**Influence of Doped Metal Center on Morphology and Pore Structure of ZIF-8**

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**Supplementary Material**

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# 1. Microwaves irradiation synthesis

## 1.2 Mixed metal Zn/Co-ZIF-8

The microwave synthesis of mixed metal Zn/Co-ZIF-8 is similar to previously reported method by our group.[1] Briefly, a solution of 2.225 mmol of Zn(NO3)2.6H2O and 2.225 mmol of Co(NO3)2.6H2O in 15 mL of methanol was prepared as mixed metal solution. A separate solution of 17.8 mmol of 2-methylimidazole in 15 mL of methanol was prepared as a ligand solution. The metal solution was then poured into the ligand solution while continuously stirring the solution for 1 min. The mixed solution was then transferred to a microwave-transparent glass tube, immediately followed by microwave irradiation with a power of 100 W for 1.5 min. The solution was then allowed to cool to room temperature by keeping it under ambient conditions for 30 min followed by centrifugation at 8000 RPM for 30 min. The precipitate was collected and dispersed in 30 mL of methanol and washed three times. The resulting powder was then dried in an oven at 60 °C for 24 hours prior to characterization.

## 1.2. ZIF-8

The microwave synthesis of ZIF-8 is similar to the mixed metal Zn/Co-ZIF-8 except that 4.45 mmol of Zn(NO3)2.6H2O were used for the metal solution and no Co(NO3)2.6H2O was added to the metal solution. The rest of the procedure in synthesis and washing steps are the same as the mixed metal Zn/Co-ZIF-8.

## 1.3. Mixed metal Cu/ZIF-8

A solution of 3.115 mmol of Zn(NO3)2.6H2O and 1.335 mmol of Cu(NO3)2.2.5H2O in 15 mL of methanol was prepared as a mixed metal solution. A separate solution of 39.5 mmol of 2-methylimidazole in 15 mL of methanol was prepared as a ligand solution. The metal solution was then poured into the ligand solution while continuously stirring the solution for 1 min. The mixed solution was then transferred to a microwave-transparent glass tube, immediately followed by microwave irradiation with a power of 100 W for 1.5 min. The solution was then allowed to cool to room temperature (by keeping it under ambient conditions for 30 min) followed by centrifugation at 8000 RPM for 30 min. The precipitate was collected and dispersed in 30 mL of methanol and washed three times. The resulting powder was then dried in an oven at 60°C for 24 hours prior to characterization.

# 2. Characterization

A Micromeritics ASAP2420® Accelerated Surface Area and Porosimetry Analyzer System, with an enhanced micropore capability (utilizing 1-Torr pressure transducer), was used to measure the pore structures of the ZIF-8, Zn/Co-ZIF-8 and Cu/ZIF-8 samples using the adsorption isotherms of nitrogen at 77 K. Prior to the adsorption measurements, the samples were regenerated in-situ for 24 h at 473 K under vacuum (1×10-4 Pa). The pore properties and surface energy distribution were obtained by built-in calculations based on the density functional theory (DFT). The morphologies ZIF-8, Zn/Co-ZIF-8 and Cu/ZIF-8 samples were observed with a FEI Nova™ nanoscanning electron microscopy 450 (Nova NanoSEM). The chemical compositions of samples were investigated by Energy-dispersive X-ray spectroscopy (EDX) attached to Nova NanoSEM. A FEI TecnaiTF20 200kV FEG high-resolution transmission electron microscope (TEM) was also used to investigate the bulk morphology. Thermogravimetric analyses (TGA) were carried out using a PerkinElmer Pyris6 TGA analyzer under an N2 gas in the range of 30oC to 800oC with heating rate 10oC/min.

# 3. Comparison study

The comparison of this work with other approaches was found in **Table S1**.

**Table S1.** Characterization comparison of ZIF-8, Zn/Co-ZIF-8 and Cu/ZIF-8 nanostructures with other similar works

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ZIF-8 | | | | | |
| **Method** | **particle size**  **(nm)** | **Pore volume**  **(cm3/g)** | **Time** | **Morphology** | **Reference** |
| Microwave-assisted  synthesis | 98.3 | 0.621 | 1.5 min | Less uniform cubic-shaped crystals | This work |
| Solvothermal synthesis | 110  nm | 1.4450 | - | Uniform cubic-shaped crystals | Ref.[2] |
| Deep eutectic method | ~ 100 nm | 0.55 | 0.5 h | Less uniform sphere nanoparticle | Ref.[3] |
| Hydrothermal  syhthesis | ~ 100 nm | 0.52 | 0.5h | Less uniform sphere nanoparticle | Ref.[3] |
| Solvothermal synthesis | 60 nm | 1.09 | 10 min | Uniform sphere nanoparticles | Ref.[4] |
| Solvothermal synthesis | 110.6 | 0.64 | 24-48 h | - | [5] |
| Cu/ZIF-8 | | | | | |
| Microwave-assisted  synthesis | 126 | 0.511 | - | Less uniform cubic-shaped crystals | This work |
| Solvothermal synthesis | ~110 | 0.4943 |  | Uniform cubic shaped crystals | Ref.[2] |
| Solvothermal Synthesis | ~60 | 0.3349 | 0.5 h | Uniform sphere nanoparticles | ReF.[6] |
| Solvothermal Synthesis | ~100 | 0.54 | 1 h | Uniform sphere nanoparticles | Ref.[7] |
| Zn/Co-ZIF-8 | | | | | |
| Microwave assisted  synthesis | 102.6nm | 0.576 | 1.5 min | Uniform cubic-shaped crystals | This work |
| Solvothermal synthesis | 0.2 mm | 0.7750 | 15 min | Uniform Cubic –shaped crystals | Ref.[8] |
| Solvothermal synthesis | 100nm-55mm | - | 2 days | Uniform Cubic –shaped crystals | Ref.[9] |

# 4. TGA thermograms

**Figure S1** shows the TGA thermograms of ZIF-8, Cu30%/ZIF-8 and Zn/Co-ZIF-8. It was observed that the thermal stability of ZIF-8 is the highest one and the thermal stability of Zn/Co-ZIF-8 represents the lowest one. The sequential order of ZIFs thermal stability is ZIF-8 > Cu30%/ZIF-8 > Zn/Co-ZIF-8. Therefore, it could be said the type of metal ion has a significant effect on the thermal stability of ZIFs if inserted into their matrix.

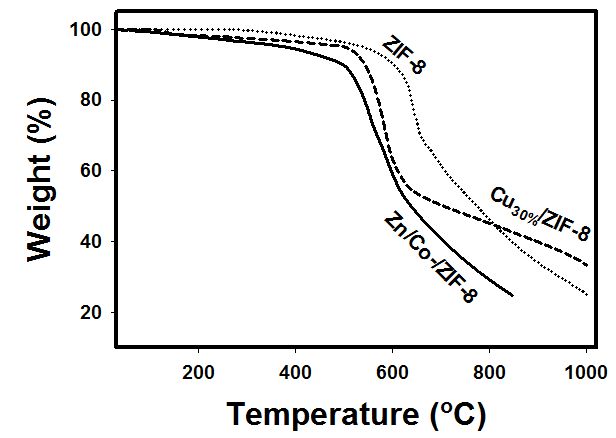


Figure S1. TGA thermograms of ZIF-8, Cu30%/ZIF-8 and Zn/Co-ZIF-8.

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