Title

Unveiling the hydrophilic nature of SDS surfactant through molecular simulations: Exploring the influence of charge distribution on interfacial properties in the vacuum/SDS/water system

Abstract

The hydrophilicity of SDS surfactant was evaluated using different charge distributions derived from atomic charges obtained by quantum mechanical calculations. The atomic charges were determined using the Hirshfeld, CM5, CHELPG, and Merz-Kollman methods. The results indicate that the correct charge distribution in the hydrophilic group has an impact on the description of the surfactant hydrophilicity, which allows us to obtain a good estimation of the interfacial properties of the vacuum/SDS/water system. Two models of charge distribution based on the point charge model were proposed for SDS surfactant, using atomic charges computed through Quantum Mechanical calculations. The charge distributions derived from CM5, Merz-Kollman, and CHELPG atomic charges consistently predict the interfacial properties such as: area occupied per molecule, interfacial thicknesses, and radial distribution functions. Using Molecular Dynamics simulations, the ability of the charge distributions combined with nonbonded parameters of the GROMOS53A6 force field to predict the interfacial properties has the following order: CM5 > Merz-Kollman ≈ CHELPG > Hirshfeld. In contrast, the charge distributions overestimated the reduction of the interfacial tension of the vacuum/SDS/water system. Interfacial properties such as interfacial tension, area occupied per SDS molecule, and molecular interaction between the hydrophilic headgroup and water molecules were evaluated. Simulations demonstrated that the high interfacial activity of the SDS surfactant is associated with the high negative charge distribution defined for the hydrophilic headgroup of the surfactant, which

enhances the ability to attract water molecules and the solvation of the hydrophilic region. © 2024 Elsevier B.V.

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Index Keywords

Atoms; Charge distribution; Distribution functions; Hydrophilicity; Molecular structure; Molecules; Quantum theory; Surface active agents; Atomic charge; Hydrophilic headgroups; Hydrophilics; Interfacial property; Molecular simulations; QM calculation; Quantum-mechanical calculation; SDS surfactants; Water molecule; Water system; Molecular dynamics

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References

Rosen M.J., Kunjappu J.T., (2012); Qi N., Chen Z., Zhao H., Wang Q., Chen H., Yuan H., Li Y., Predicting and controlling the effect of solubilized flavor oil on foam properties of surfactant through study of the adsorption activity and configuration, J. Surfactants Deterg., 23, pp. 347-358, (2020); Wei Y., Wang X., Dong L., Liu G., Xia Q., Yuan S., Molecular dynamics study on the effect of surfactant mixture on their packing states in mixed micelles, Colloids Surf. A Physicochem. Eng. Asp., 631, (2021); Duan M., Ding Z., Wang H., Xiong Y., Fang S., Shi P., Liu S., Evolution of oil/water interface in the presence of SDBS detected by dual polarization

interferometry, Appl. Surf. Sci., 427, pp. 917-926, (2018); Kumar V., Pal N., Jangir A.K., Manyala D.L., Varade D., Mandal A., Kuperkar K., Dynamic interfacial properties and tuning aqueous foamability stabilized by cationic surfactants in terms of their structural hydrophobicity, free drainage and bubble extent, Colloids Surfaces A Physicochem. Eng. Asp., 588, (2020); Al Yousef Z.A., Almobarky M.A., Schechter D.S., Surfactant and a mixture of surfactant and nanoparticles to stabilize CO2/brine foam, control gas mobility, and enhance oil recovery, J. Pet. Explor. Prod. Technol., 10, pp. 439-445, (2020); Almobarky M.A., AlYousif Z., Schechter D., Gas/water foams stabilized with a newly developed anionic surfactant for gas mobility control applications, Pet. Sci., 17, pp. 1025-1036, (2020); Ma L., Zhu M., Liu T., Effects of chain length of surfactants and their adsorption on nanoparticles on stability of CO2-in-water emulsions, Colloids Surf. A Physicochem. Eng. Asp., 644, (2022); Su L., Sun J., Ding F., Gao X., Zheng L., Molecular insight into photoresponsive surfactant regulated reversible emulsification and demulsification processes, J. Mol. Liq., 335, (2021); Burlatsky S.F., Atrazhev V.V., Dmitriev D.V., Sultanov V.I., Timokhina E.N., Ugolkova E.A., Tulyani S., Vincitore A., Surface tension model for surfactant solutions at the critical micelle concentration, J. Colloid Interface Sci., 393, pp. 151-160, (2013); Tadros T.F., Physical chemistry of surfactant solutions, Appl. Surfactants, (2005); Calvo E., Bravo R., Amigo A., Gracia-Fadrique J., Dynamic surface tension, critical micelle concentration, and activity coefficients of aqueous solutions of nonyl phenol ethoxylates, Fluid Phase Equilib., 282, pp. 14-19, (2009); Wang C., Morgner H., Effects of counterions on adsorption behavior of anionic surfactants on solution surface, Langmuir, 26, pp. 3121-3125, (2010); Ivanov I.B., Ananthapadmanabhan K.P., Lips A., Adsorption and structure of the adsorbed layer of ionic surfactants, Adv. Colloid Interface Sci., 123-126, pp. 189-212, (2006); Yazhgur P., Vierros S., Hannoy D., Sammalkorpi M., Salonen A., Surfactant interactions and organization at the gas-water Interface (CTAB with added salt), Langmuir, 34, pp. 1855-1864, (2018); Wang L., Drainage and rupture of thin foam

