Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Targeted Design of a Cubic Boron Imidazolate Cage with Sensing and Reducing Functions

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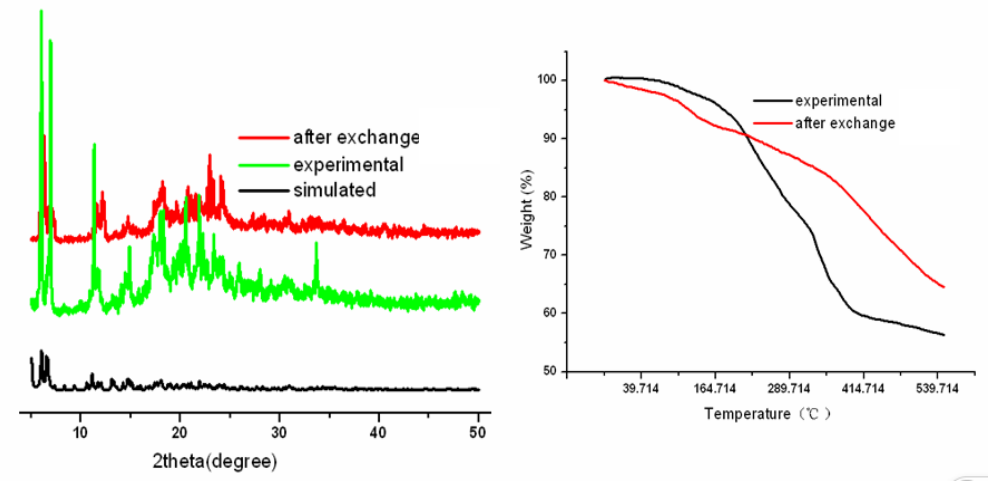

Figure S1. The PXRD and TGA curve of **BIF-28**.

Procedure for anion exchange

As-synthesized **BIF-28** (0.1 mmol) was immersed in an aqueous solution (4.5 mL) of $K_2Cr_2O_7$ (0.00068 mol·L^{-1}) at room temperature for 9h. The anion exchange process was monitored by liquid UV-vis spectroscopy based on typical absorption of $Cr_2O_7^{2-}$ at 257 nm. The aqueous $K_2Cr_2O_7$ solution was pipetted at different time interval to measure the UV-vis adsorption intensity. The anion exchange capacity of **BIF-28** were evaluated by measuring the decolorization rate of aqueous $K_2Cr_2O_7$ solution, which was calculated by the following formula:

$$D = (C_0 - C_1)/C_0 \times 100\% = (A_0 - A_1)/A_0 \times 100\%$$

Where D is adsorption capacity, C_0, A_0 and C_1, A_1 are the concentration and absorbency of aqueous $K_2Cr_2O_7$ solution at the peak of 257 nm in adsorption equilibrium before and after anion exchange, respectively. The adsorption intensity of solution decreases from 0.932 to 0.382 with continuous exchange in 3h, which means 55% $Cr_2O_7^{2-}$ was exchanged into the cationic framework. After anion exchange, the crystals were filtered, rinsed with deionized water and dried in the air.

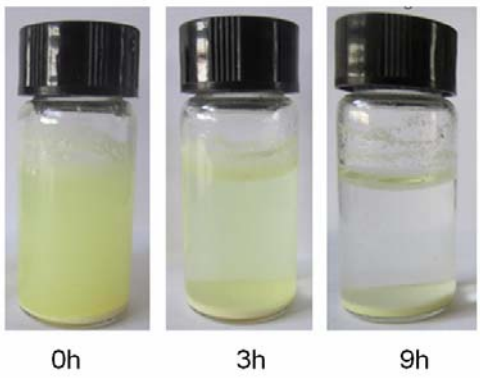

Figure S2. Photographs of the sample **BIF-28** show aqueous $K_2Cr_2O_7$ solution changes with increasing exchange time at room temperature.

