Supporting Information to

Adsorption of n-Alkanes in MFI and MEL: Quasi-Equilibrated Thermodesorption Combined with Molecular Simulations

by

A. Sławek, J. M. Vicent-Luna, B. Marszałek, S. R. G. Balestra, W. Makowski, S. Calero

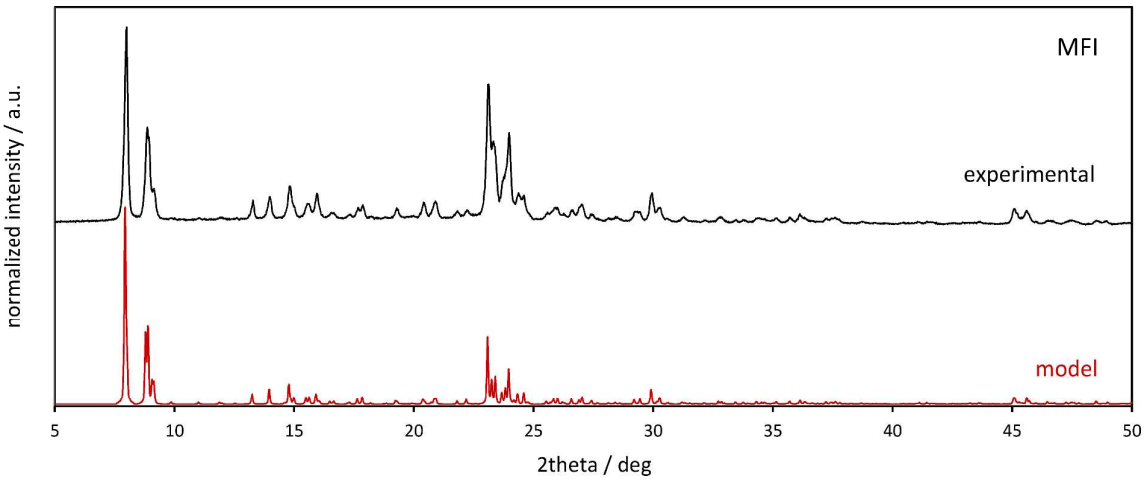

Figure S1. Comparison of the ¡experimental and modelled XRD pattern of the studied zeolite ZSM-5 based on MFI structure from IZA structure database[1].

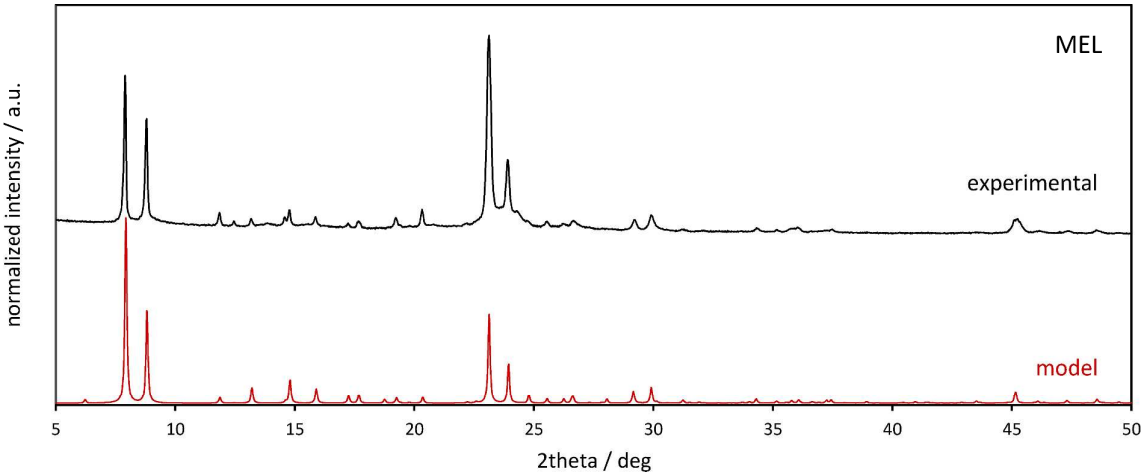

Figure S2. Comparison of the experimental and modelled XRD pattern of the studied zeolite ZSM-11 based on MEL structure from IZA structure database[2].