films in the presence of ionic and non-ionic surfactants, Int. J. Miner. Process., 102-103, pp. 58-68, (2012); Tagashira H., Takata Y., Hyono A., Ohshima H., Adsorption of surfactant ions and binding of their counterions at an air/water interface, J. Oleo Sci., 58, pp. 285-293, (2009); Li J., Wang J., Zhao Y., Zhou P., Carter J., Li Z., Waigh T.A., Lu J.R., Xu H., Surfactant-like peptides: From molecular design to controllable self-assembly with applications, Coord. Chem. Rev., 421, (2020); Petkov J.T., Tucker I.M., Penfold J., Thomas R.K., Petsev D.N., Dong C.C., Golding S., Grillo I., The impact of multivalent counterions, Al3+, on the surface adsorption and self-assembly of the anionic surfactant alkyloxyethylene sulfate and anionic/nonionic surfactant mixtures, Langmuir, 26, pp. 16699-16709, (2010); Johnson C.M., Tyrode E., Study of the adsorption of sodium dodecyl sulfate (SDS) at the air/water interface: Targeting the sulfate headgroup using vibrational sum frequency spectroscopy, Phys. Chem. Chem. Phys., 7, pp. 2635-2640, (2005); Pan H., Sun Y., Cao L., Li D., Sun K., Song X., Cao X., Li Y., Study of the interfacial array behaviour of surfactant at very low concentration by second harmonic generation and molecular dynamic simulation, Optik (Stuttg)., 130, pp. 1445-1453, (2017); Phan C.M., (2018); Peng M., Nguyen A.V., Adsorption of ionic surfactants at the air-water interface: the gap between theory and experiment, Adv. Colloid Interface Sci., 275, pp. 1-20, (2020); Peng M., Duignan T.T., Nguyen A.V., Significant effect of surfactant adsorption layer thickness in equilibrium foam films, J. Phys. Chem. B, 124, pp. 5301-5310, (2020); Nguyen K.T., Nguyen A.V., New evidence of head-to-tail complex formation of SDS-DOH mixtures adsorbed at the air-water Interface as revealed by vibrational sum frequency generation spectroscopy and isotope labelling, Langmuir, 35, pp. 4825-4833, (2019); Ivanov I.B., Marinova K.G., Danov K.D., Dimitrova D., Ananthapadmanabhan K.P., Lips A., Role of the counterions on the adsorption of ionic surfactants, Adv. Colloid Interface Sci., 134-135, pp. 105-124, (2007); Bahramian A., Zarbakhsh A., Interfacial equation of state for ionized surfactants at oil/water interfaces, Soft Matter, 11, pp. 6482-6491, (2015); Dehghan

