Chemical Communications Supporting Information

Facile Xenon Capture and Release at Room Temperature using a Metal-Organic Framework: A Comparison with activated Charcoal

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MOF-5 synthesis:

Benzene 1,4-dicarboxylic acid (30mg, Aldrich) and zinc nitrate hexahydrate (300 mg, Aldrich) were dissolved in 10 mL of *N*,*N*-dimethylformamide (Fisher) with stirring in a 20 ml vial and tightly capped and placed in a oven at 110 °C for 20 h to yield MOF-5 crystals. After decanting the hot mother liquor the product was washed with DMF and dried in air for several hours. To produce the porous form of MOF-5, the resulting material was soaked overnight in 20 ml of chloroform solution for at least 2-3 times in 3 days to replace the trapped DMF molecules. The trapped chloroform will be removed at high temperature under vacuum to get a porous MOF-5. The simulated and experimental PXRD of MOF-5 is identical that confirms the successful synthesis of MOF-5.

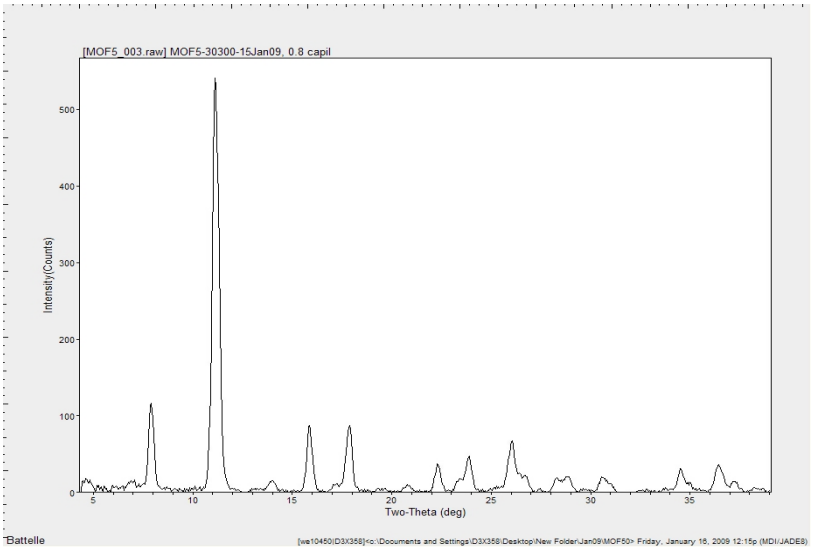

Figure S1. Experimental PXRD of MOF-5 (slightly shift in peak position is due to the different X-ray source)

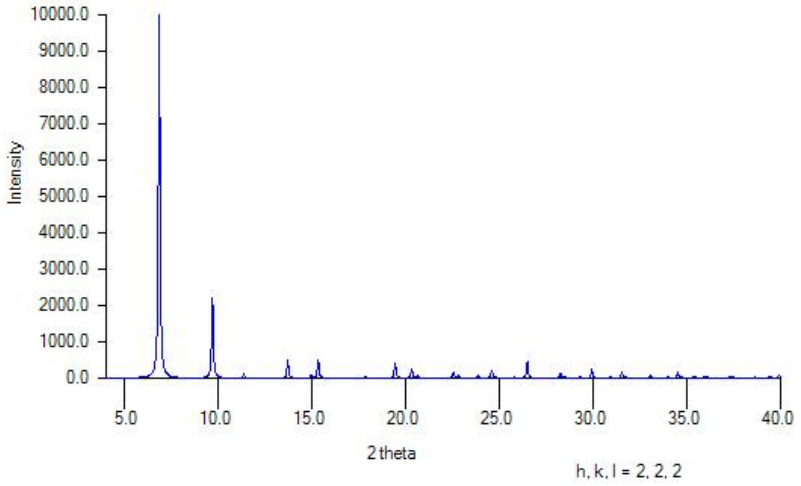

Figure S2. Simulated PXRD of MOF-5.