Table S1 Force field and model parameters used in the work

- Intermolecular interactions: Lennard-Jones parameters[3] (σ_{ij} in *Å* and ε_{ij}/k_B in *K*)

	O		$CH_3(sp^3)$		$CH_2(sp^3)$	
	σ_{ij}	ε_{ij}/k_B	σ_{ij}	ε_{ij}/k_B	σ_{ij}	ε_{ij}/k_B
$CH_3(sp^3)$	3.48	93	3.76	108	3.86	77.77
$CH_2(sp^2)$	3.58	60.5	3.86	77.77	3.96	56

- Intramolecular interactions[3]

$$U^{intra} = U^{bond} + U^{bend} + U^{torsion}$$

$$U^{bond} = \frac{1}{2}k_1(r - r_0)^2$$

$CH_x - CH_x$ $\quad k_1 / k_B = 96500\ K/Å^2$ $\quad r_0 = 1.54\ Å$ subscript *x* = 2 or 3

$$U^{bend} = \frac{1}{2}k_2(\theta - \theta_0)^2$$

$CH_x - CH_2 - CH_x$ $\quad k_2 / k_B = 62500\ K/rad^2$ $\quad \theta_0 = 114°$ subscript x = 2 or 3

$$U^{torsion} = p_0 + p_1[1 + cos\emptyset_{ijkl}] + p_2[1 - cos2\emptyset_{ijkl}] + p_3[1 + cos3\emptyset_{ijkl}]$$

$CH_x - CH_2 - CH_2 - CH_x$ $\quad p_0 / k_B = 0.0\ K$ $\quad p_1 / k_B = 335.03\ K$

$p_2 / k_B = -68.19\ K$ $\quad p_3 / k_B = 791.32\ K$

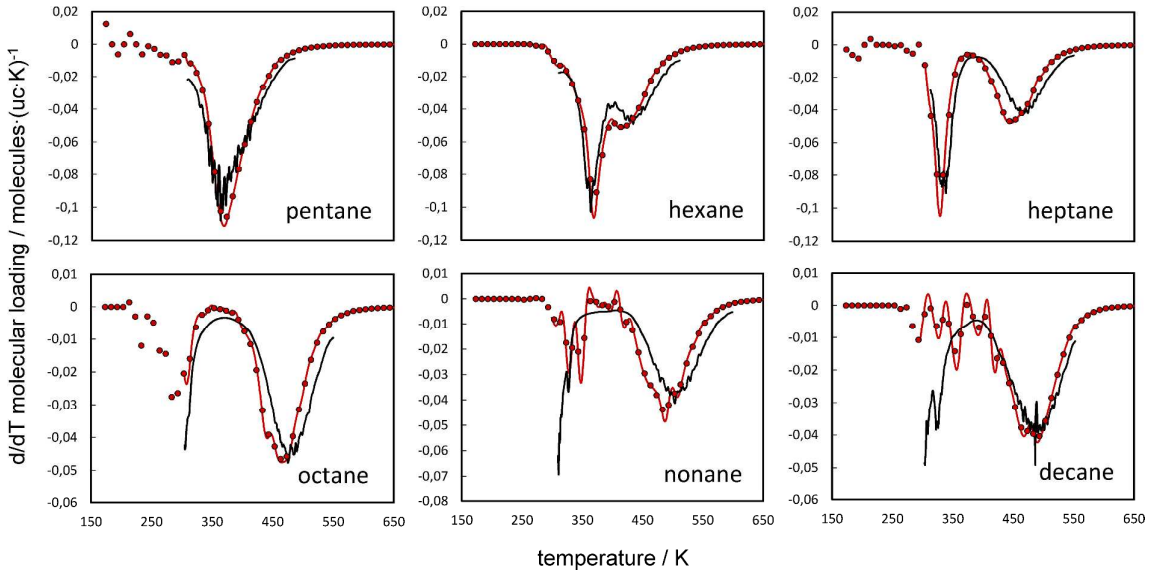

Figure S3. Temperature derivatives of the experimental (black lines) and simulated (red points) adsorption isobars of alkanes in MFI (orthorhombic). The red lines, calculated as derivatives of the spline functions interpolating the original simulated isobars, serve as guides to the eye.