A.A., Masihi M., Ayatollahi S., Phase behavior and interfacial tension evaluation of a newly designed surfactant on heavy oil displacement efficiency; effects of salinity, wettability, and capillary pressure, Fluid Phase Equilib., 396, pp. 20-27, (2015); Fainerman V.B., Aksenenko E.V., Kovalchuk V.I., Mucic N., Javadi A., Liggieri L., Ravera F., Loglio G., Makievski A.V., Schneck E., Miller R., New view of the adsorption of surfactants at water/alkane interfaces – competitive and cooperative effects of surfactant and alkane molecules, Adv. Colloid Interface Sci., 279, (2020); Tostado C.P., Xu J.H., Du A.W., Luo G.S., Experimental study on dynamic interfacial tension with mixture of SDS-PEG as surfactants in a coflowing microfluidic device, Langmuir, 28, pp. 3120-3128, (2012); Qazi M.J., Schlegel S.J., Backus E.H.G., Bonn M., Bonn D., Shahidzadeh N., Dynamic surface tension of surfactants in the presence of high salt concentrations, Langmuir, 36, pp. 7956-7964, (2020); Fainerman V.B., Aksenenko E.V., Kovalchuk V.I., Mucic N., Javadi A., Liggieri L., Ravera F., Loglio G., Makievski A.V., Schneck E., Miller R., New view of the adsorption of surfactants at water/alkane interfaces – competitive and cooperative effects of surfactant and alkane molecules, Adv. Colloid Interface Sci., 279, (2020); Sett S., Karakashev S.I., Smoukov S.K., Yarin A.L., Ion-specific effects in foams Ion-specific effects in foams, Adv. Colloid Interface Sci., 225, pp. 98-113, (2015); Mumtaz M., Tan I.M., Mushtaq M., Synergistic effects of surfactants mixture for foam stability measurements for enhanced oil recovery applications, Soc. Pet. Eng. - SPE Saudi Arab. Sect. Annu. Tech. Symp. Exhib., (2015); Briceno-Ahumada Z., Maldonado A., Imperor-Clerc M., Langevin D., On the stability of foams made with surfactant bilayer phases, Soft Matter, 12, pp. 1459-1467, (2016); Kamal M.S., Hussein I.A., Sultan A.S., Review on surfactant flooding: Phase behavior, retention, IFT, and field applications, Energy Fuel, 31, pp. 7701-7720, (2017); James-Smith M.A., Alforda K., Shah D.O., A novel method to quantify the amount of surfactant at the oil/water interface and to determine total interfacial area of emulsions, J. Colloid Interface Sci., 310, pp. 590-598, (2007); Dominguez H., Computer simulation studies

of surfactant monolayer mixtures at the water/oil interface: Charge distribution effects, J. Colloid Interface Sci., 274, pp. 665-672, (2004); Zhang G., Chen Y., Sui X., Kang M., Feng Y., Yin H., Nonionic surfactant stabilized polytetrafluoroethylene dispersion: Effect of molecular structure and topology, J. Mol. Liq., 345, (2022); Abdel-Azeim S., Revisiting OPLS-AA force field for the simulation of anionic surfactants in concentrated electrolyte solutions, J. Chem. Theory Comput., 16, pp. 1136-1145, (2020); Farafonov V.S., Lebed A.V., Developing and validating a set of all-atom potential models for sodium dodecyl sulfate, J. Chem. Theory Comput., 13, pp. 2742-2750, (2017); Taddese T., Anderson R.L., Bray D.J., Warren P.B., Recent advances in particle-based simulation of surfactants, Curr. Opin. Colloid Interface Sci., 48, pp. 137-148, (2020); Matsumiya M., Hata K., Tsunashima K., Self-diffusion behaviors of ionic liquids by MD simulation based on united-atom force field introduced charge scaling by ab initio MO simulation, J. Mol. Liq., 203, pp. 125-130, (2015); Barbosa G.D., Liu X., O'Harra K.E., Bara J.E., Turner C.H., Charge scaling parameter evaluation for multivalent ionic liquids with fixed point charge force fields, J. Ion. Liq., 2, (2022); Riniker S., Fixed-charge atomistic force fields for molecular dynamics simulations in the condensed phase: An overview, J. Chem. Inf. Model., 58, pp. 565-578, (2018); Wang Z., Li P., Ma K., Chen Y., Campana M., Penfold J., Thomas R.K., Roberts D.W., Xu H., Petkov J.T., Yan Z., Impact of molecular structure, headgroup and alkyl chain geometry, on the adsorption of the anionic ester sulfonate surfactants at the air-solution interface, in the presence and absence of electrolyte, J. Colloid Interface Sci., 544, pp. 293-302, (2019); Xu Z., He Z., Quan X., Sun D., Miao Z., Yu H., Yang S., Chen Z., Zeng J., Zhou J., Molecular simulations of charged complex fluids: A review, Chin. J. Chem. Eng., 31, pp. 206-226, (2021); Zhao G.X., Zhu B.Y., Dou Z.P., Yan P., Xiao J.X., Effect of charge distribution along surfactant molecules on physico-chemical properties of surfactant systems, Colloids Surf. A Physicochem. Eng. Asp., 327, pp. 122-126, (2008); Fizer M., Fizer O.; Aspects P.P., Chapter 3 Hydrophile-lipophile balance of surfactants 3, (2000); Yamashita Y.,

