Supplementary Information

for

Interfacial Solvation and Slow Transport of Hydrated Excess Protons in Non-ionic Reverse Micelles

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1. Simulation Details

The following table (Table S1) shows the parameters for MS-RMD 5. Detailed explanation of the definition of each parameter can be found in ref [1].

Table S1. Parameters for MS-RMD 5.

D_{OH}	79.0864	kcal/mol		C	4.8104436742	kcal/mol
a_{OH}	2.0834	Å^{-1}		c	0.8789513630	Å^{-1}
R^0_{OH}	0.98	Å		d^0_{OH}	1.0	Å
k_a	77.4868	kcal/mol/rad^2		V^{ij}_{const}	−26.8448507041	kcal/mol
a_0	111.7269	deg		$q^{\mathrm{ex}}_{\mathrm{O}}$	−0.0895456	e
$\varepsilon_{\mathrm{O^*O^*}}$	0.098609686	kcal/mol		$q^{\mathrm{ex}}_{\mathrm{H}}$	0.0252683	e
$\sigma_{\mathrm{O^*O^*}}$	3.118508	Å		$q^{\mathrm{ex}}_{\mathrm{H^*}}$	0.0780180	e
$\varepsilon_{\mathrm{H^*H^*}}$	0.000 040 458	kcal/mol		γ	0.9255057577	Å^{-2}
$\sigma_{\mathrm{H^*H^*}}$	0.0	Å		P	0.6709512773	
$\varepsilon_{\mathrm{O^*H_W}}$	1.5	k		k	4.3082944586	Å^{-2}
$\sigma_{\mathrm{O^*H_W}}$	1.6	Å		D_{OO}	2.7665199244	Å
$q^{\mathrm{H_3O^+}}_{\mathrm{O}}$	−0.32	e		β	5.5765348350	Å^{-1}
$q^{\mathrm{H_3O^+}}_{\mathrm{H}}$	0.44	e		R^0_{OO}	3.0571843103	Å
B	12.8946159531	kcal/mol		P'	5.7250801272	Å^{-1}
b	0.9652626593	Å^{-1}		a	7.2620326328	Å^{-1}
b'	2.9007507545	Å^{-2}		r^0_{OO}	1.7870085767	Å

d_{OO}^{0}	2.4	Å				

The following figure (Figure S1) shows the charges generated from *ab initio* calculations by R.E.D. Server for the atoms in the surfactant molecules. The parameters of bonds, angles and dihedrals are from General Amber Force Field (GAFF). Information about GAFF can be found in ref [2].

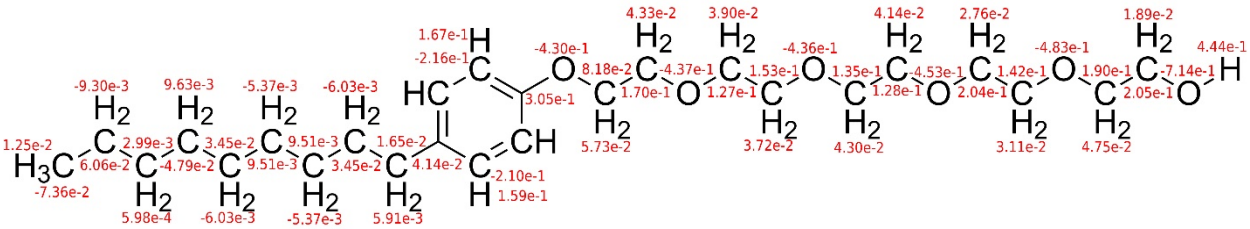

Figure S1. Charge of each atom in the surfactant molecule, generated by R.E.D. server.

The following table (Table S2) shows the parameters for aSPC/fw water model used in this research. Detailed explanation of the definition of each parameter can be found in ref [3].

Table S2. Parameters for aSPC/fw water model.

r_{OH}^{eq}	0.995	Å
D_{OH}	116.09	kcal/mol
α_{OH}	2.287	$Å^{-1}$
K_{HOH}	75.9	kcal/mol/rad^2
θ_{HOH}^{eq}	112.5	deg
q_O	-0.8350	e
q_H	0.4175	e
ϵ_{OO}	0.1554253	kcal/mol
σ_{OO}	3.165492	Å

References:

[1] Chen, C., Arntsen, C., & Voth, G. A. (2017). Development of reactive force fields using ab initio molecular dynamics simulation minimally biased to experimental data. *The Journal of Chemical Physics*, *147*, 161719.

[2] Wang, J., Wolf, R. M., Caldwell, J. W., Kollman, P. A., & Case, D. A. (2004). Development and testing of a general amber force field. *Journal of Computational Chemistry*, *25*, 1157-1174.

[3] Wu, Y., Tepper, H. L., & Voth, G. A. (2006). Flexible simple point-charge water model with improved liquid-state properties. *The Journal of Chemical Physics*, *124*, 024503.