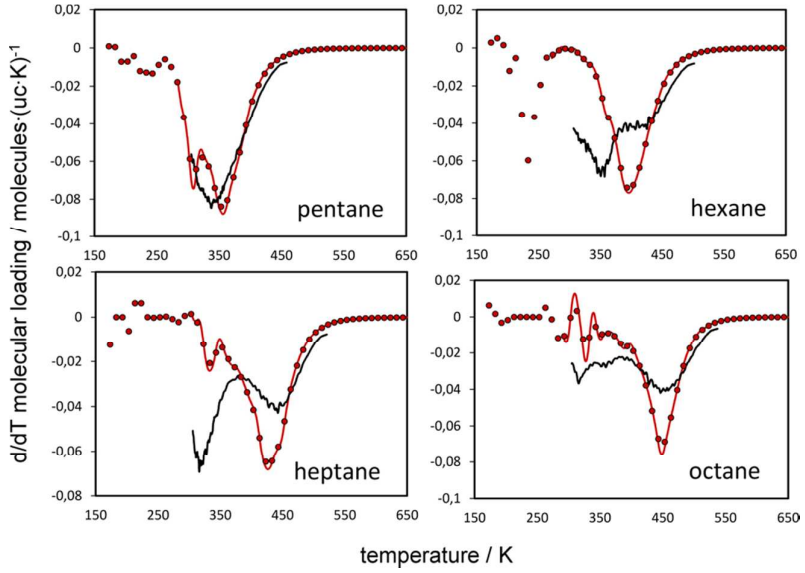

Figure S4. Temperature derivatives of the experimental (black lines) and simulated (red points) adsorption isobars of alkanes in MEL ($I\bar{4}m2$). The red lines, calculated as derivatives of the spline functions interpolating the original simulated isobars, serve as guides to the eye.

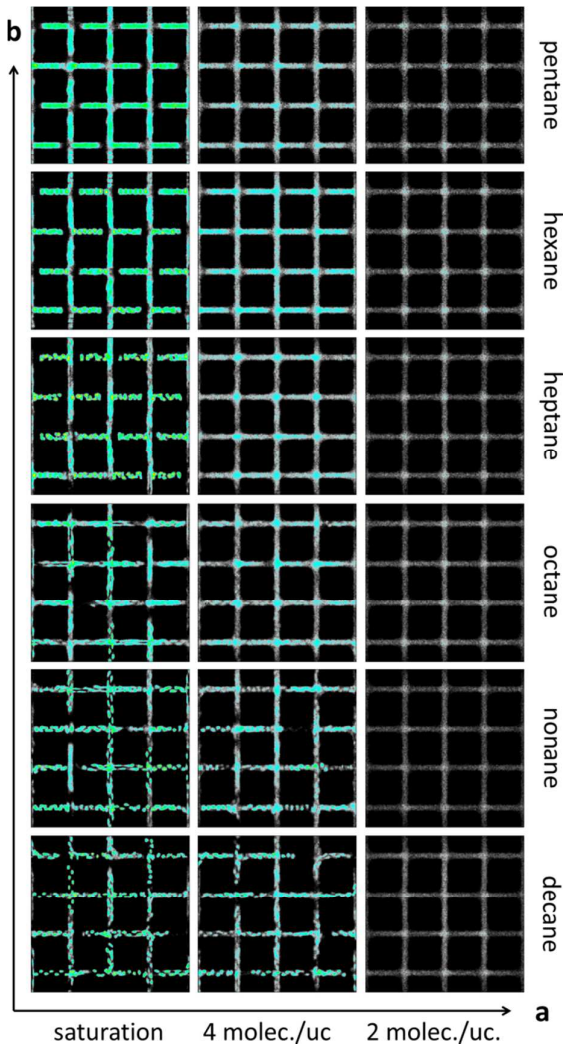

Figure S5. Average occupation profiles, MFI (orthorhombic), *xy* plane.