Sakamoto K., Hydrophilic-lipophilic balance (HLB): Classical indexation and novel indexation of surfactant, Encycl. Biocolloid Biointerface Sci. 2V Set., 1, pp. 570-574, (2016); Nakahara H., Shibata O., Moroi Y., Examination of surface adsorption of cetyltrimethylammonium bromide and sodium dodecyl sulfate, J. Phys. Chem. B, 115, pp. 9077-9086, (2011); Casandra A., Chung M.C., Noskov B.A., Lin S.Y., Adsorption kinetics of sodium dodecyl sulfate on perturbed air-water interfaces, Colloids Surf. A Physicochem. Eng. Asp., 518, pp. 241-248, (2017); Dominguez H., Rivera M., Mixtures of sodium dodecyl sulfate/dodecanol at the air/water interface by computer simulations, Langmuir, 21, pp. 7257-7262, (2005); Shi L., Tummala N.R., Striolo A., C12E6 and SDS surfactants simulated at the vacuum?water interface, Langmuir, 26, pp. 5462-5474, (2010); Wang C., Jiang Z., Xu L., Kan A., Fu H., Lin X., Surface structure of aqueous ionic surfactant solutions and effects of solvent therein—A computer simulation study, Colloid Polym. Sci., 294, pp. 575-581, (2016); Zhang J., Zhang H., Wu T., Wang Q., Van Der Spoel D., Comparison of implicit and explicit solvent models for the calculation of solvation free energy in organic solvents, J. Chem. Theory Comput., 13, pp. 1034-1043, (2017); Bresme F., Chacon E., Martinez H., Tarazona P., Adhesive transitions in Newton black films: A computer simulation study, J. Chem. Phys., 134, (2011); Bresme F., Artacho E., Electronic structure computations of Newton black films, J. Mater. Chem., 20, pp. 10351-10358, (2010); Truong V.N.T., Wang X., Dang L.X., Miller J.D., (2019); Chen M.L., Wang Z.W., Tao F.M., DFT investigation of alkyl sulfate surfactant adsorption at the air-water interface, J. Dispers. Sci. Technol., 30, pp. 185-189, (2009); Chen M., Wang Z., Wang H., Zhang G., Tao F., Investigation of adsorption of surfactant at the air-water interface with quantum chemistry method, Chin. Sci. Bull., 52, pp. 1451-1455, (2007); Paluch A.S., Cryan D.D., Maginn E.J., Predicting the solubility of the sparingly soluble solids 1,2,4,5-tetramethylbenzene, phenanthrene, and fluorene in various organic solvents by molecular simulation, J. Chem. Eng. Data, 56, pp. 1587-1595, (2011); Lebecque S., Crowet J.M., Nasir M.N., Deleu M., Lins L.,

