Energetic Performances of the Metal-Organic Framework ZIF-8 by
High Pressure Water Intrusion-Extrusion Experiments

Guillaume Ortiz, Habiba Nouali, Claire Marichal, Gérald Chaplais, Joël Patarin

Equipe Matériaux à Porosité Contrôlée (MPC), Institut de Sciences des Matériaux de Mulhouse (IS2M), UMR 7361 CNRS-UHA, Institut Jean-Baptiste Donnet, 3 bis rue Alfred Werner 68093 Mulhouse, France

Corresponding authors: gerald.chaplais@uha.fr; joel.patarin@uha.fr

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**Water Intrusion-Extrusion Experiments**

The intrusion-extrusion experiments of water on ZIF-8 samples were performed at room temperature using a modified mercury porosimeter (Micromeritics Model Autopore IV). ZIF-8 powder was directly introduced in the cell. This latter, which contains the “MOF-water” system, consists in a polypropylene cylinder of 2 cm$^3$ sealed by a mobile piston. Then this cell is introduced in a 15 cm$^3$ penetrometer of the porosimeter which is filled with mercury. The volume variation is determined through a capacity measurement which depends on the mercury height in the capillary tube of the penetrometer. The experimental intrusion-extrusion curve is obtained after correction of the curve corresponding to the compressibility of pure water. The value of the intrusion ($P_{int}$) and extrusion ($P_{ext}$) pressures correspond to the pressure where the variation of the intruded / extruded volume is maximal. Pressure is expressed in MPa, and volume variation in mL per gram of sample. The experimental error is estimated to 1 % on the pressure and on the volume.

**Powder X-ray Diffraction**

The powder XRD patterns of the different samples was collected between 5 and 50° (2θ) (step 0.01°) on a STOE STADI-P diffractometer in Debye-Scherrer geometry, equipped with a linear position-sensitive detector (6° in 2θ) and employing Ge monochromated CuKα$_1$ radiation ($λ= 1.5406$ Å).

**Thermogravimetric Analyses**

The measures were performed under air until 900 °C (rate of 2 °C min$^{-1}$) using a METTLER-TOLEDO TGA 851e apparatus.

**Scanning Electron Microscopy**

The size and the morphology of ZIF-8 nanoparticles were determined using a Philips XL 30 FEG microscope.

**Nitrogen Adsorption-Desorption Measurements**

Nitrogen adsorption-desorption isotherms were carried out using a Micromeritics ASAP 2420 apparatus. Prior to the adsorption measurements, samples were outgassed at 90 °C overnight under vacuum. BET surface ($S_{BET}$) areas for ZIF-8, before and after water intrusion-extrusion experiments, were calculated according to the criteria given in the literature,$^{1,2}$ namely in the $0.001 \leq P/P_0 \leq 0.018$ range. Langmuir surface ($S_{Lang}$) areas were calculated by the apparent Langmuir equations assuming a monolayer coverage of N$_2$ and a cross-sectional area of 16.2 Å$^2$ per molecule in the same range as BET surface. The micropore volume ($V_{micro}$) was determined by t-plot method.
**Figure S1.** Water intrusion-extrusion diagrams of the “ZIF-8-water” system in linear scale for pressure values.

**Figure S2.** Mercury porosimetry on ZIF-8.
Figure S3. Powder X-ray diffraction patterns of ZIF-8 before (blue line) and after (red line) three water intrusion-extrusion cycles.

Figure S4. SEM images of ZIF-8 before (a) and after (b) three water intrusion-extrusion cycles.
Figure S5. TG curves under air of ZIF-8 before (blue line) and after (red line) three water intrusion-extrusion cycles.

Figure S6. Nitrogen adsorption (full square)-desorption (empty square) isotherms of ZIF-8 before (blue line) and after (red line) water intrusion-extrusion experiments.
References