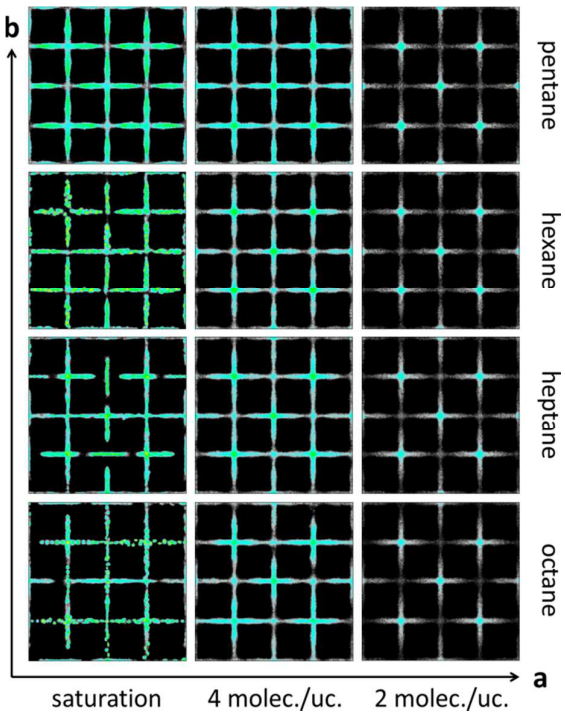

Figure S6. Average occupation profiles, MEL ($I\bar{4}m2$), *xy* plane.

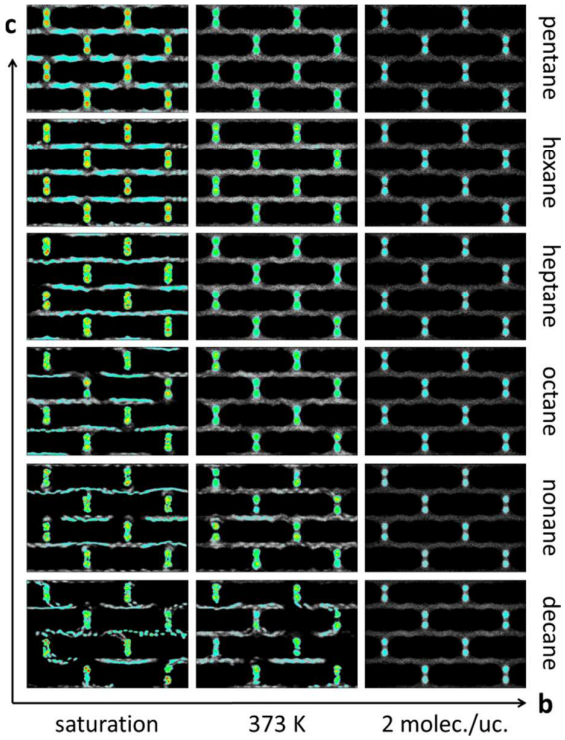

Figure S7. Average occupation profiles, MFI (orthorhombic), *yz* plane.

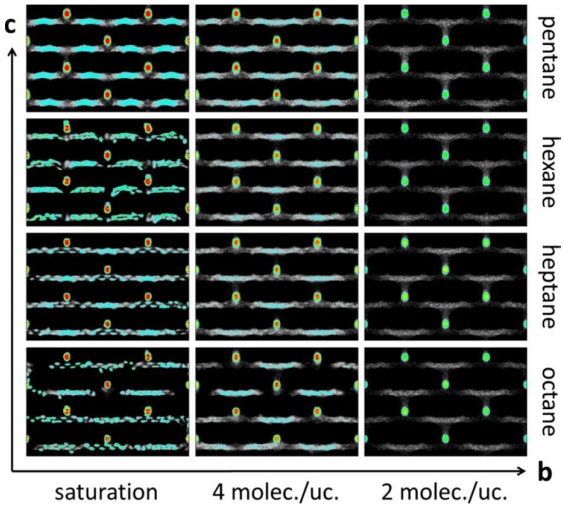

Figure S8. Average occupation profiles, MEL ($I\bar{4}m2$), *yz* plane.

