPs, corresponding to (A) and (B).

The K_m and ν_{max} values of CD-IrNPs when choosing TMB as substance were calculate to be 0.0619 mM and 0.011 mM/s, respectively. And the values were 0.64 mM and 0.014 mM/s when choosing H_2O_2 as substrate.

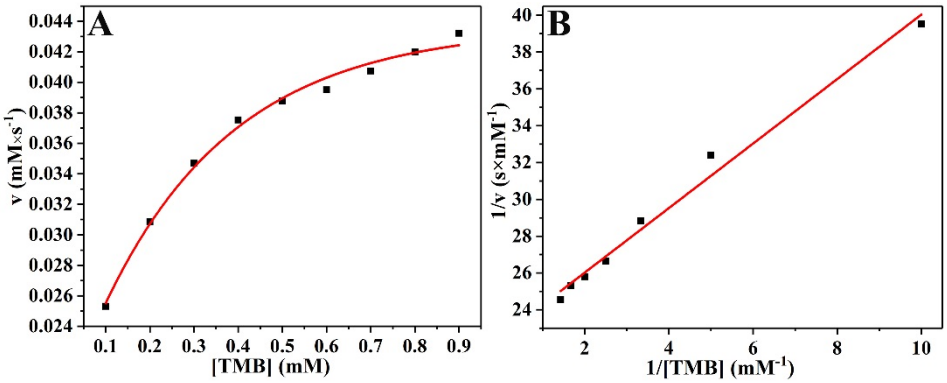

Fig.S5 (A) Steady state kinetic assay of oxidase-like activity of CD-IrNPs in HAc-NaAc buffer (0.01 M, pH 3.86) versus varying concentration of TMB at room temperature. (B) Double-reciprocal plots of oxidase-like activity of CD-IrNPs. Accordingly, the K_m and v_{max} of CD-IrNPs were calculated to be 0.082 mM and 0.045 mM/s, respectively.

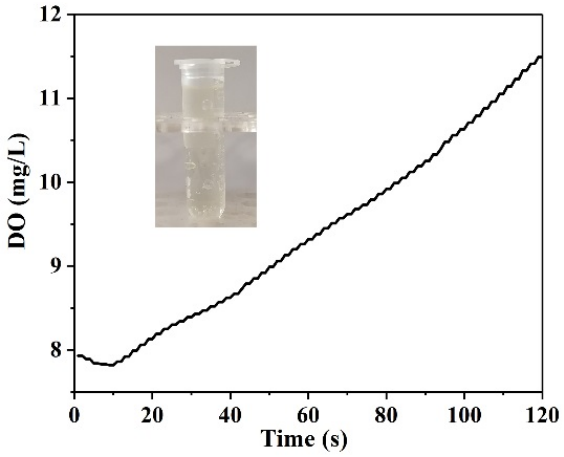

Fig.S6 Dissolved oxygen generation catalyzed by TA-IrNPs. Reaction conditions: 30 μL, 3 mg/mL TA-IrNPs were incubated in 5 mM H_2O_2 solution for minutes at room temperature.

Table S1. The enzyme mimic properties of different IrNPs

	crystal plane				catalytic activity		
	(111)	(200)	(220)	(311)	oxidase-like activity	peroxidase-like activity	catalase-like activity
TA-IrNPs	✓					✓	✓
PVP-IrNPs	✓					✓	✓
Cit-IrNPs	✓	✓	✓	✓	✓	✓	✓
CD-IrNPs	✓		✓		✓	✓	✓

Table S2. Calculated energy of adsorption for oxygen at different crystal faces and distance d between adsorb ate and surface.

site	ΔE_{ad} (eV)	d (Å)
(111)	-2.33	1.98
(200)	-2.88	1.96
(220)	-3.41	1.96
(311)	-3.38	1.94

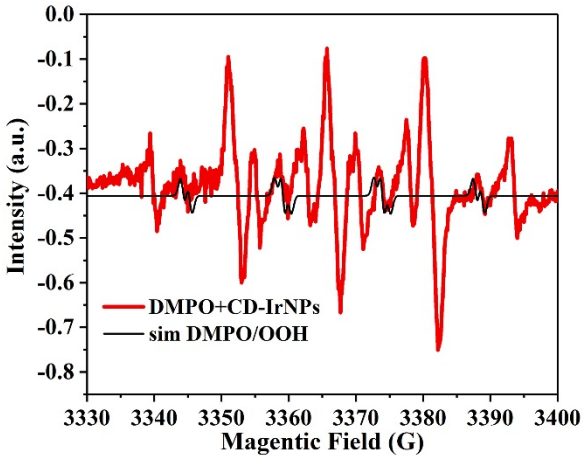

Fig.S7 ESR spectrum of CD-IrNPs/DMPO sample (red line) and the simulated DMPO/·OOH spectrum (black line).

In the ESR tests, an amount of 100 μL CD-IrNPs aqueous suspension (3 mg/mL) and 20 μL of DMPO was mixed with 0.5 mL of H_2O. The mixed solution was monitored by ESR spectrometer immediately.