Molecular dynamics study of micelles properties according to their size, J. Mol. Graph. Model., 72, pp. 6-15, (2017); Sammalkorpi M., Karttunen M., Haataja M., Structural properties of ionic detergent aggregates: A large-scale molecular dynamics study of sodium dodecyl sulfate, J. Phys. Chem. B, 111, pp. 11722-11733, (2007); Chun B.J., Il Choi J., Jang S.S., Molecular dynamics simulation study of sodium dodecyl sulfate micelle: Water penetration and sodium dodecyl sulfate dissociation, Colloids Surf. A Physicochem. Eng. Asp., 474, pp. 36-43, (2015); Tang X., Koenig P.H., Larson R.G., Molecular dynamics simulations of sodium dodecyl sulfate micelles in water - The effect of the force field, J. Phys. Chem. B, 118, pp. 3864-3880, (2014); Hirshfeld F.L., Bonded-atom fragments for describing molecular charge densities, Theor. Chim. Acta, 44, pp. 129-138, (1977); Marenich A.V., Jerome S.V., Cramer C.J., Truhlar D.G., Charge model 5: An extension of Hirshfeld population analysis for the accurate description of molecular interactions in gaseous and condensed phases, J. Chem. Theory Comput., 8, pp. 527-541, (2012); Singh U.C., Kollman P.A.; Breneman C.M., Wiberg K.B.; Oostenbrink C., Soares T.A., Van Der Vegt N.F.A., Van Gunsteren W.F., Validation of the 53A6 GROMOS force field, Eur. Biophys. J., 34, pp. 273-284, (2005); Oostenbrink C., Villa A., Mark A.E., Van Gunsteren W.F., A biomolecular force field based on the free enthalpy of hydration and solvation: The GROMOS force-field parameter sets 53A5 and 53A6, J. Comput. Chem., 25, pp. 1656-1676, (2004); Van Der Spoel D., Lindahl E., Hess B., Groenhof G., Mark A.E., Berendsen H.J.C., GROMACS: Fast, flexible, and free, J. Comput. Chem., 26, pp. 1701-1718, (2005); Hess B., Kutzner C., Van Der Spoel D., Lindahl E., GRGMACS 4: Algorithms for highly efficient, load-balanced, and scalable molecular simulation, J. Chem. Theory Comput., 4, pp. 435-447, (2008); Zahariev F., Xu P., Westheimer B.M., Webb S., Galvez Vallejo J., Tiwari A., Sundriyal V., Sosonkina M., Shen J., Schoendorff G., Schlinsog M., Sattasathuchana T., Ruedenberg K., Roskop L.B., Rendell A.P., Poole D., Piecuch P., Pham B.Q., Mironov V., Mato J., Leonard S., Leang S.S., Ivanic J., Hayes J., Harville T., Gururangan K., Guidez E., Gerasimov I.S.,

Friedl C., Ferreras K.N., Elliott G., Datta D., Del Angel Cruz D., Carrington L., Bertoni C., Barca G.M.J., Alkan M., Gordon M.S., The general atomic and molecular electronic structure system (GAMESS): Novel methods on novel architectures, J. Chem. Theory Comput., 19, pp. 7031-7055, (2023); Hanwell M.D., Curtis D.E., Lonie D.C., Vandermeerschd T., Zurek E., Hutchison G.R., Avogadro: An advanced semantic chemical editor, visualization, and analysis platform, J. Cheminform., 4, (2012); Sousa S.F., Fernandes P.A., Ramos M.J., General performance of density functionals, J. Phys. Chem. A, 111, pp. 10439-10452, (2007); Tirado-Rives J., Jorgensen W.L., Performance of B3LYP density functional methods for a large set of organic molecules, J. Chem. Theory Comput., 4, pp. 297-306, (2008); Rassolov V.A., Pople J.A., Ratner M.A., Windus T.L., 6–31G* basis set for atoms K through Zn, J. Chem. Phys., 109, (1998); Zhao Y., Truhlar D.G., A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions, J. Chem. Phys., 125, (2006); Zhao Y., Truhlar D.G., The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: Two new functionals and systematic testing of four M06-class functionals and 12 other functionals, Theor. Chem. Acc., 120, pp. 215-241, (2008); Demir S., Cakmak S., Dege N., Kutuk H., Odabasoglu M., Kepekci R.A., A novel 3-acetoxy-2-methyl-N-(4-methoxyphenyl)benzamide: Molecular structural describe, antioxidant activity with use X-ray diffractions and DFT calculations, J. Mol. Struct., 1100, pp. 582-591, (2015); Vidal A.V., De Vicente Poutas L.C., Faza O.N., Lopez C.S., On the use of popular basis sets: Impact of the intramolecular basis set superposition error, Molecules, 24, (2019); Cossi M., Rega N., Scalmani G., Barone V., Energies, structures, and electronic properties of molecules in solution with the C-PCM solvation model, J. Comput. Chem., 24, pp. 669-681, (2003); Marenich A.V., Cramer C.J., Truhlar D.G., Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric