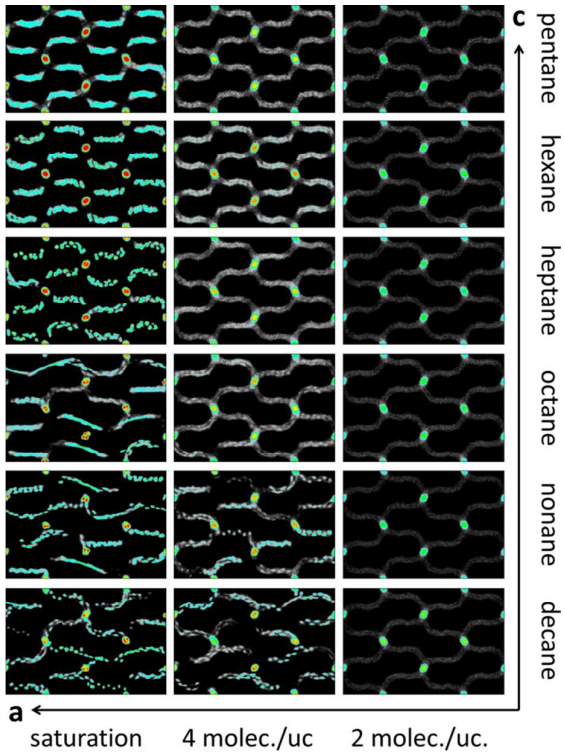

Figure S9. Average occupation profiles, MFI (orthorhombic), *zx* plane.

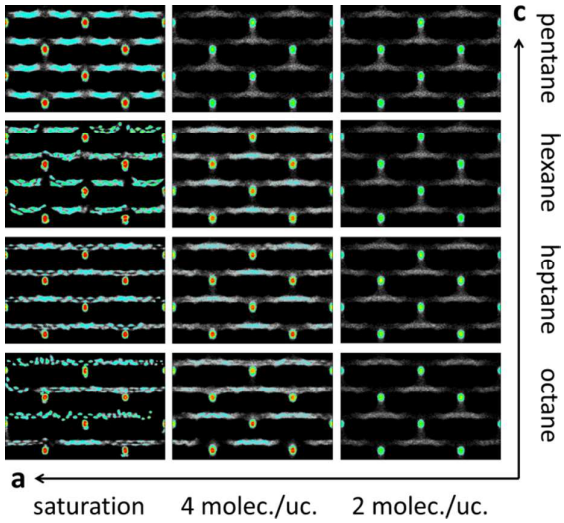

Figure S10. Average occupation profiles, MEL ($I\bar{4}m2$), *zx* plane.

