Supporting Information for

Properties of Phenol Confined in Realistic Carbon Micropore Model: Experiment and Simulation

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Details of interaction energy calculations

The interaction energy between molecule pairs was calculated as the sum of interaction between pairs of centers:

$$U_{ff}(r,\omega_{1},\omega_{2}) = \sum_{i=1}^{13} \sum_{j=1}^{13} \left[U_{LJ}^{ij}(r_{ij}) + U_{electr}^{ij}(r_{ij}) \right]$$
(S1)

where *r* is the distance between molecules, ω_1 and ω_2 determine their angular orientation, r_{ij} is the distance between the pair of centers, U_{LJ}^{ij} and U_{electr}^{ij} represent the energy of dispersive and electrostatic interactions between them, respectively. The dispersive interactions are modeled using Lennard-Jones potential.^{S1} Cut-offs are realized by the switching function in a quintic form:^{S2}

$$U_{LJ}^{ij}\left(r_{ij}\right) = 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6} \right] \times S\left(r_{ij}\right)$$
(S2)

where σ_{ij} and ε_{ij} are the collision diameter and the potential well depth, respectively, and *S* is the switching function:^{S2}

$$S(r_{ij}) = \begin{cases} 1 & r_{ij} \leq r_{on} \\ -6\left(\frac{r_{ij} - r_{on}}{r_{cut} - r_{on}}\right)^{5} + 15\left(\frac{r_{ij} - r_{on}}{r_{cut} - r_{on}}\right)^{4} - 10\left(\frac{r_{ij} - r_{on}}{r_{cut} - r_{on}}\right)^{3} + 1 & r_{on} < r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases}$$
(S3)

 r_{cut} is the cut-off distance and r_{on} is the distance at which the switching function starts to apply.

The energy of electrostatic interactions is calculated using the potential proposed by Fennel and Gezelter:^{S3}

$$U_{electr}^{ij}\left(r_{ij}\right) = \begin{cases} \frac{q_{i}q_{j}}{4\pi\varepsilon_{0}} \left[\frac{\operatorname{erfc}\left(\alpha r_{ij}\right)}{r_{ij}} - \frac{\operatorname{erfc}\left(\alpha r_{cut}\right)}{r_{cut}} + \left(\frac{\operatorname{erfc}\left(\alpha r_{cut}\right)}{r_{cut}^{2}} + \frac{2\alpha}{\sqrt{\pi}} \times \frac{\exp\left(-\alpha^{2} r_{cut}^{2}\right)}{r_{cut}}\right) \left(r_{ij} - r_{cut}\right) \right] & r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases}$$

$$(S4)$$

where q_i and q_j are the values of the charges of the centers, $\varepsilon_0 = 8.8543 \times 10^{-12} \text{ C}^2/\text{J/m}$ is the dielectric permittivity of free space, and $\alpha = 2.0 \text{ nm}^{-1}$ is the damping factor.^{S3} Eq. (S4) is a simple alternative to the Ewald summation.^{S3} The same value of r_{cut} (equal to 1.5 nm) is used for both dispersive and electrostatic interactions. Additionally, the value of r_{on} is assumed as equal to 1.4 nm.

The energy of solid-fluid interactions for a molecule at a given location is calculated as the sum of dispersive interaction:

$$U_{sf} = \sum_{i=1}^{N_c} \sum_{j=1}^{13} U_{LJ}^{ij} \left(r_{ij} \right)$$
(S5)

where N_C is the number of carbon atoms in the adsorbent structure.

References

- (S1) Frenkel, D.; Smit, B. Understanding Molecular Simulation. Academic Press: San Diego, 1996.
- (S2) Lau K. F.; Alper H. E.; Thacher, T. S.; Stouch, T. R. Effects of switching functions on the behavior of liquid water in molecular dynamics simulations. *J. Phys. Chem.* 1994, 98, 8785–8792.
- (S3) Fennel, C.J.; Gezelter, D. Is the Ewald summation still necessary? Pairwise alternatives to the accepted standard for long-range electrostatics. *J Chem Phys.* 2006, 124, 234104.