Electronic Supporting Information

Confined toluene within InOF-1: CO_2 capture enhancement

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1. Powder X-ray diffraction patterns of InOF-1

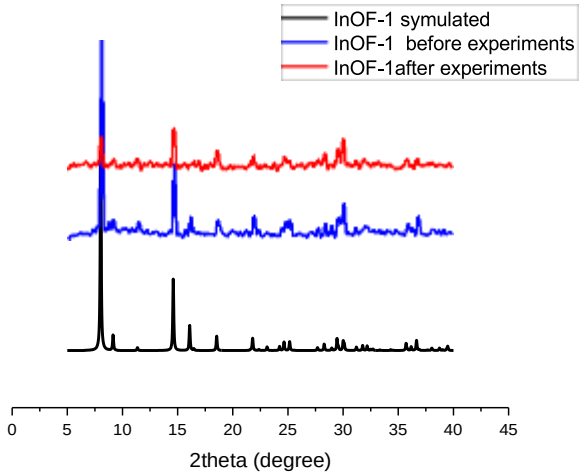

Fig. S1. Powder X-ray diffraction patterns of calculated (black); before experiments, as synthesized (blue); and after-adsorption experiments, without activation (red) InOF-1.

2. Adsorption isotherms for toluene

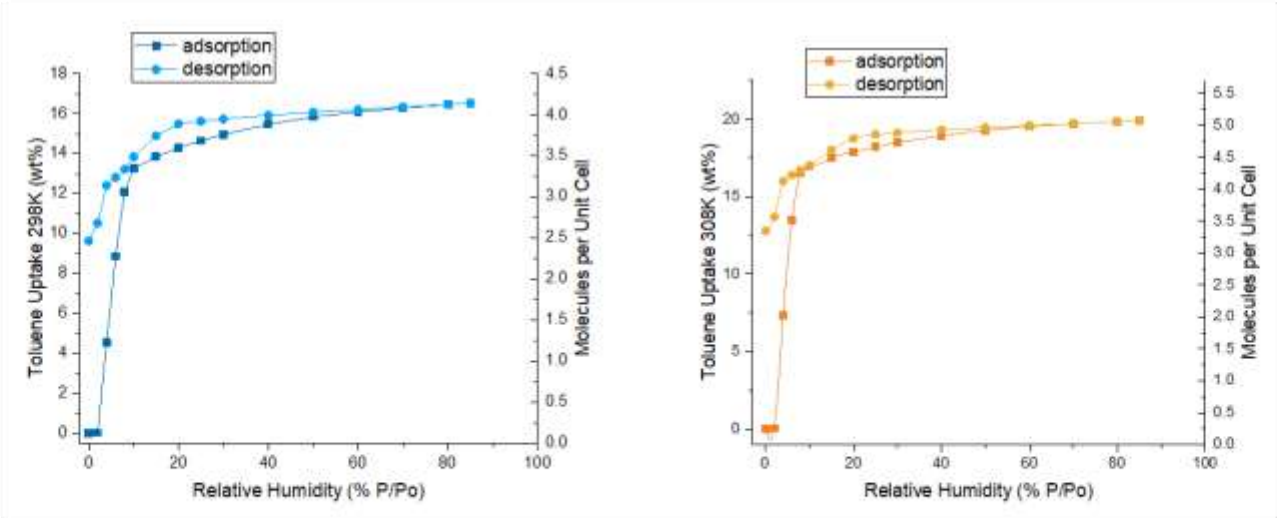

Fig. S2. Toluene adsorption isotherms at 298K (blue) and 308K (orange) for InOF-1 from *from %P/P0= 0 to 85. Squares* show adsorption phase, while circles show desorption phase

3. Derivation of the isosteric enthalpy of adsorption for toluene

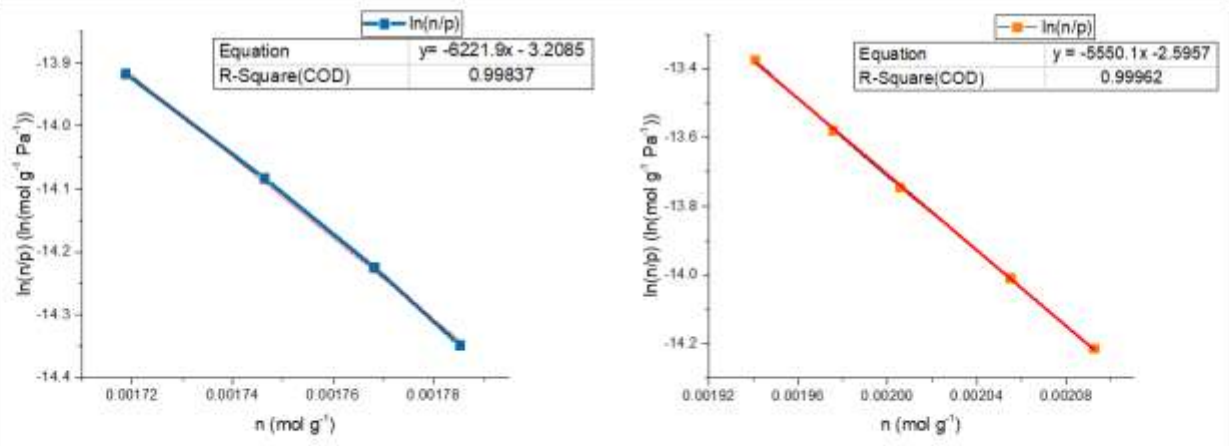

Fig. S3. Viral fitting plot for the adsorption of toluene on InOF-1 at 298 K (left) and 308 K (right)