constant and atomic surface tensions, J. Phys. Chem. B, 113, pp. 6378-6396, (2009); Lu T., Chen F., Multiwfn: A multifunctional wavefunction analyzer, J. Comput. Chem., 33, pp. 580-592, (2012); Parra J.G., Aray Y.R., Iza P., Zarate X., Schott E., Behavior of the SDS/1-butanol and SDS/2-butanol mixtures at the water/n-octane interface through molecular dynamics simulations, Chem. Phys., 523, (2019); Dominguez H., Computer studies on the effects of long chain alcohols on sodium dodecyl sulfate (SDS) molecules in SDS/dodecanol and SDS/hexadecanol monolayers at the air/water interface, J. Phys. Chem. B, 110, pp. 13151-13157, (2006); Bussi G., Donadio D., Parrinello M., Canonical sampling through velocity rescaling, J. Chem. Phys., 126, (2007); Berendsen H.J., Postma J.P.M., van Gunsteren W.F., DiNola A.R.H.J., Haak J.R., Molecular dynamics with coupling to an external bath, J. Chem. Phys., 81, pp. 3684-3690, (1984); Petersen H.G., Accuracy and efficiency of the particle mesh Ewald method, J. Chem. Phys., 103, pp. 3668-3679, (1995); Humphrey W., Dalke A., Schulten K., VMD: Visual molecular dynamics, J. Mol. Graph., 14, pp. 33-38, (1996); Plazzer M.B., Henry D.J., Yiapanis G., Yarovsky I., Comparative study of commonly used molecular dynamics force fields for modeling organic monolayers on water, J. Phys. Chem. B, 115, pp. 3964-3971, (2011); da Silva G.C.Q., Silva G.M., Tavares F.W., Fleming F.P., Horta B.A.C., Are all-atom any better than united-atom force fields for the description of liquid properties of alkanes?, J. Mol. Model., 26, (2020); Aray Y., Parra J.G., Paredes R., (2020); Cao X., Qin X., Chen J., Li X., Xia W., Bian J., Zhang P., Adsorption kinetics investigation of surfactant molecules at the short-chain alkane-water interface, Colloids Surf. A Physicochem. Eng. Asp., 660, (2023); Ivanova A.A., Phan C.M., Cheremisin A.N., Barifcani A., Molecular behaviour of a surfactant layer under an external electrostatic field, J. Mol. Liq., 362, (2022); Malde A.K., Zuo L., Breeze M., Stroet M., Poger D., Nair P.C., Oostenbrink C., Mark A.E., Malde2011, J. Chem. Theory Comput., 7, pp. 4026-4037, (2011); Berendsen H., Postma J., (1981); Parra J.G., Iza P., Dominguez H., Schott E., Zarate X., Effect of triton X-100 surfactant on the interfacial activity of ionic surfactants SDS, CTAB and

