

Electronic Supplementary Information

Iridium nanoparticles stabilized by metal organic framework (IrNPs@ZIF- 8): synthesis, structural properties and catalytic performance

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Characterization

The amounts of iridium loading into ZIF-8 framework and leaching into the solution were determined by inductively couple plasma mass spectroscopy (ICP-MS) by using Perkin Elmer DRC II model. X-ray diffraction (XRD) analyses were carried out on Rigaku Ultima-IV in the range of $2\theta = 5-60^\circ$. ^{13}C MAS NMR spectra were taken on a Bruker Superconducting FT-NMR Spectrometer Avance TM 300 MHz WB. ^1H NMR spectra were recorded on a Bruker Avance DPX 400 MHz spectrometer. The transmission electron microscopy (TEM), high resolution-TEM (HR-TEM), and STEM images were taken on JEOL JEM-2010F (FEG, 80-200 kV). Oxford EDXS system and Inca software were used to collect and process STEM/EDS data. XPS analyses were performed on a Physical Electronics 5800 spectrometer equipped with a hemispherical analyzer and using monochromatic Al-K α radiation (1486.6 eV, the X-ray tube working at 15 kV, 350 W and pass energy of 23.5 keV). Diffuse reflectance UV-vis analyses were performed from solid samples on Shimadzu UV-3600. The nitrogen adsorption/desorption experiments were carried out at 77 K using a NOVA 3000 series instrument (Quantachrome Instruments). The sample was out gassed under vacuum at 573 K for 3 h before the adsorption of nitrogen. The GC analyses were performed on a TRB-WAX column (30 m 0.25 mm 0.25 μm) with a Shimadzu GC-2010 equipped with a FID detector.

Control experiment ZIF-8 catalyzed hydrogenation of cyclohexene and phenylacetylene

In a control experiment the catalytic activity of ZIF-8 (100 mg) was tested in the hydrogenation of 1.0 mL (9.8 mmol) cyclohexene by following the procedure described in the previous section.

Isolability, bottlability and reusability of IrNPs@ZIF-8

After the first run of the hydrogenation of 1.0 mL of cyclohexene, catalyzed by 100 mg of

IrNPs@ZIF-8, the FP bottle was detached from the line, taken into the drybox, the suspension in the culture tube was transferred into a Schlenk tube, resealed, and connected to a vacuum line. After the evaporation of volatiles, the solid residue was weighed and used again in the hydrogenation of 1.0 mL of cyclohexene under the same conditions (25 ± 0.1 °C and 3 bar initial H₂ pressure). The results were expressed as *initial* TOF values of IrNPs@ZIF-8 retained in the successive runs of cyclohexene hydrogenation.

