

Electronic Supporting Information

Aluminum hydride nanoparticles nested in the porous Zeolitic Imidazolate Framework-8

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Experimental Methods and Instrumentation

All chemicals were purchased from Sigma Aldrich and used without further purification. ZIF-8 was activated in vacuum at 473 K for 70 h prior use to remove guest solvent molecules and kept in the glove box under argon atmosphere. All preparation steps were carried out in an argon-filled glove box ($O_2 < 1$ ppm; $H_2O < 1$ ppm).

alane@ZIF-8 synthesis: Alane was loaded into ZIF-8 by solution infiltration method. Dimethylethylamine alane (DMEAAI) toluene solution (0.5 M) was added to the activated ZIF-8 powder. The molar ratio of reactants was 10:1 (DMEAAI: ZIF-8). The mixture was vigorously stirred for 16 h. The sample was heated to 323 K at around 0.7 mbar for 8 h to remove free toluene and to dissociate amine-alane adduct.

Characterization

All samples were handled under nitrogen unless otherwise mentioned.

Powder X-ray diffraction data (PXRD) were collected on a PANalytical X'pert Pro powder diffractometer with Cu-K α radiation ($\lambda=1.541874$ Å). The voltage and the current were set to be 45 kV and 40 mA, respectively. Phase identity was verified by the match search in the ICDD database (Powder Diffraction File-4+, editions 2007-2010).

The FTIR spectra were collected on a Varian 3100 FT with a DTGS detector in the 4000-400 cm^{-1} range. The spectral resolution was 4 cm^{-1} and 64 scans were averaged. Samples have been prepared using Nujol as a mulling agent and sandwiched between KBr plates.

The volumetric Ar sorption measurements were carried out on a Micromeritics ASAP2010 gas adsorption analyzer equipped with additional 1 mmHg and 10 mmHg pressure transducers in order to achieve high resolution in the low pressure range. Prior to the actual adsorption measurement, the samples were in-situ degassed at 323 K during 24 h. Handling of the samples was done in a glove box under nitrogen. The free space volume of the sample cell was determined in a separate measurement, in order to avoid the so-called helium entrapment phenomenon, which adversely affects adsorption in the low pressure range. The specific surface area was calculated using the BET model in the adapted relative pressure range of 0.01-0.10. Non-Local Density Functional Theory (NLDFT) pore size models were applied to fit the experimental isotherms. The model describing argon adsorption (at 87 K) in spherical pores for zeolite/silica surfaces turned out to be the most adequate model, but required the modelling to be limited to the relative pressure range 10^{-7} up to 0.3.

TEM analyses were performed using JEOL2100F microscope operating at 200kV. The samples were suspended in dry and degassed toluene. One drop of a solution was placed on the copper TEM grid with lacey carbon support film and left for drying. The sample was transferred to the microscope under inert conditions.

The elemental analyses were performed on Spectro Ciros Vision ICP-OES spectrometer.

DSC measurement were conducted on Mettler-Toledo DSC 1 module instrument. The samples were heated from RT till 600°C (10°C/min) in a flow of nitrogen gas (60 ml/min).

