Supporting Information of

Synthesis of magnesium ZIF-8 from $Mg(BH_4)_2$

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1. **Synthesis of [Mg(2 mim)$_2$] (Mg-ZIF-8, 2 mimH = 2-methyl imidazole)**
   10 mL of an acetonitrile solution of 2 mimH (82.1 mg, 100 mM) was slowly added dropwise to 10 mL of an acetonitrile solution of $Mg(BH_4)_2$ (27.0 mg, 50 mM) at 298 K inside an Ar-filled glove box. Consequently, a white precipitate was generated when half of the ligand solution was added. The suspension was transferred to a hydrothermal bomb with a Teflon vial; the bomb was tightly sealed and heated at 373 K for 2 days. The white precipitate was filtered, and the powder was washed several times with acetonitrile and dried overnight at room temperature inside the glove box.

2. **Characterizations**
   Powder X-ray diffraction (PXRD) data were collected on a Rigaku RINT 2200 Ultima diffractrometer with Cu *K*α radiation. The differential scanning calorimetry (DSC) was carried out with a DSC6220 (SII Nano Technology Inc.) at the heating rate of 10 K min^{-1}. Nitrogen adsorption isotherms were measured at 77 K and carbon dioxide adsorption isotherms were measured at 195 K by BELSORP-mini.

3. **Theoretical calculation**
   Total energy calculations were performed with in the density functional theory using DMol code.[1] The generalized gradient approximation (GGA) with in Perdew-Burke-Ernzerhof (PBE) parameterization was used to describe exchange and correlation.[2] The double numerical all electron basis set (DNP) were employed.[3] The formation energy was defined as the difference of total energy between [M(2 mim)$_2$] per unit cell and the isolated corresponding ions, M^{2+} and mim^-. Both lattice constants and geometry were optimized for [M(2 mim)$_2$]unit cell, and the force convergence criteria were 0.05 eV Å^{-1}. The optimized lattice constants were 17.81 and 17.94 Å for [Zn(2

mim)$_2$] and [Mg(2 mim)$_2$], respectively. The errors were less than 5 % when compared with experimental values of 17.01 and 17.29 Å. In order to investigate the charge on metal ions in M(2 mim)$_2$, conventional Mulliken atomic charges were calculated.

[1] Delley, B. *J. Chem. Phys.*, 1990, 92, 508.
[2] Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.*, 1996, 77, 3865.
[3] Delley, B. *J. Chem. Phys.*, 2000, 113, 7756.

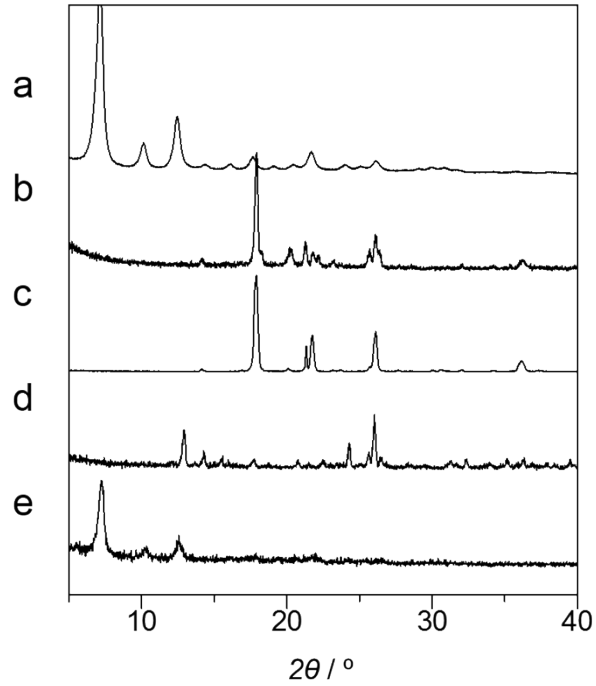

Figure S1. PXRD patterns of (a) Mg-ZIF-8 under Ar prepared by optimized synthesis condition (b) Mg-ZIF-8 after 10 min of air exposure (c) 2-methyl imidazole (d) $MnCl_2$(2 mimH)$_3$ synthesised from $MgCl_2$ (e) Mg-ZIF-8 under Ar synthesised by tetrahydrofuran.

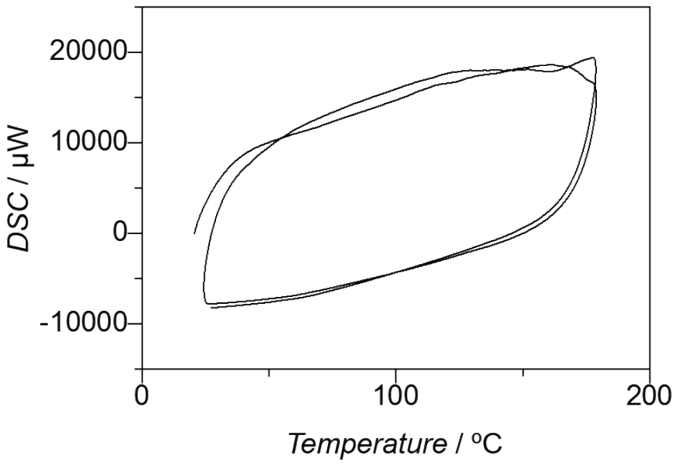

Figure S2. Differential scanning calorimetry profile of Mg-ZIF-8 under N_2 atmosphere.

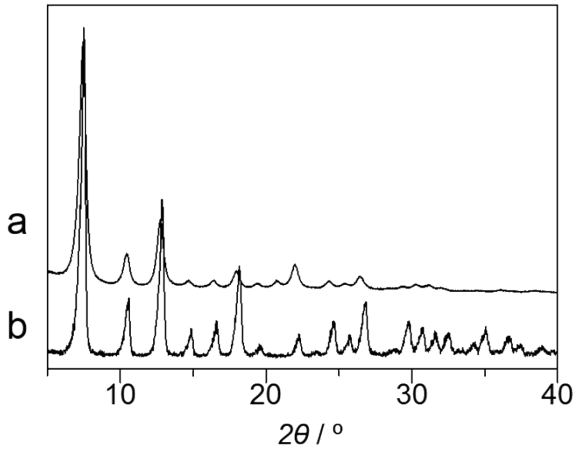

Figure S3. PXRD patterns of (a) Mg-ZIF-8 (b) Zn-ZIF-8 under Ar.