Supporting Information

Electrocatalytic water oxidation enabling the highly selective oxidation of styrene to benzaldehyde

Chenxing Li [a, b], Qingqing Cheng [b*], Chengyu Wu [a, b], Qiansen Wang [a, b], Weibo Hu [b], Liangliang Zou [b], Ke Wen [a, b], Hui Yang [a,b*]

[a] School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China;

[b] Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai 201210, China

[*]Corresponding authors, E-mail: chengqq@sari.ac.cn; yangh@sari.ac.cn

Experimental details

Synthesis of Pt black

Clean Pt sheet was used as working electrode. Another Pt electrode and saturated calomel electrode were used as counter electrode and reference electrode. Pt black electrode was prepared by an electrochemical deposition method. H_2PtCl_6 ($3.3x10^{-2}$ mol/L, 30 mL), HCl (0.5 mol/L) and Pb $(Ac)_2$ ($3.3x10^{-5}$ mol/L) were added into a single electrolytic cell with a current density of 60 $mAcm^{-2}$.

Electrochemical experiments

Electrochemical experiments were conducted using a separated compartment cell. MeCN with 0.1 M nBu_4PF_6 was used as the electrolyte with varying concentrations of ST and water. Platinum and graphite plates were used as the working and counter electrodes, respectively. An Ag/AgCl (Innovative Instruments) used as the reference electrode. All electrochemical measurements were performed at a temperature of ca. 25 ^oC using a CHI 760E workstation.

Post treatment experiments

After the reaction period, extract 5 mL of reaction solution with 2.5 mL of water and excess NaCl, and take supernatant and dry it with anhydrous Na_2SO_4. The collected samples were analyzed on a GC (ThermoFish Trace1300) with FID and a GC/MS (ThermoFish Trace1300 ISQ). The GC and GC/MS signals were calibrated against those of standard samples. EPR spectra were recorded on a Bruker A300 spectrometer. ^1H NMR spectra were recorded on a 500 MHz Bruker Advance III HD spectrometer.

Computational formulas

$$Conversation\ (\%) = \frac{initial\ substrate\ (mM) - final\ substrate\ (mM)}{initial\ substrate\ (mM)}$$

$$Yield_{BzH}\ (mM/h) = \frac{BzH\ (mM)}{time\ (h)}$$

$$Selectivity_{BzH}\ (\%) = \frac{BzH\ (mM)}{total\ products\ observed\ (mM)}$$

$$Faradaic\ efficiency_{BzH}\ (\%) = \frac{BzH\ (mM)}{theoretical\ yield_{BzH}\ (mM)}$$