Electronic Supplementary Information (ESI) for

## **Redox-active Cu(I) Boron Imidazolate Framework for Mechanochromic and Catalysis**

Tian Wen<sup>a</sup>, De-Xiang Zhang<sup>a</sup>, Hai-Xia Zhang<sup>a</sup>, Hua-Bin Zhang<sup>a</sup>, Jian Zhang<sup>a</sup>, \* and Dong-Sheng

Li<sup>b,</sup>\*

<sup>a</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of

Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China. E-mail:

zhj@fjirsm.ac.cn

<sup>b</sup>College of Materials & Chemical Engineering, China Three Gorges University, Yichang 443002, P. R. China. E-mail: lidongsheng1@126.com

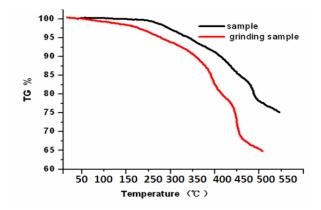


Fig. S1 Thermogravimetric analyses of BIF-34 and its ground sample.

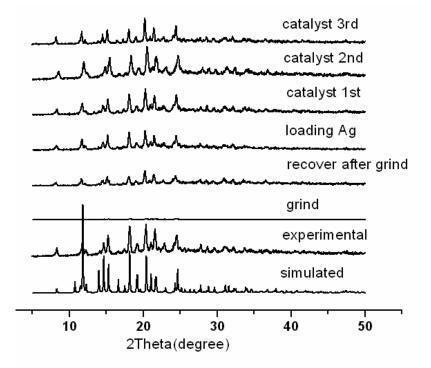


Fig. S2 The PXRD patterns of BIF-34 under different conditions.

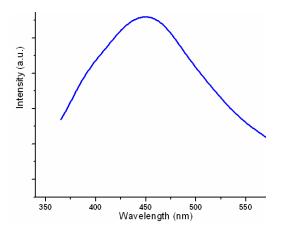


Fig. S3 The solid-state emission spectra ( $\lambda ex = 355 \text{ nm}$ ) for the ligand sample of KBH (dm-bim)<sub>3</sub>.

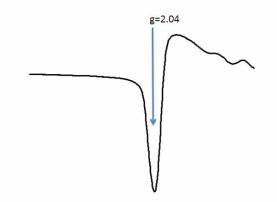


Fig. S4 EPR spectrum of Ag@BIF-34.

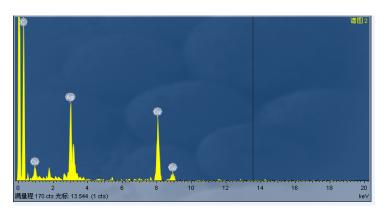


Fig. S5 EDS of Ag@BIF-34.

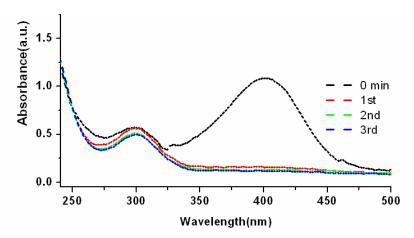
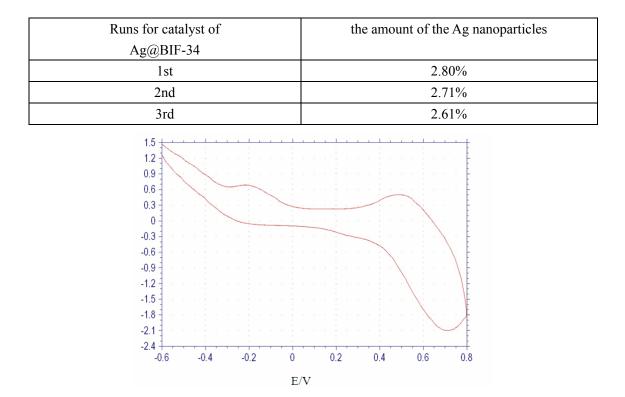
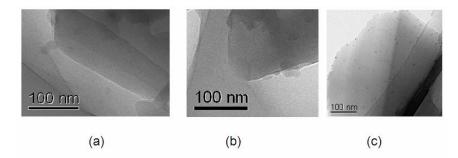


Fig. S6 Recycling test on reduction of 4-NP over Ag@BIF-34.

**Table S1**. The test the amount of the Ag nanoparticles after each cycle of the catalytic reaction for the reduction of 4-nitrophenol by ICP-AES.



**Fig. S7** Cyclic voltammograms of **BIF-34** films on FTO substrates measured in DMF solution at a scan rate of 50 mVs<sup>-1</sup>.



**Fig. S8** (FE)TEM images immersed in a aqueous solution of  $AgNO_3(a: BIF-1-Cu, b: kB(im)_{4,} c: KBH(dm-bim)_3)$ . In order to investigate the active B–H bonds from tridentate coordinated BH(dm-bim)\_3<sup>-</sup> ligands, we did some control experiments. We chose the tetradentate coordinated **BIF-1-Cu** and tetradentate B(im)\_4<sup>-</sup> ligand<sup>1</sup>. Ag(0) nanoparticles can not be obtained under the same conditions as **Ag@ BIF-34**. However, the potentially active B–H bonds from tridentate coordinated BH(**dm-bim**)\_3<sup>-</sup> ligand could sever as the reducing agent and contribute to the direct formation of Ag nanoparticles.

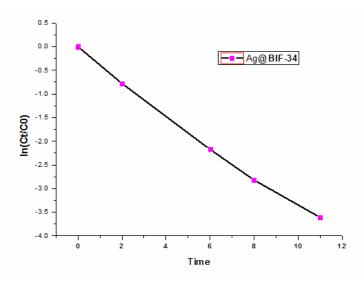


Fig. S9 The kinetics study of the catalytic reaction on reduction of 4-NP over Ag@BIF-34.

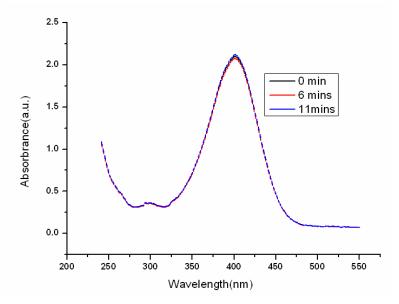


Fig. S10 View of UV-vis spectra BIF-34 immersed 4-NP (showing no gradual reduction).