Reduction on Specific Lattice Planes for Metal-organic Frameworks/Poly-pyrrole Composites with Dilated Porosity

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1. Experimental section

1.1 Materials

All chemicals in this work were analytical grade and used without further purification. copper nitrate $[Cu(NO_3)_2]$, benzenetricarboxylic acid (H₃BTC), pyrrole (Py), styrene, and tertbutyl hydroperoxide (TBHP) were purchased from Energy Chemical (Shanghai). Dichloromethane (CH₂Cl₂), acetonitrile (CH₃CN), N, N-Dimethylformamide (DMF), EtOH, and MeOH were purchased from Sinopharm Chemical Reagent Co. Ltd. Water used in this work was deionized water.

1.2 Characterization

The morphology of as-synthesized samples was examined by a field-emission scanning electron microscope (FE-SEM, Hitachi SU8010) and corresponding elemental mapping images were obtained by energy-dispersive X-ray (EDX, Oxford Instruments). Transmission electron microscopes (TEM, FEI TALOS F200X) were applied to get more structural information of as-synthesized samples. The crystalline structure information of as-synthesized samples was determined by Powder X-ray diffraction (XRD, Shimadzu XRD-6000) with Cu K α radiation source (k =1.54056 Å) at room temperature. The elemental analyses were collected by X-ray photoelectron spectroscopy (XPS, Thermo Scientific ESCALAB 250). The organic groups of the as-synthesized samples were characterized by Fourier transform infrared spectroscopy (FT-IR, Bruker VERTEX 70). TGA profiles were obtained by thermogravimetric analyzer (TGA5500) from 30 to 600 °C with a heating rate of 10 °C min⁻¹ in air flow. The content of N elements of sample is analyzed by organic element analyzer (EA, Elementar Unicube).



Fig. S1 Molecular size of pyrrole.



Fig. S2 Optical microscope images of Cu-BTC (a, c) and Cu-BTC/PPy (b, d).



Fig. S3 The UV-vis spectrum of pure H₃BTC and washing solution of Cu-BTC/PPy.



Fig. S4 Optical images of collapsed Cu-BTC/PPy.



Fig. S5 The XRD pattern of Cu-BTC, Cu-BTC/PPy (80 °C), and Cu-BTC/PPy (90 °C).

Cu-BTC/PPy (60°C)

Cu-BTC/PPy (80°C)



Fig. S6 The optical microscope images of Cu-BTC/PPy (60°C) and Cu-BTC/PPy (80°C).



Fig. S7 Molecular size of styrene.



Fig. S8 The selectivity of three catalysts on styrene oxidation in oil bath.



Fig. S9 The XPS spectra for Cu 2p (a) and N 1s (b) of Cu-BTC/PPy(Fe³⁺).



Fig. S10 The conversion and yield of PPy, Cu-BTC, Cu-BTC/PPy, and Cu-BTC/PPy(Fe³⁺) on styrene oxidation in oil bath.



Fig. S11 SEM images of Cu-BTC/PPy after 4 cycles in oil bath.



Fig. S12 XRD pattern of Cu-BTC/PPy after 4 cycles in oil bath.



Fig. S13 SEM images of Cu-BTC/PPy after 4 cycles under Xe lamp.



Fig. S14 XRD pattern of Cu-BTC/PPy after 4 cycles under Xe lamp.