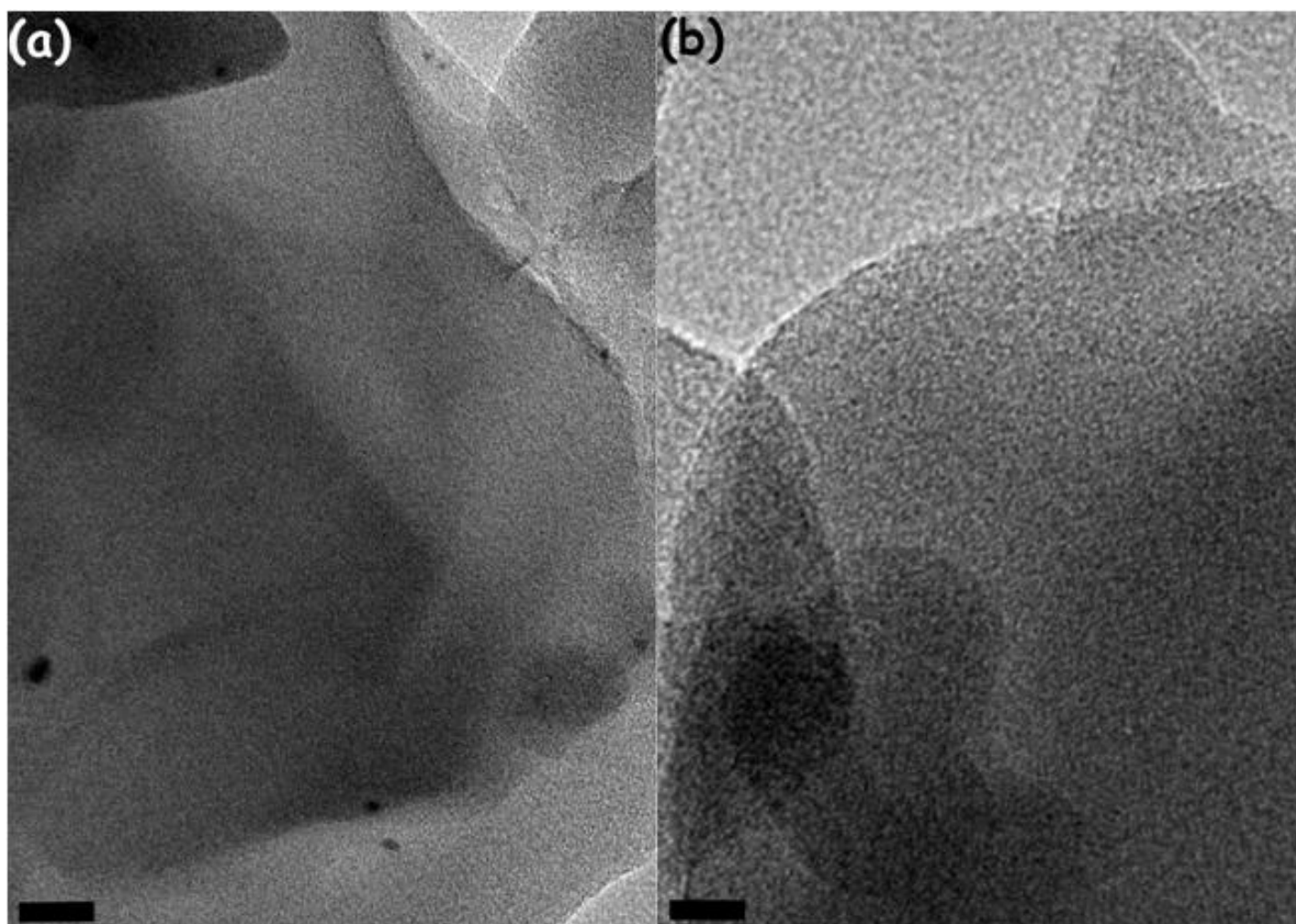


Fig. ESI-1 TEM images of (a) IrNPs@ZIF-8 and (b) plain ZIF-8 (scale bars equal to 10 nm).

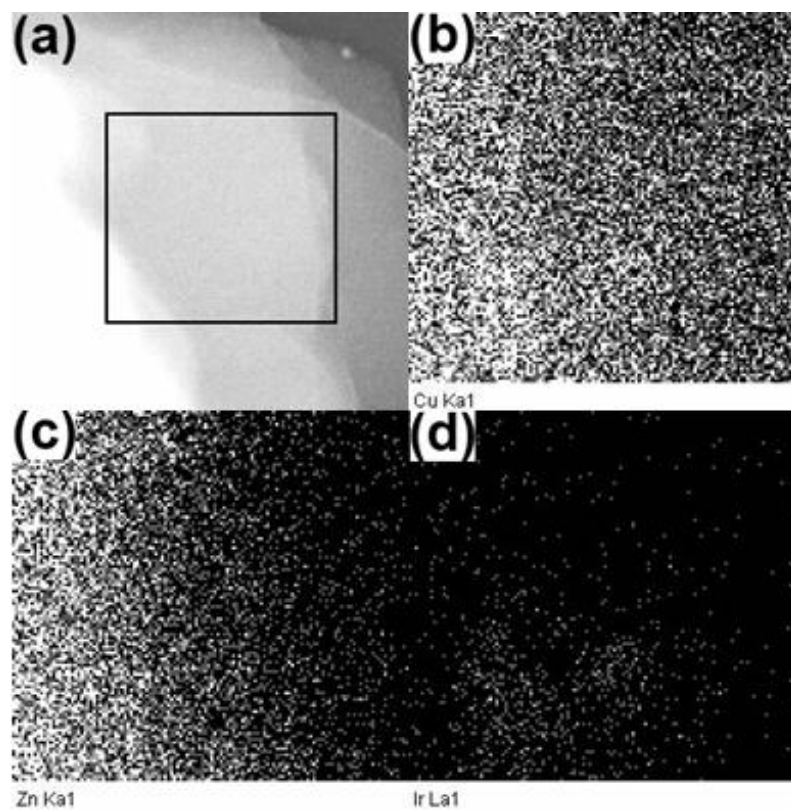


Fig. ESI-2 (a) HAADF-STEM image of IrNPs@ZIF-8 and its elemental mapping collected from the selected region given in (a) for (b) Cu, (c) Zn, and (d) Ir.