NiDOBDC Synthesis and Characterization:

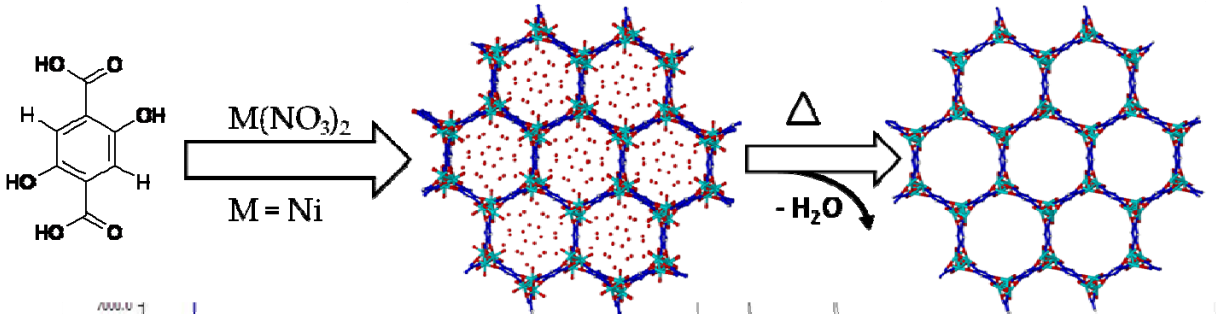

Figure S3. Synthesis and characterization of NiDOBDC using PXRD.

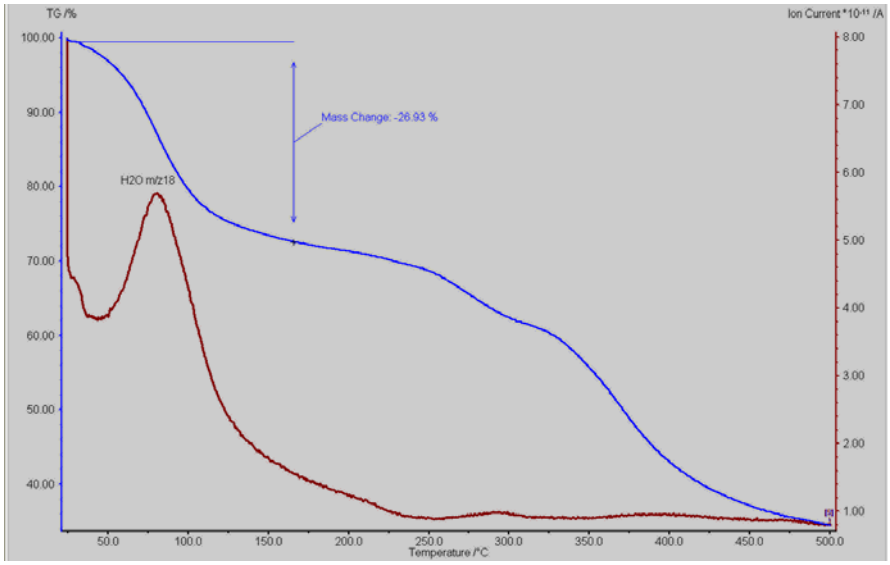

Figure S4. Thermogravimetric analysis of NiDOBDC between room temperature and 500 C under flowing Nitrogen.