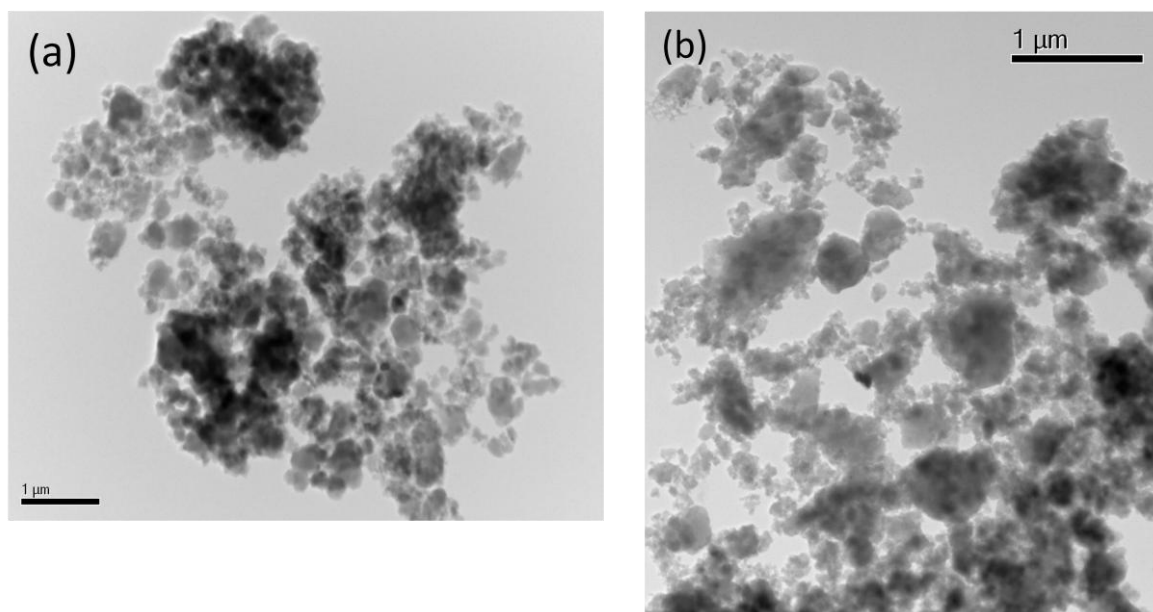


Fig. S1 Bright-field TEM image of (a) ZIF-8 and (b) alane@ZIF-8 sample.

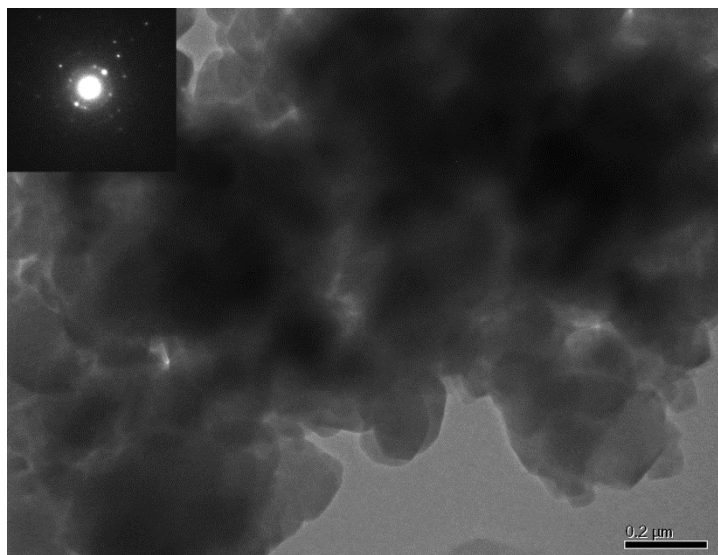


Fig. S2 Bright-field TEM image of ZIF-8. The inset diffraction pattern evidences the cubic structure of ZIF-8 material and confirms that the structure is still largely intact.

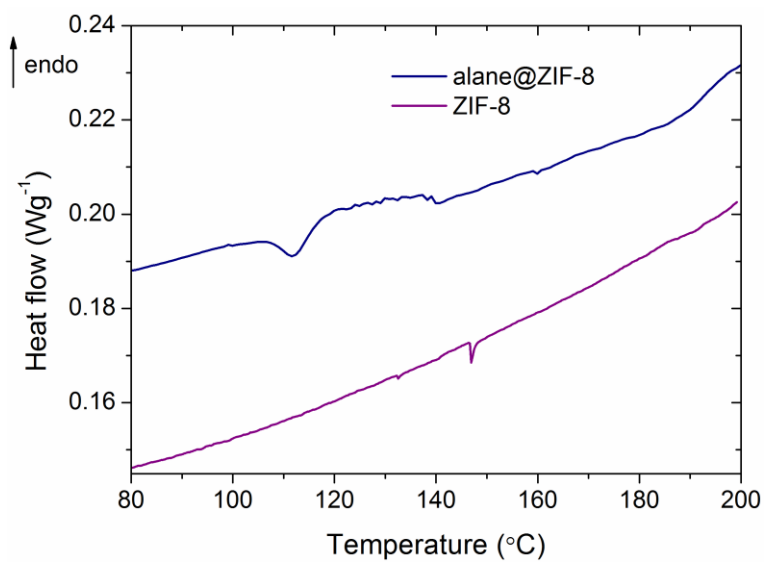


Fig. S3 Differential scanning calorimetry profiles for nanoconfined alane and empty ZIF-8 material.