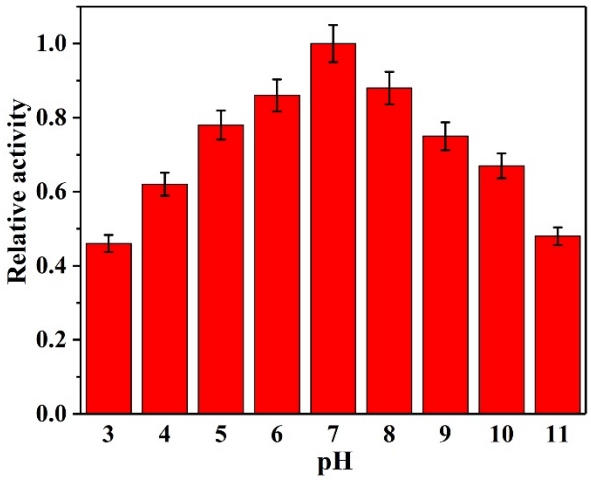

Fig.S8 Effect of pH on the catalase-like activity of CD-IrNPs.

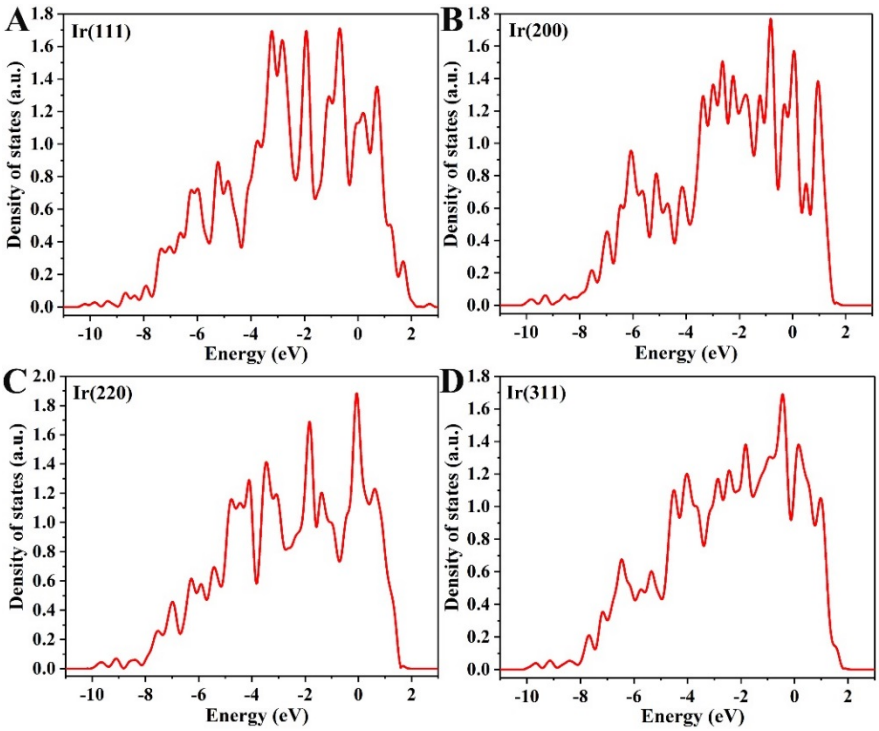

Fig.S9 DOS projections onto states for Ir atoms on Ir(111) plane (A), Ir(200) plane (B), Ir(220) plane (C) and Ir(311) plane (D).

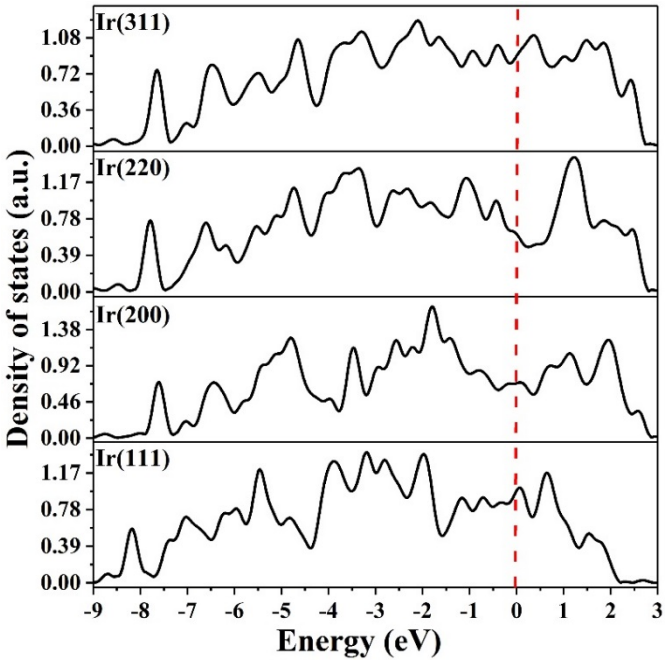

Fig.S10 DOS projections onto states for Ir atom on different Ir lattice planes after interact with ·OOH.