Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for: "Effect of Confinement on the Adsorption Behavior of Inorganic and Organic Ions at Aqueous-Cyclohexane Interfaces: A Molecular Dynamics Study"

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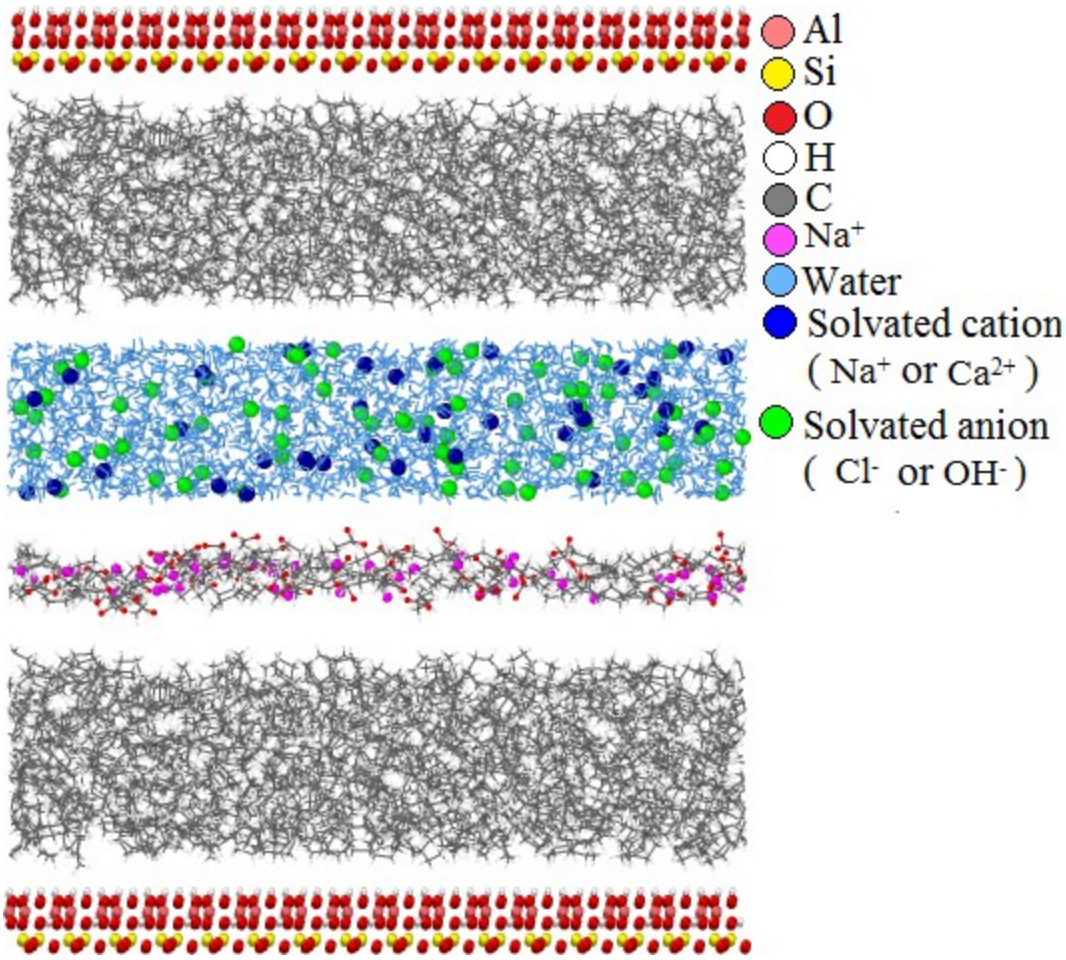

Figure $S1$**.** The initial structure, composed of kaolinite (001) surfaces (octahedral sheet at the bottom and tetrahedral sheet at the top), cyclohexane phase (1000 molecules, $28\ wt\%$ on a dry clay basis), 50 decanoate molecules (with equal number of sodium ions), and the water phase (2000 molecules, $12.12\ wt\%$ on a dry clay basis) with 0.5 or $1.0\ M$ concentration of NaCl, NaOH, $CaCl_2$ or $Ca(OH)_2$.