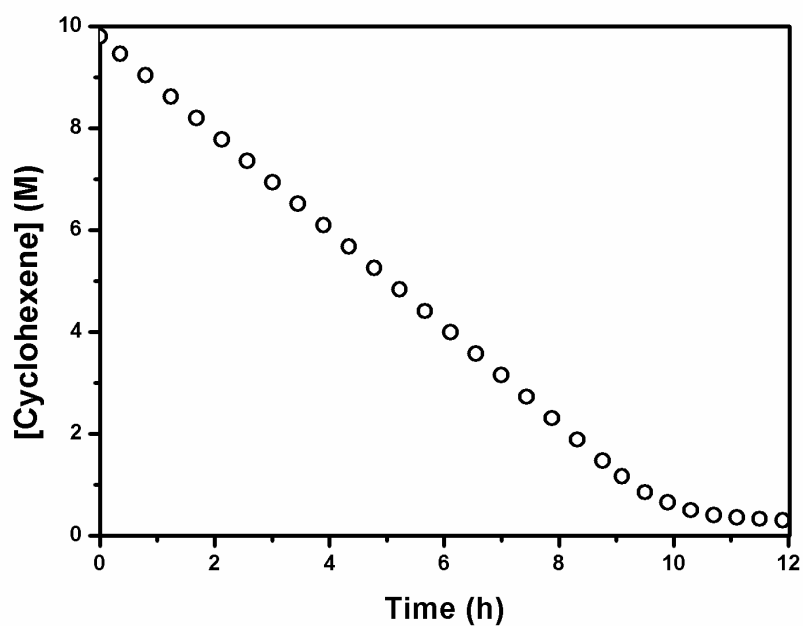


Fig. ESI-3. Plot of the concentration of cyclohexene (M) versus time (h) for the hydrogenation of neat cyclohexene (1.0 mL, 9.8 mmol) catalyzed by IrNPs@ZIF-8 (100 mg with iridium loading of 1.5 % wt corresponds to 7.8 μmol) at 25 ± 0.1 °C with 3 bar initial H_2 pressure.