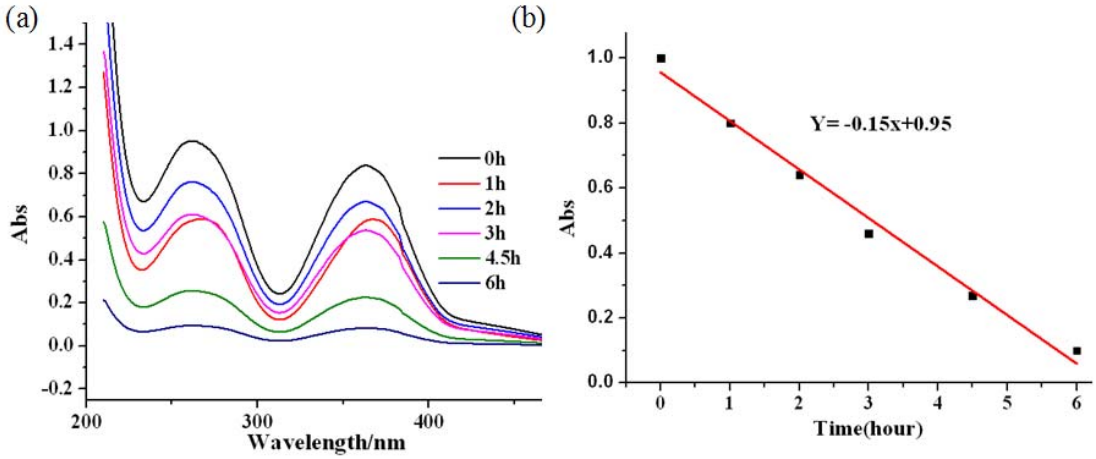

Figure S3. UV-vis spectra of aqueous $K_2Cr_2O_7$ solution during anion exchange and fit curves of the exchange of $Cr_2O_7^{2-}$ in the first 6 h.

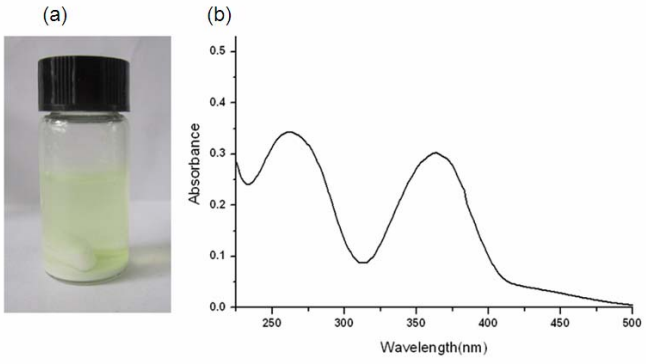

Figure S4. (a) Photographs of the regeneration of **BIF-28** from Cr_2O_7 exchanged sample **BIF-28**-Cr_2O_7 in aqueous KNO_3 solution. (b) UV-vis spectra of released $Cr_2O_7^{2-}$ solution.

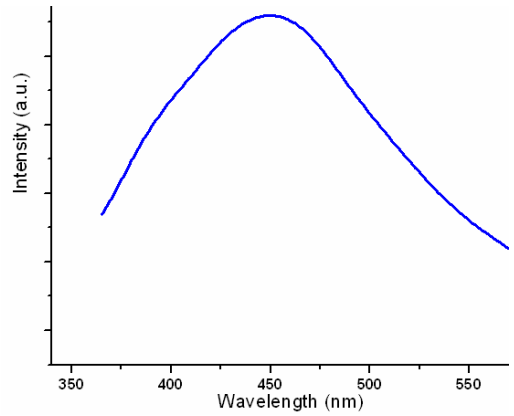

Figure S5. The solid-state emission spectra (λex = 355 nm) for the KBH(dm-bim)$_3$ sample.

Figure S6. Photographs of the sample **BIF-28**: Showing luminescence changes with exchange time at room temperature under ambient light and 365 nm UV lamp, respectively.

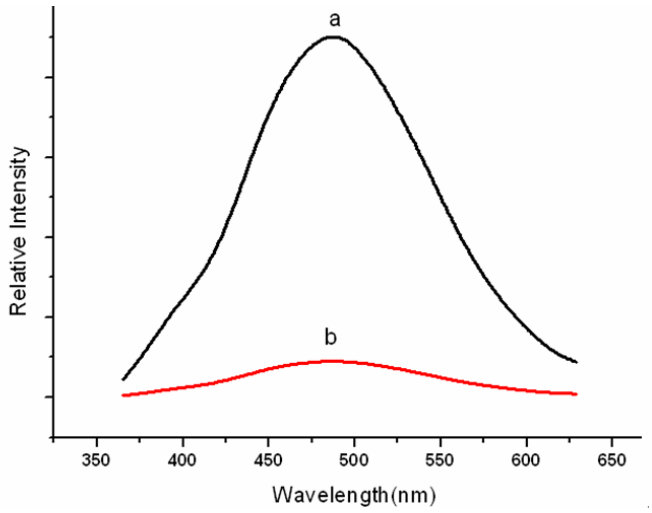

Figure S7. The solid-state emission spectra (λex = 350 nm) for the **BIF-28** sample (black line: before exchange $Cr_2O_7^{2-}$, red line: after exchange $Cr_2O_7^{2-}$).