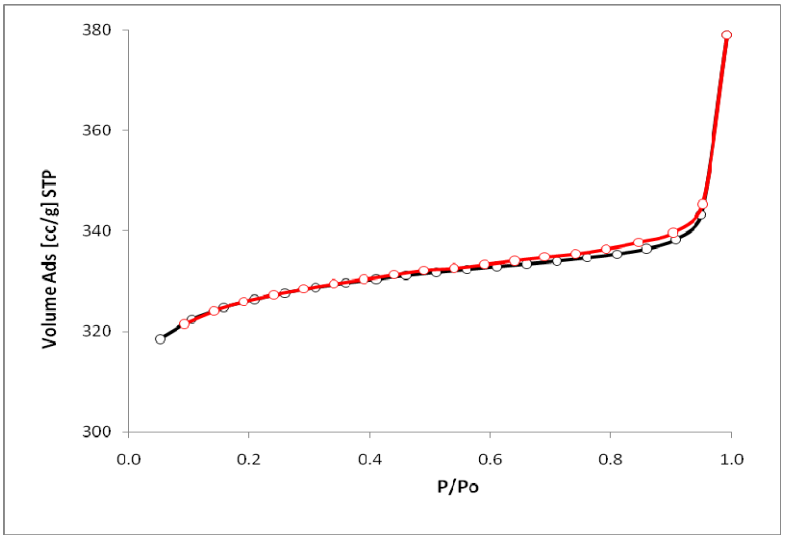

Figure S5. BET plot of NiDOBDC using N_2 at 77K and 1 bar pressure

Gas Adsorption Isotherms: Prior to adsorption measurement, the NiDOBDC sample was placed in a container of the IGA chamber and recorded the weight of the sample before activation. The temperature of the furnace was increased up to 250 °C under vacuum at a rate of 5°C/min to remove the trapped solvent molecules. The sample was cooled to RT and its dry mass was set and the experimental temperature 25°C was maintained by IGA water bath. The static mode of IGA was used to measure the xenon, krypton adsorption isotherms. The pressure points were set beforehand using IGA software. The pressure was maintained at the set point by active computer control of the inlet/outlet valves throughout the duration of the experiment. For low pressure experiments, 100 mbar of xenon was introduced into the sample chamber with an equilibration time of 10min and increased weight of the sample was plotted against the pressure. After equilibrium was established the pressure was increased to the next set pressure value, and the subsequent uptake was measured until equilibrium was re-established. The increase in weight due to adsorption for each pressure step was plotted against the pressure.

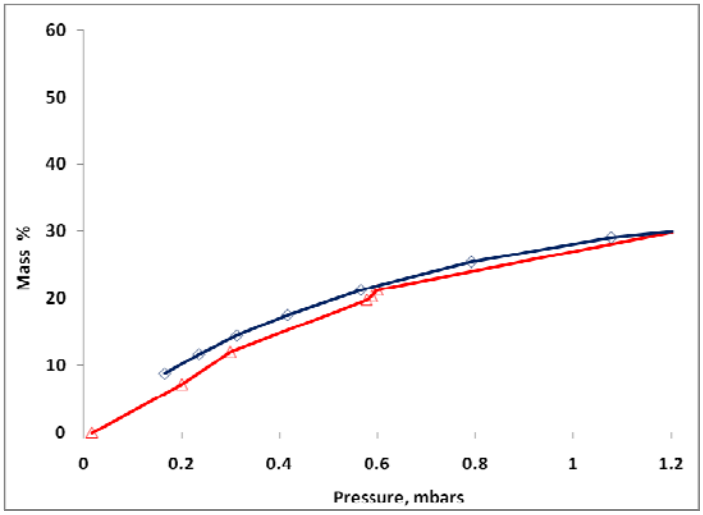

Figure S6. Uptake of Xenon by MOF-5. Adsorption (Δ) and Desorption data points (◊)

NiDOBDC Adsorption and Desorption Isotherms of Xenon at different Temeperature:

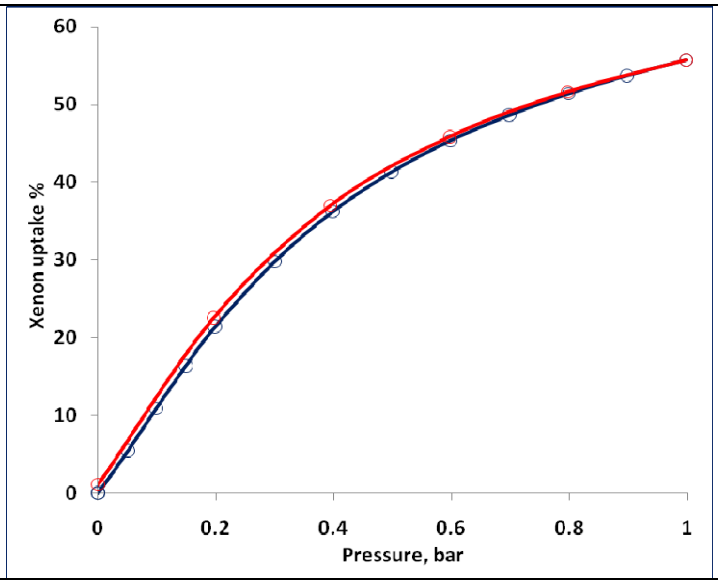

Figure S7. Xenon adsorption (blue) and desorption (red) at room temperature

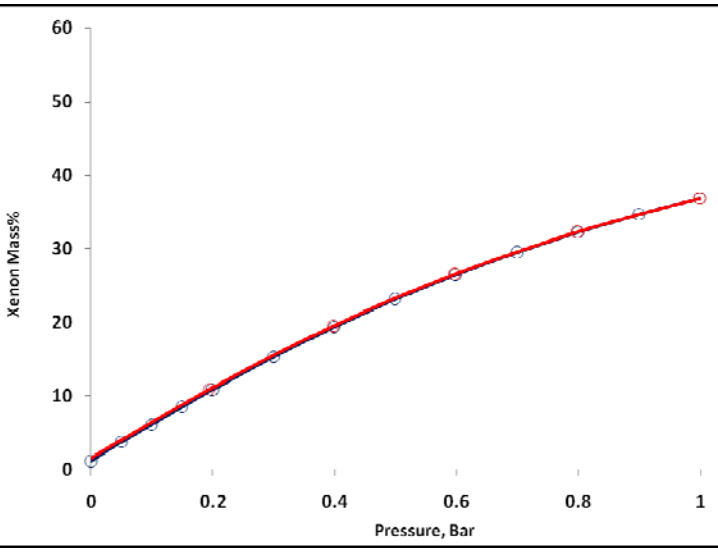

Figure S8. Xenon adsorption (blue) and desorption (red) at 50 °C

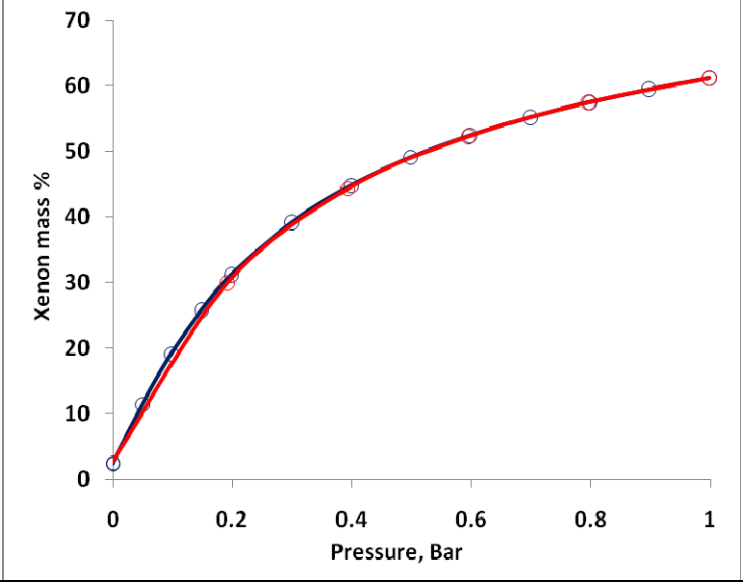

Figure S9. Xenon adsorption (blue) and desorption (red) at 10 °C

Activated Carbon Adsorption and Desorption Isotherms of Xenon at different Temeperature:

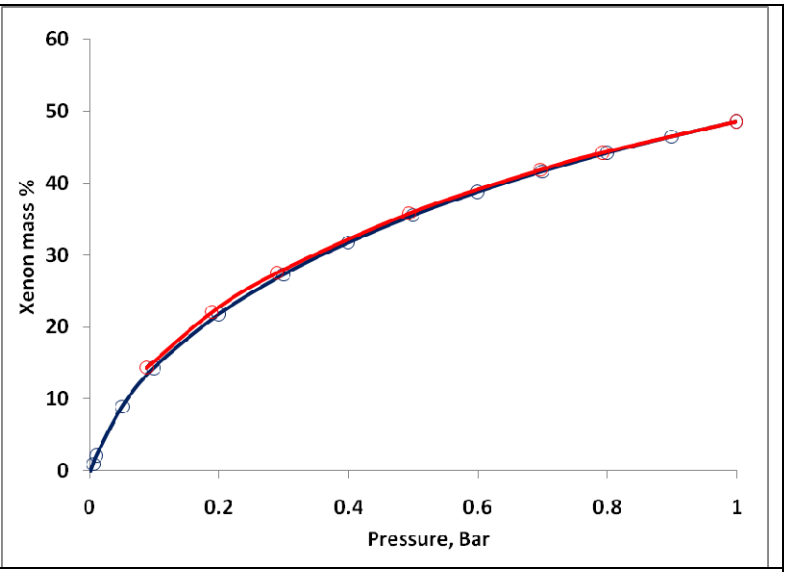

Figure S10. Xenon adsorption (blue) and desorption (red) at room temperature

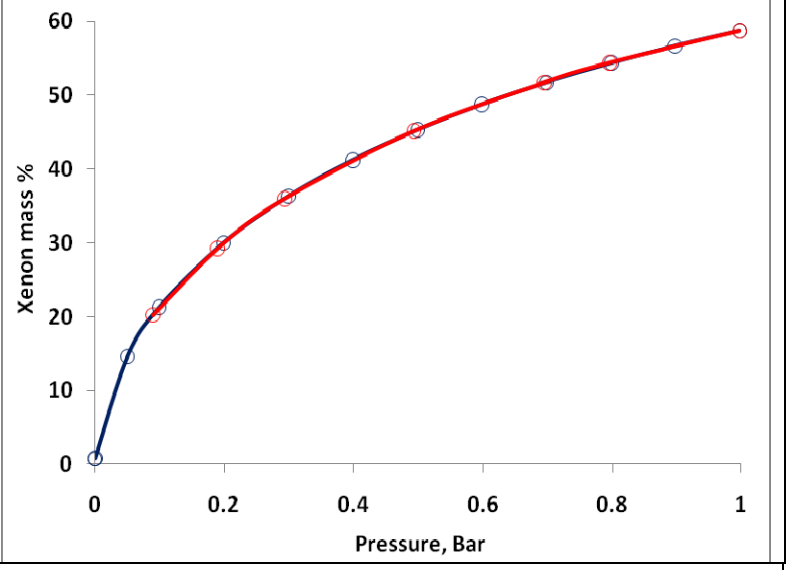

Figure S11. Xenon adsorption (blue) and desorption (red) at 10 °C

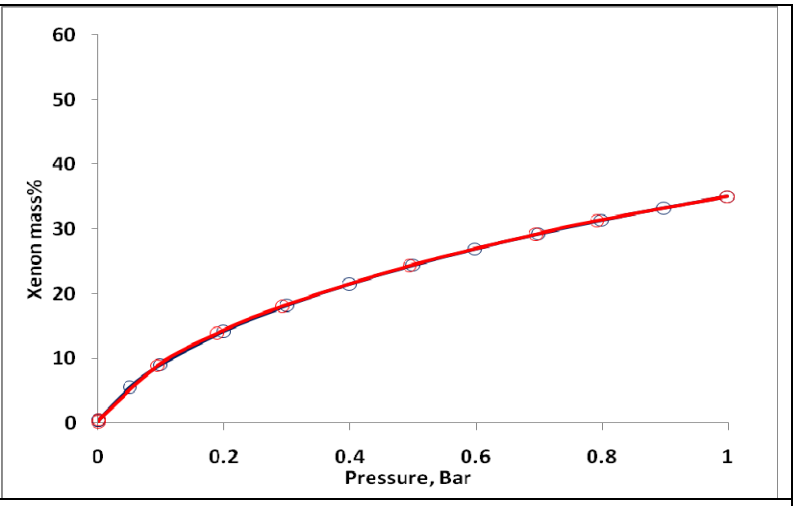

Figure S12. Xenon adsorption (blue) and desorption (red) at 50 °C

Dubinin-Radushkevich (DR) equation

$$\ln W = \ln W_0 - \left(\frac{RT}{\beta E_0}\right)^2 \left(\ln\left(\frac{P_0}{P}\right)\right)^2$$

