Supplemental Material

Potential theory for gate adsorption on soft porous crystals

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Table S1 Adsorption potentials from equation (8) and those from $k_B T \ln (P_0/P_{\text{gate}})$

T^*	0.8	0.85	0.9	0.95	1.0	1.1	1.2
$A(P_{\text{gate}})$	3.46	3.45	3.46	3.47	3.50	3.55	3.59
$k_B T \ln (P_0/P_{\text{gate}})$	3.48	3.51	3.50	3.57	3.61	3.71	3.96

$T^* = k_B T / \epsilon_{\text{gg}}$ and the other values are reduced by ϵ_{gg} .

Table S2 Values of the terms in equations (19), (20), and $C_m = C + P_0 v_{\text{liq}} - P_{\text{gate}} v_{\text{guest}}$

T^*	0.8	0.85	0.9	0.95	1.0	1.1	1.2
$A(P_{\text{gate}})$	3.46	3.45	3.46	3.47	3.50	3.55	3.59
C	-3.62	-3.55	-3.46	-3.39	-3.31	-3.15	-2.99
$-u_{\text{gh}} - \Delta G_{\text{host}}/N + C$	3.44	3.44	3.45	3.46	3.45	3.45	3.45
$P_0/\rho_{\text{liq}} - P_{\text{gate}}/\rho_{\text{guest}}$	5.84×10^{-3}	4.20×10^{-3}	1.54×10^{-2}	9.68×10^{-3}	3.51×10^{-2}	6.86×10^{-2}	1.33×10^{-1}
C_m	-3.61	-3.55	-3.45	-3.38	-3.28	-3.08	-2.85
$-u_{\text{gh}} - \Delta G_{\text{host}}/N + C_m$	3.45	3.44	3.47	3.47	3.48	3.52	3.59

$T^* = k_B T / \epsilon_{\text{gg}}$ and the other values are reduced by ϵ_{gg} .

Figure S1 Comparison of the adsorption potential at the gate adsorption pressure $A(P_{\text{gate}})$: equation (8), $-u_{\text{gh}} - \Delta G_{\text{host}}/N$: the right hand side of equation (14), and $-u_{\text{gh}} - \Delta G_{\text{host}}/N + C_m$: where $C_m = C + P_0 v_{\text{liq}} - P_{\text{gate}} v_{\text{guest}}$, which are reduced by ϵ_{gg} , at $T^* = k_B T / \epsilon_{\text{gg}} = 0.8, 0.85, 0.9, 0.95, 1.0, 1.1$, and 1.2 . u_{gh} is the guest-host interaction potential per one guest molecule, $\Delta G_{\text{host}}/N$ is the Gibbs free energy change due to the host framework deformation per guest molecule, C is a correction term originating from spatial constraint of adsorbed guest molecules in the host, v_{liq} and v_{guest} are the volumes of the bulk liquid and adsorbed phase per molecule, and P_0 is the saturated vapour pressure, respectively. The v_{guest} value is the pore volume where the solid-fluid interaction potential is less than zero. The lines are guide to eyes.