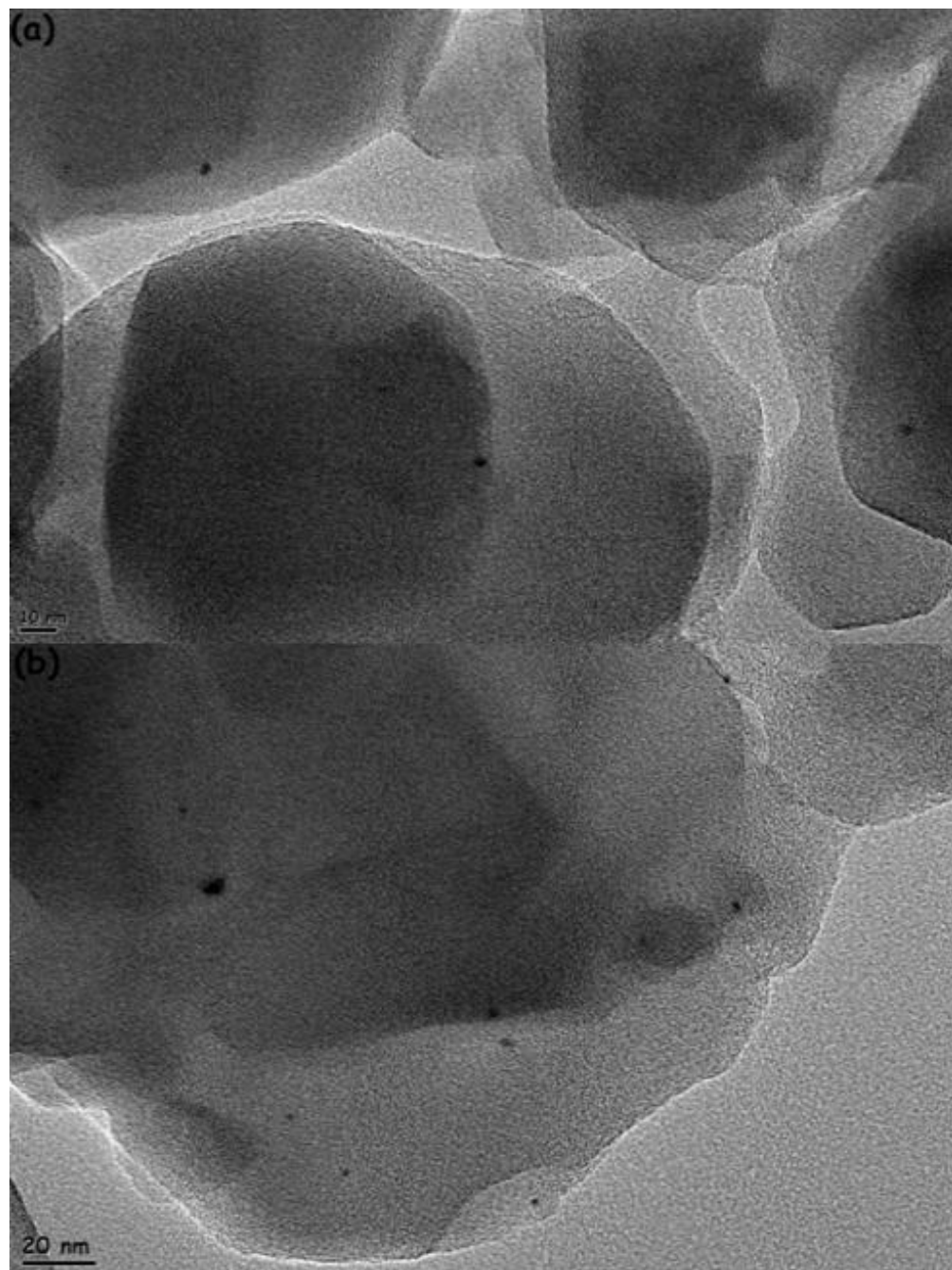


Fig. ESI-4 TEM images of IrNPs@ZIF-8 containing (a) 2.3 wt % (b) 3.8 wt % Ir.

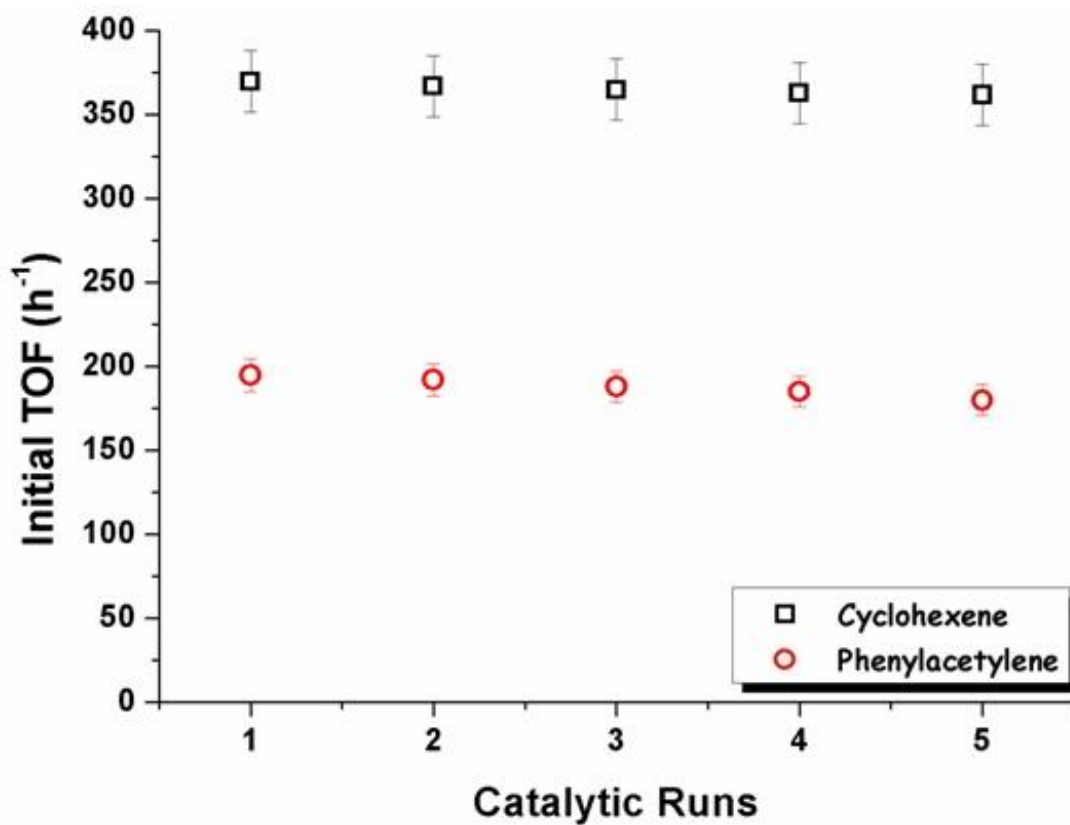


Fig. ESI-5 *Initial* TOF values vs catalytic runs determined for the IrNPs@ZIF-8-catalyzed hydrogenation of cyclohexene (square) and phenylacetylene (circle). *Initial* TOF values were determined at conversion levels of $\leq 20\%$.