In the form of Y=A+BX

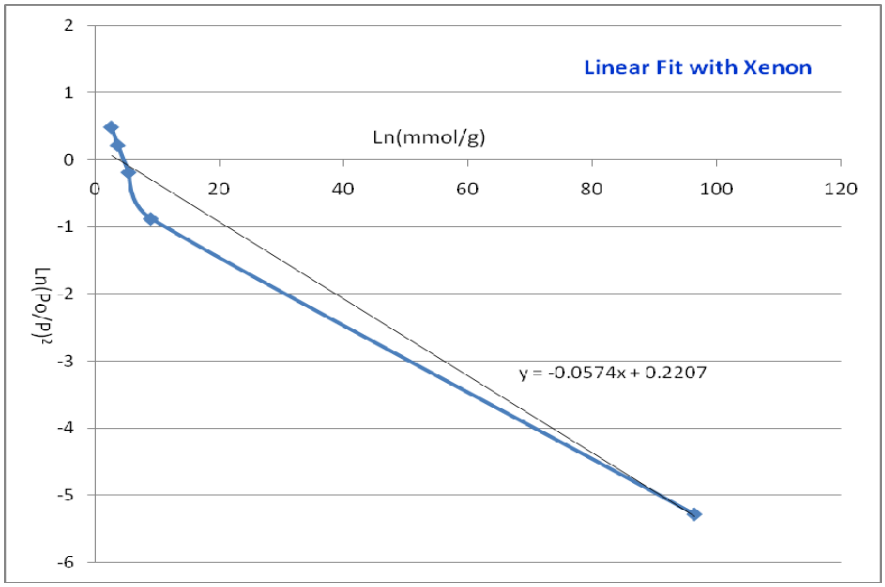

Figure S13. NiDOBDC linear fit with Xenon using DR equation

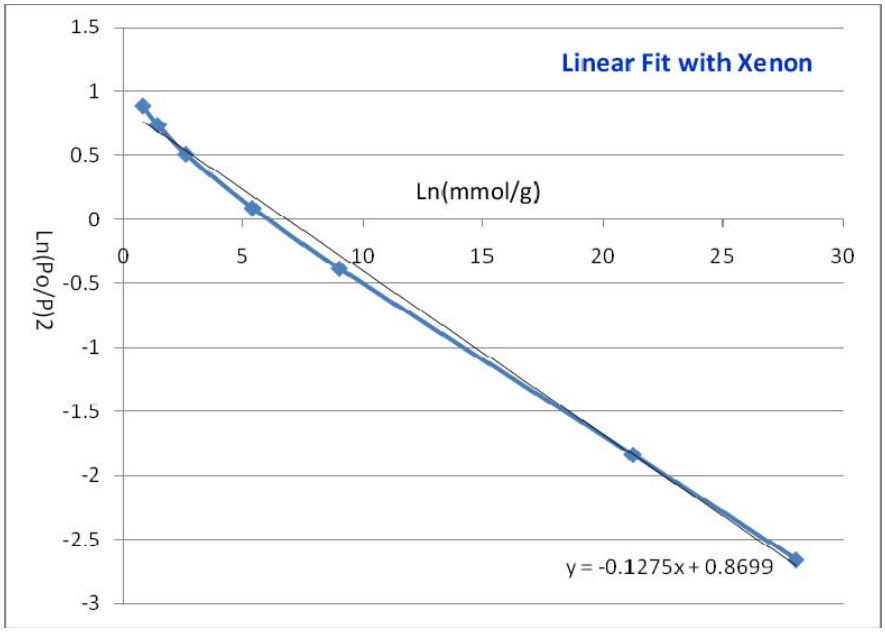

Figure S14. Charcoal linear fit with Xenon using DR equation