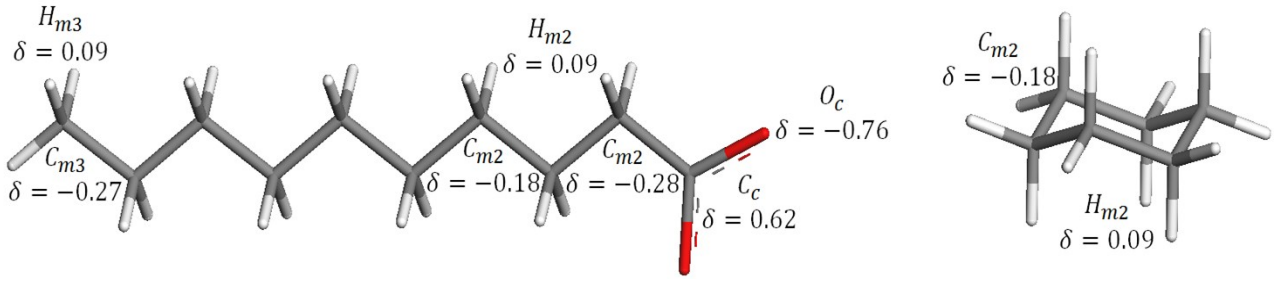

Table $S1$**.** Non-bond and bond parameters for hydroxide [47], cyclohexane and decanoate [52]

Non-bonded Interactions ($12-6$ **LJ)**		
Atom Type	$\varepsilon\ (kcal/mol)$	σ (Å)
$O_h(O_{hydroxide})$	0.161	3.670
$O_c(O_{carboxylate})$	0.120	3.029
$C_c(C_{carboxylate})$	0.070	3.564
$C_{m2}(C_{methylene-bridge})$	0.056	3.581
$C_{m3}(C_{methyl})$	0.078	3.653
$H_{m2}(H_{methylene-bridge})$	0.035	2.388
$H_{m3}(H_{methyl})$	0.024	2.388
Bonded Interactions		
Harmonic Bond $\left[E_b = K_b(r-r_0)^2\right]$	$K_b\left(kcal/(mol\ Å^2)\right)$	r_0 (Å)
$O_h - H_h$	---	1.00
$O_c - C_c$	525.000	1.26
$C_c - C_{m2}$	200.000	1.52
$C_{m2} - C_{m3}$	222.500	1.53
$C_{m2} - H_{m2}$	309.000	1.11
$C_{m3} - H_{m3}$	322.000	1.11
Harmonic Angle $\left[E_b = K_b(r-r_0)^2\right]$	$K_a\left(kcal/(mol\ rad^2)\right)$	$\theta\ (degrees)$
$O_c - C_c - O_c$	100.00	128.00
$O_c - C_c - C_{m2}$	40.00	116.00
$C_c - C_{m2} - C_{m2}$	52.00	108.00
$C_c - C_{m2} - H_{m2}$	33.00	109.50
$C_{m2} - C_{m2} - C_{m2}$	58.35	113.60
$C_{m2} - C_{m2} - H_{m2}$	26.50	110.10
$H_{m2} - C_{m2} - H_{m2}$	35.50	109.00
$C_{m2} - C_{m2} - C_{m3}$	58.00	115.00
$H_{m2} - C_{m2} - C_{m3}$	34.60	110.10
$C_{m2} - C_{m3} - H_{m3}$	34.60	110.10
$H_{m3} - C_{m3} - H_{m3}$	35.50	108.40

Table $S1$ - Continued

Bonded Interactions			
Charmm Dihedral $[E_d = K_d(1 + cos(n\varphi - d))]$	$K_d(kcal/mol)$	n	d
$O_c - C_c - C_{m2} - C_{m2}$	0.050	6	180
$O_c - C_c - C_{m2} - H_{m2}$	0.05	6	180
$C_c - C_{m2} - C_{m2} - C_{m2}$	0.065	2	0
$C_c - C_{m2} - C_{m2} - H_{m2}$	0.195	3	0
$C_{m2} - C_{m2} - C_{m2} - H_{m2}$	0.195	3	0
$H_{m2} - C_{m2} - C_{m2} - H_{m2}$	0.220	3	0
$C_{m2} - C_{m2} - C_{m2} - C_{m3}$	0.151	2	0
$H_{m2} - C_{m2} - C_{m2} - C_{m3}$	0.180	3	0
$C_{m2} - C_{m2} - C_{m3} - H_{m3}$	0.160	3	0
$H_{m2} - C_{m2} - C_{m3} - H_{m3}$	0.160	3	0

