SUPPLEMENTARY INFORMATION

Inelastic Neutron Scattering Study of Binding of Para-hydrogen in an Ultra-Microporous Metal-Organic Framework

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A Langmuir plot (1) was used to estimate the maximum uptake of supercritical hydrogen at 77K in NOTT-300:

$$\frac{P}{W} = \frac{1}{W_0} P + \frac{1}{W_0 \bullet K} \qquad (1)$$

where W is the amount adsorbed at the pressure of P, W_0 is the amount adsorbed at saturation, and K is a coefficient. Linear fitting of (P/W) vs P is shown in Figure S1, and the maximum uptake is estimated as 26 cc/g, consistent with the experimental saturated uptake at 4 bar.

The H_2 adsorption isotherm was also studied using the Dubinin-Radushkelvich (DR) equation (2) which was then converted into a linear format (3) to analyse the porosity:

$$\sqrt{\ln(\frac{W_0}{W})} = (\frac{RT}{\beta E_0})(\ln(P_0) - \ln(P)) \qquad (2)$$

$$RT \ln P = RT \ln P_{0q} - \beta E_0 \sqrt{\ln\left(\frac{W_0}{W}\right)} \quad (3)$$

where W_0 is the estimated maximum uptake obtained from Langmuir plot, and P_{0q} is the saturated vapour pressure of the quasi-vaporized supercritical H_2. In the high pressure region, the DR plot has a linear relationship which was used to estimate the adsorption energy βE_0 and the isosteric heat of gas adsorption (Q_{st}) at the loading of 1/e by using equation (4):

$$Q_{st}\,(1/e) = \Delta H_v + \beta E_0 \quad (4)$$

where the ΔH_V is the vaporisation heat of H_2 at its boiling point (H_2 = 0.91 kJ mol^{-1} at 20.39 K). The linear fitting of equation (3) is shown in Figure S2, and the heat of adsorption at 1/e loading is estimated as 6.5 kJ/mol.

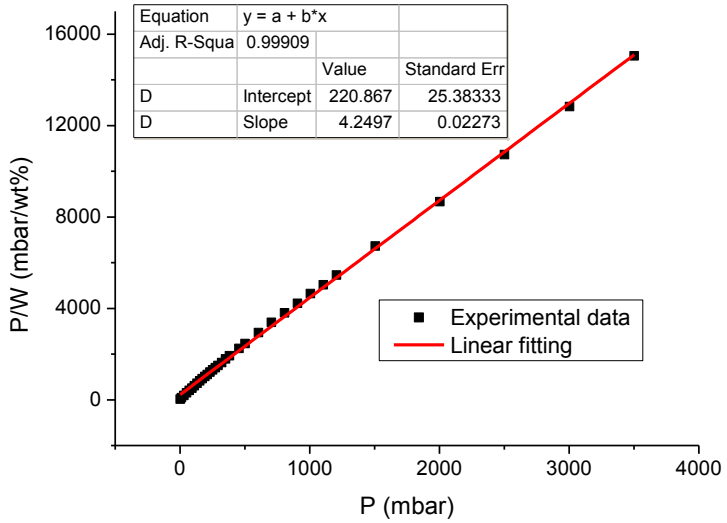

Figure S1. Linear fitting plot for H_2 adsorption isotherm of NOTT-300 by Langmuir equation.

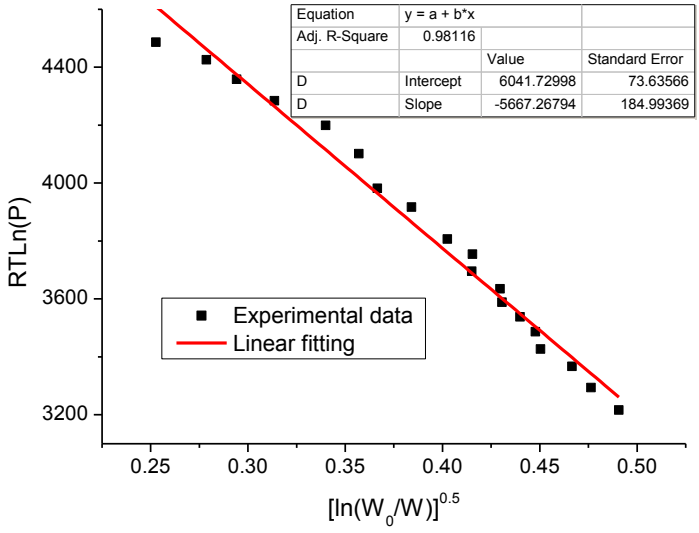

Figure S2. Linear fitting plot for H_2 adsorption isotherm of NOTT-300 by DR equation.