Supporting Information to accompany:

Behaviour of the Enthalpy of Adsorption in Nanoporous Materials Close to Saturation

Ariana Torres-Knoop*[1], Ali Poursaeidesfahani[2], Thijs J. H. Vlugt [2] and David Dubbeldam[1]

[1]Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, 1098XH, Amsterdam, The Netherlands
[2]Delft University of Technology, Proicess and Energy Department, Leegwaterstraat 39, 2628CB Delft, The Netherlands

March 14, 2017

*A.TorresKnoop@uva.nl

Table S1: *Variables/parameters definitions*

	General parameters
p	pressure of the system
p_0	pressure of reference state (perfect gas)
T	temperature
k_B	Boltzmann constant
β	$1/k_\mathrm{B}T$
N	number of adsorbed molecules
U	total energy of the system (host and adsorbed molecules)
ΔU	difference in the energy between the old and the new configuration
V	volume
R	gas constant (8.314464919 J mol^{-1} K^{-1})
Λ	thermal de Broglie wavelength
λ	CFCMC non-bonded interactions scaling parameter
$u_\mathrm{LJ}(r)$	Lennard Jones (LJ)energy
$u_\mathrm{Coul}(r)$	Coulombic energy
ϵ	LJ strength parameter
σ	LJ size parameter
f	fugacity of the system
μ^0_{IG}	chemical potential of the reference state (ideal gas)
ε_0	dielectric constant in vacuum
q_i, q_j	atomic charges
$\Delta\lambda_\mathrm{max}$	maximum displacement in λ-space
Δx_max	maximum displacement of the particles in the adsorbent
	Langmuir isotherm parameters
n	amount adsorbed (equilibrium loading)
m	Langmuir isotherm model saturation loading
c	Langmuir isotherm model parameter
ν	Langmuir-Freundlich isotherm model exponent (heterogeneity factor)
k_1, k_2, k_3, k_4	arbitrary constants in the temperature dependence of m and ν
A	constant in the temperature dependence of c (entropic factor)
B	constant in the temperature dependance of c (enthalpy factor)
$m1, m2$	dual-Langmuir saturation loading parameters
$c1, c2$	dual-Langmuir parameters
ν_1, ν_2	Langmuir-Freundlich isotherm model exponents
	Theoretical model
ϕ	the total potential for N particles adsorbed
r	interparticle distance (same for all neighboring particles)
$\langle N\rangle$	average number of adsorbed particles
$\langle r\rangle$	average interparticle distance
	CFCMC derivation parameters
$\langle U_g\rangle$	average energy of a single molecule in the gas phase
$\langle U_h\rangle$	average energy of the host system
$\langle\cdots\rangle_\mu$	average in the grand-canonical ensemble
$\langle\cdots\rangle_\mathrm{CFCMC}$	average in the grand-canonical CFCMC ensemble
Q_CFCMC	partition function CFCMC-ensemble
U_CFCMC	total energy of the system (including the fractional particle) obtained using CFCMC algorithm
N_CFCMC	total number of particles (including the fractional particle) obtained using the CFCMC algorithm
U_int	total energy of the integer particles in CFCMC
U_frac	total energy of the fractional particle in CFCMC
U_total	total energy of the system (integer + fractional particles), same as U_{CFCMC}??
N_int	total number of integer particles in CFCMC
$\eta(\lambda)$	biasing in λ-space
$\delta_{\lambda=0}$	Dirac delta at $\lambda = 0$
	Thermodynamic parameters
Q	heat of adsorption
$\Delta\bar{h}$	differential enthalpy of adsorption
Δh_ads	isosteric enthalpy of adsorption
ΔH	enthalpy of adsorption
ΔG	free energy between the fluid phase and the adsorbed phase
ΔS	entropy of adsorption
ΔH_imm	enthalpy changes associated with isothermal immersion
ΔH_comp	enthalpy changes associated with isothermal compression
ΔS_imm	entropy changes associated with isothermal immersion
ΔS_comp	entropy changes associated with isothermal compression
ΔG_imm	free energy changes associated with isothermal immersion
ΔG_comp	free energy changes associated with isothermal compression
ΔF_imm	helmholtz free energy changes associated with isothermal immersion
ΔF_comp	helmholtz free energy changes associated with isothermal compression
Ω	grand potential, free energy change associated with the isothermal immersion
μ_s	chemical potential of the adsorbent in its clean state in vacuo (unadsorbed)