The isosteric heat of adsorption (ΔH_{ads}) was calculated with the help of toluene adsorption isotherms using the isosteric method, $Q_{"\#}$, by fitting a virial-type equation to both 298 and 308 K toluene adsorption isotherms. The following virial-type equation was used to fit both isotherms:

$$\ln\left(\frac{n}{p}\right) = A_{-} + A_{/}n + A_0 n^0 \cdots$$

Where p is the pressure, n is the amount absorbed by the material InOF-1, and A_{-}, $A_{/}$, etc. are the virial coefficients, A_0 and higher terms can be ignored.

A plot of $\ln\left(\frac{4}{5}6\right)$ versus n should give a straight line at low surface coverage. Once obtained the plots, $Q_{"\#}$ was calculated with the help of the Clausius-Clapeyron equation, obtaining a value of 46.81 kJ mol^{-1}:

$$Q_{"\#} = R\left(\frac{8_9 * 8}{8 < 8}6\right) ln\left(\frac{>_9}{>}6\right)$$

4. Theoretical calculations

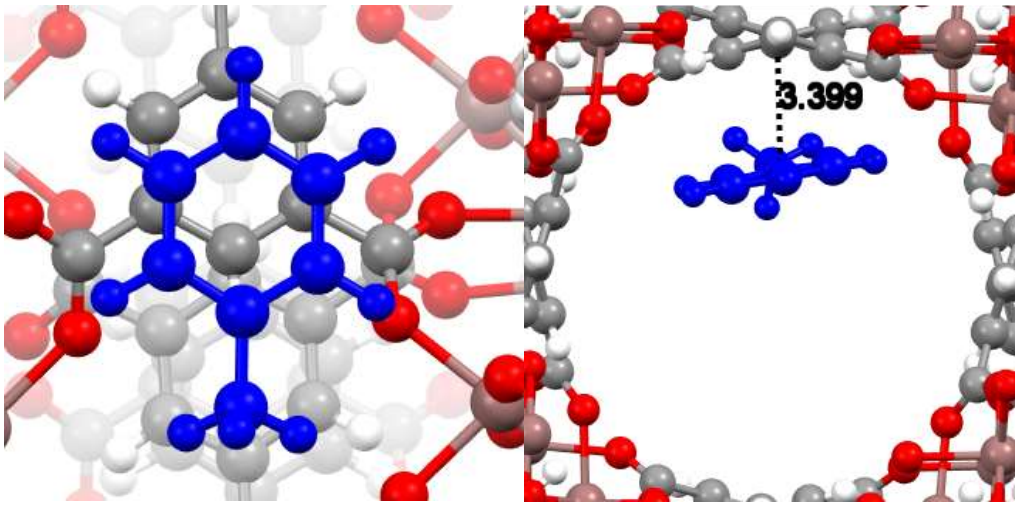

Fig. S4. Pore channel (*top*) and close up (*bottom*) views of an additional optimized structure of the toluene molecule (shown in blue) adsorbed within InOF-1 in a parallel displaced geometry. Pink, red, grey and white colors represent indium, oxygen, carbon and hydrogen atoms, correspondingly. Intermolecular distances are depicted in black (Å).

Table S1. Electron density ($\rho_{@}$), its laplacian ($\nabla^0\rho_{@}$), the kinetic and potential energy densities ratio $|V_{@}/G_{@}|$ and the electron energy density ($H_{@}$) values evaluated at the bond critical points for each contact found in the toluene@InOF-1 system. All values (a.u.) are indicative of non-covalent interactions. The strongest H···H interaction is highlighted in black.

Interaction	$\rho_{@}$	$\nabla^0\rho_{@}$	$\|V_{@}/G_{@}\|$	$H_{@}$
C···C	0.0075	0.0271	0.7	0.0014
C···C	0.0076	0.0271	0.7	0.0014
C···C	0.0076	0.0285	0.7	0.0015
C···O	0.0080	0.0286	0.7	0.0015
H···H	0.0089	0.0294	0.8	0.0013
H···H	0.0080	0.0278	0.7	0.0014
H···H	**0.0152**	**0.0491**	**0.9**	**0.0014**
C-H···O	0.0083	0.0297	0.7	0.0014
C-H···O	0.0071	0.0241	0.7	0.0014
C-H···O	0.0017	0.0064	0.7	0.0015