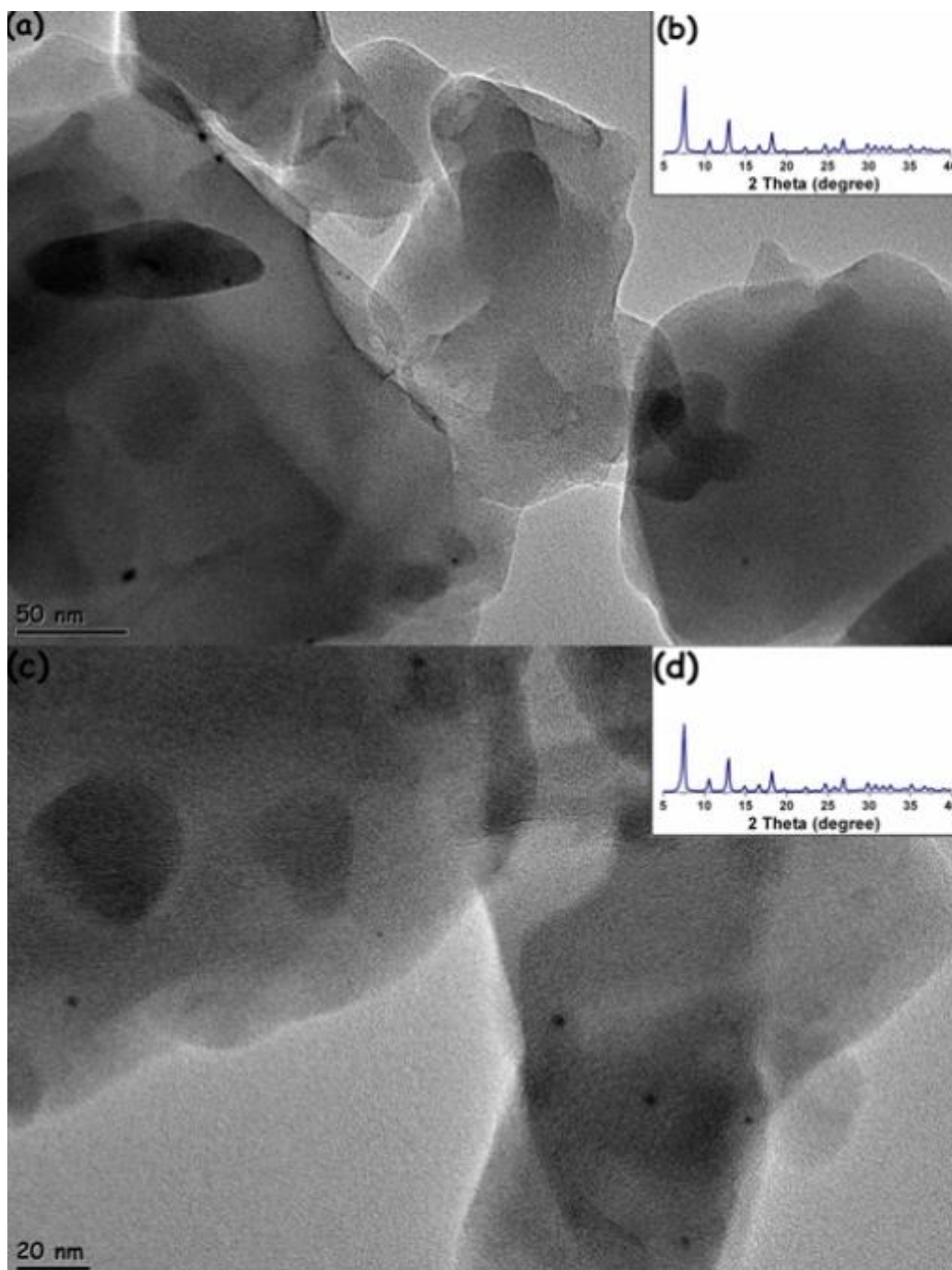


Fig. ESI-6 (a) TEM image (b) PXRD pattern of IrNPs@ZIF-8 isolated from the fifth catalytic run in the hydrogenation of neat cyclohexene, (c) TEM image (d) PXRD pattern of IrNPs@ZIF-8 isolated from the fifth catalytic run in the hydrogenation of phenylacetylene.