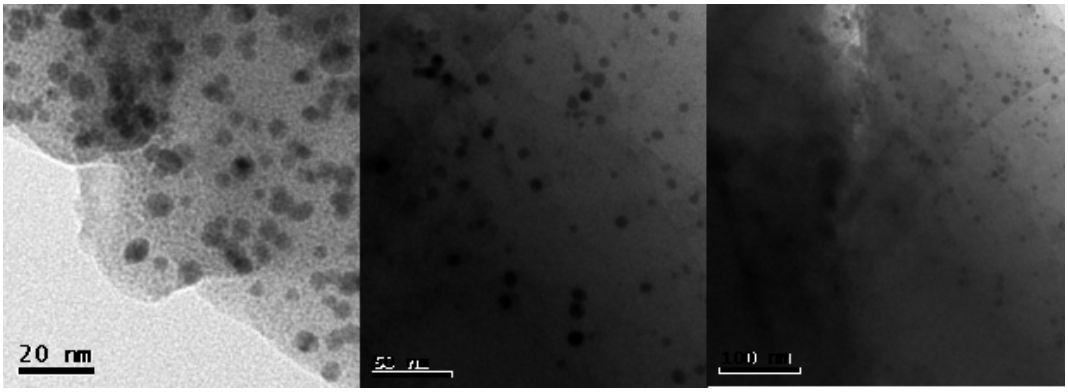

Figure S8. TEM images of the prepared **Au@BIF-28** in water solution

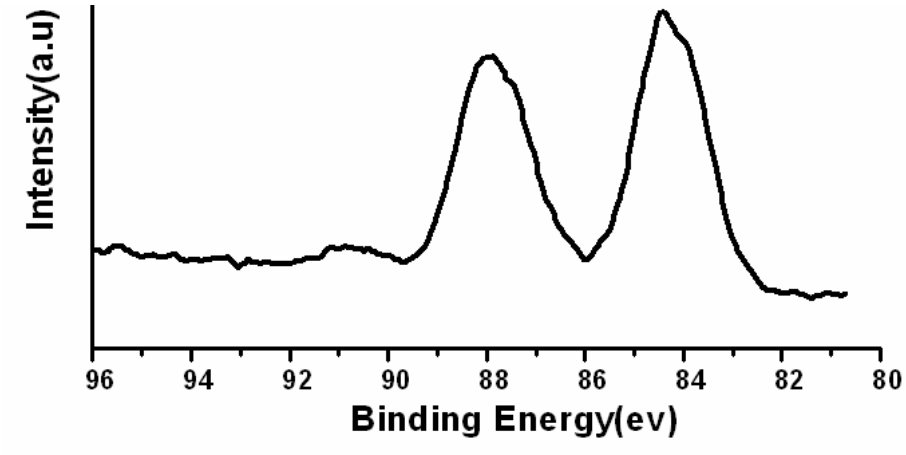

Figure S9. XPS spectrum of **Au@BIF-28**

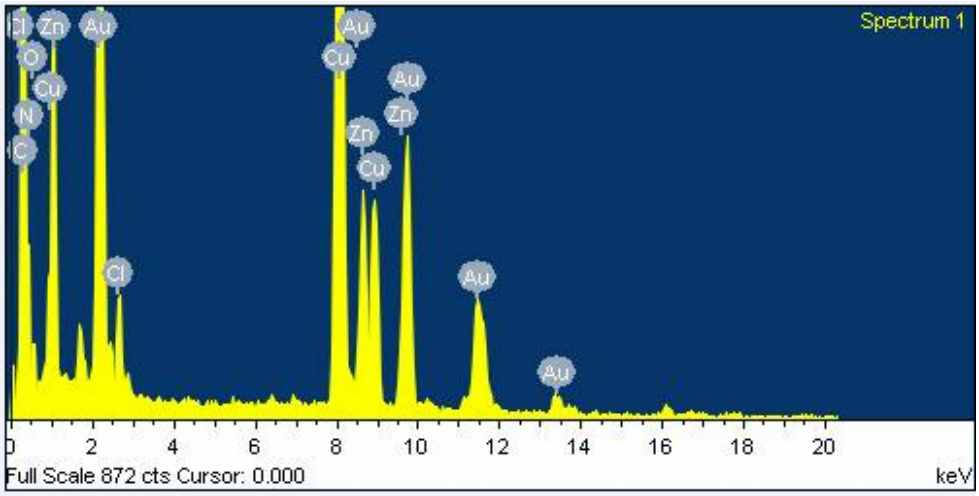

Figure S10. EDX spectrum of **Au@BIF-28**