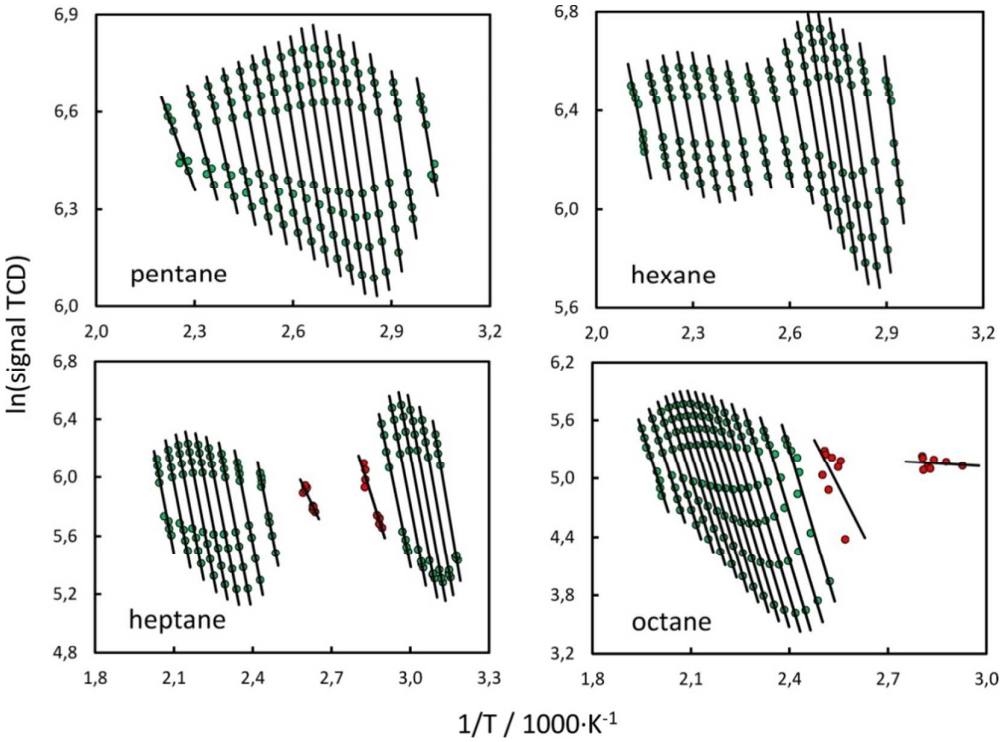

Figure S11. Experimental isosters used to calculate the isosteric heats of adsorption of n-alkanes in MFI (green dots). Excluded isosters are marked with red dots. The heating/cooling rates for pentane, hexane, heptane are 10, 8, 6, 4 °C/min and 8, 6, 4, 2 °C/min for octane.

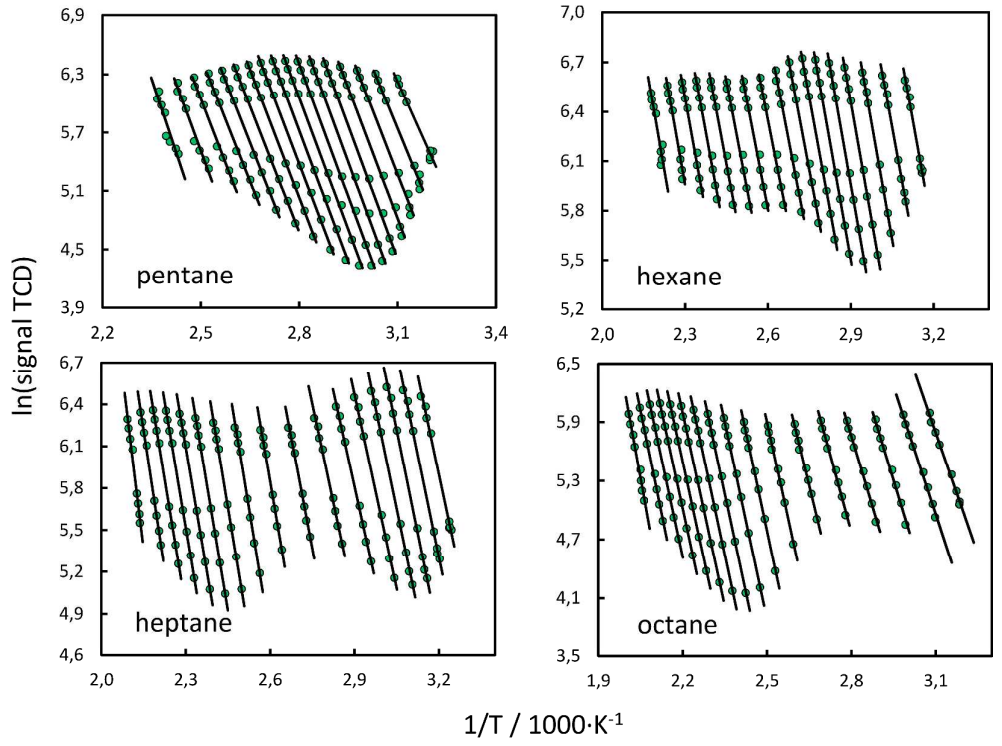

Figure S12. Experimental isosters used to calculate the isosteric heats of adsorption of n-alkanes in MEL (green dots). The heating/cooling rates for pentane, hexane, heptane are 10, 8, 6, 4 °C/min and 8, 6, 4, 2 °C/min for octane.

References

(1) van Koningsveld, H.; Jansen, J. C.; Bekkum, H. The Monoclinic Framework Structure of Zeolite ZSM-5. Comparison with the Orthorhombic Framework of as-Synthesized ZSM-5. *Zeolites* **1990**, *10*, 235–242.
(2) Terasaki, O.; Ohsuna, T.; Sakuma, H.; Watanabe, D.; Nakagawa, Y.; Medrud, R. C. Direct Observation of „Pure MEL Type" Zeolite. *Chem. Mater.* **1996**, *8*, 463–468.
(3) Dubbeldam, D.; Calero, S.; Vlugh T. J. H.; Krishna, R.; Maesen, T. L. M.; Smit, B. United Atom Force Field for Alkanes in Nanoporous Materials. *J. Phys. Chem. B* **2004**, *108*, 12301–12313