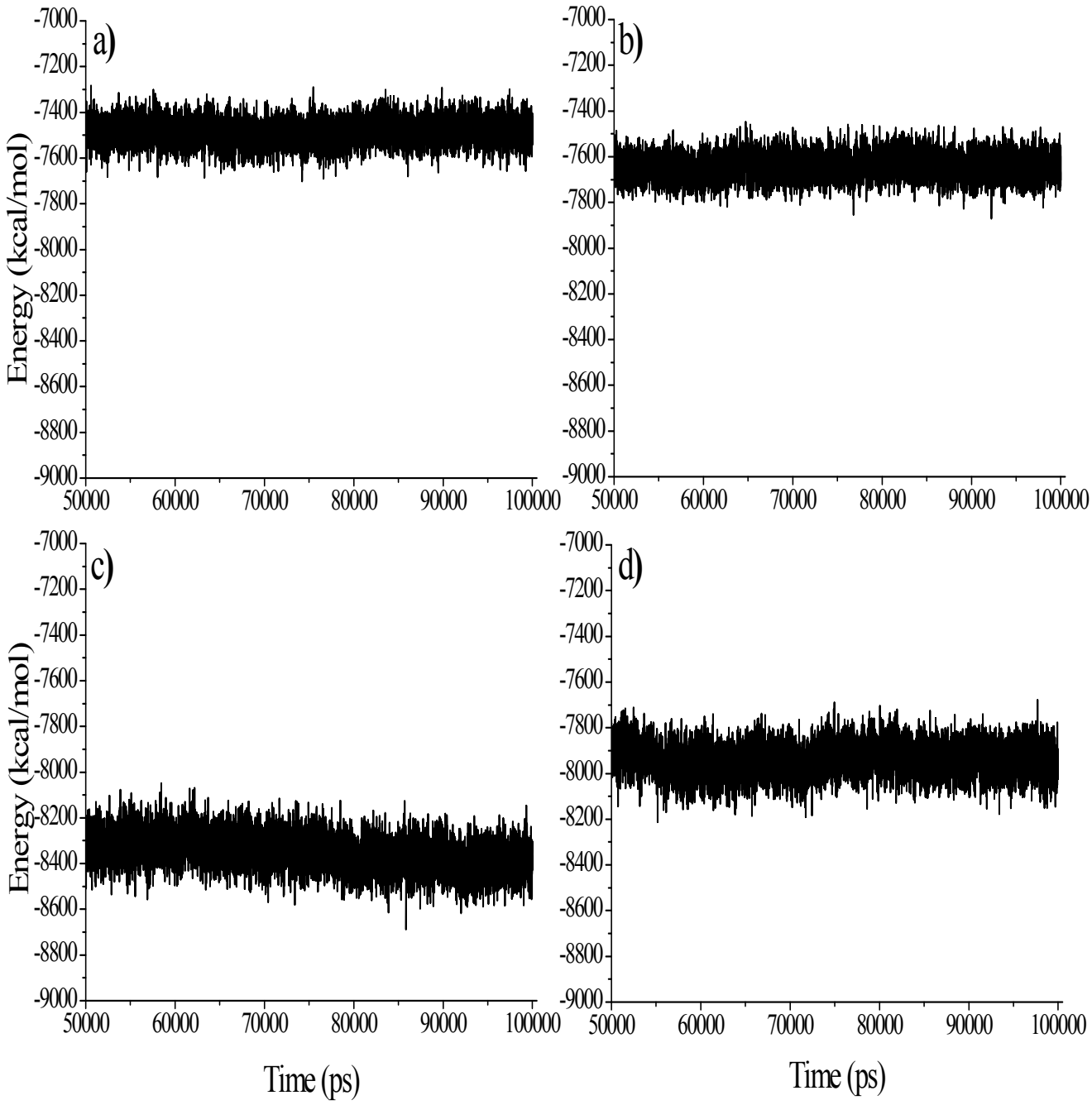

Figure $S2$**.** Potential-energy profile of the decanoate head-group oxygens in the presence of $1.0\ M$ solution of a) NaCl, b) NaOH, c) $CaCl_2$ and d) $Ca(OH)_2$ in between kaolinite surfaces.