SDBS at the air/water interface: A study using molecular dynamic simulations, Colloids Surf. A Physicochem. Eng. Asp., 603, (2020); Barone V., Cossi M., Quantum calculation of molecular energies and energy gradients in solution by a conductor solvent model, J. Phys. Chem. A, 102, pp. 1995-2001, (1998); (2019); (1994); Fedorov D.G., Analysis of solute-solvent interactions using the solvation model density combined with the fragment molecular orbital method, Chem. Phys. Lett., 702, pp. 111-116, (2018); Wang P., Shi R., Su Y., Tang L., Huang X., Zhao J., Hydrated sodium ion clusters [Na+(H2O)n (n = 1–6)]: An ab initio study on structures and non-covalent interaction, Front. Chem., 7, (2019); Huibers P.D.T., Quantum-chemical calculations of the charge distribution in ionic surfactants, Langmuir, 15, pp. 7546-7550, (1999); Roussel G., Michaux C., Perpete E.A., Multiscale molecular dynamics simulations of sodium dodecyl sulfate micelles: From coarse-grained to all-atom resolution, J. Mol. Model., 20, (2014); Bruce C.D., Senapati S., Berkowitz M.L., Perera L., Forbes M.D.E., Molecular dynamics simulations of sodium dodecyl sulfate micelle in water: The behavior of water, J. Phys. Chem. B, 106, pp. 10902-10907, (2002); Wang S., Larson R.G., Coarse-grained molecular dynamics simulation of self-assembly and surface adsorption of ionic surfactants using an implicit water model, Langmuir, 31, pp. 1262-1271, (2015); Bernardes C.E.S., Joseph A., Evaluation of the OPLS-AA force field for the study of structural and energetic aspects of molecular organic crystals, J. Phys. Chem. a., 119, pp. 3023-3034, (2015); Kroger L.C., Muller S., Smirnova I., Leonhard K., Prediction of solvation free energies of ionic solutes in neutral solvents, J. Phys. Chem. A, 124, pp. 4171-4181, (2020); Galabov B., Ilieva S., Cheshmedzhieva D., Nikolova V., Popov V.A., Hadjieva B., Schaefer H.F., Mini-review on structure-reactivity relationship for aromatic molecules: Recent advances, ACS Omega, 7, pp. 8199-8208, (2022); Tahoon M.A., Gomaa E.A., Suleiman M.H.A., Aqueous micro-hydration of Na + (H 2 O) n=1-7 clusters: DFT study, Open Chem., 17, pp. 260-269, (2019); Xu J., Zhang Y., Chen H., Wang P., Xie Z., Yao Y., Zhang J.,

Effect of surfactant headgroups on the oil/water interface: An interfacial tension measurement and simulation study, J. Mol. Struct., 1052, pp. 50-56, (2013); Ghosh M.K., Re S., Feig M., Sugita Y., Choi C.H., Interionic hydration structures of NaCl in aqueous solution: A combined study of quantum mechanical cluster calculations and QM/EFP-MD simulations, J. Phys. Chem. B, 117, pp. 289-295, (2013); Neela Y.I., Mahadevi A.S., Sastry G.N., First principles study and database analyses of structural preferences for sodium ion (Na+) solvation and coordination, Struct. Chem., 24, pp. 67-79, (2013); Shi Y., Wang P., Li W., Su Y., Effects of Na+ and Cl− on hydrated clusters by ab initio study, J. Chem. Phys., 159, (2023); Rehfeld S.J., Adsorption of sodium dodecyl sulfate at various hydrocarbon-water interfaces, J. Phys. Chem., 71, pp. 738-745, (1967); Bergfreund J., Siegenthaler S., Lutz-bueno V., Bertsch P., Fischer P., Surfactant adsorption to different fluid, Interfaces, (2021); Lu J.R., Simister E.A., Lee E.M., Thomas R.K., Rennie A.R., Penfold J., Direct determination by neutron reflection of the penetration of water into surfactant layers at the air/water interface, Langmuir, 8, pp. 1837-1844, (1992); Lu J.R., Thomas R.K., Penfold J., Surfactant layers at the air/water interface: structure and composition, Adv. Colloid Interface Sci., 84, pp. 143-304, (2000); Zeron I.M., Abascal J.L.F., Vega C., A force field of Li+, Na+, K+, Mg2+, Ca2+, Cl-, and S O 4 2 - in aqueous solution based on the TIP4P/2005 water model and scaled charges for the ions, J. Chem. Phys., 151, (2019); Cui K., Yethiraj A., Schmidt J.R., Influence of charge scaling on the solvation properties of ionic liquid solutions, J. Phys. Chem. B, 123, pp. 9222-9229, (2019); Lu J.R., Marrocco A., Su T.J., Thomas R.K., Penfold J., Adsorption of dodecyl sulfate surfactants with monovalent metal counterions at the air-water interface studied by neutron reflection and surface tension, J. Colloid Interface Sci., 158, pp. 303-316, (1993); Jose Salas F., Arlette Mendez-Maldonado G., Nunez-Rojas E., Eloy Aguilar-Pineda G., Dominguez H., Alejandre J., Systematic procedure to parametrize force fields for molecular fluids, J. Chem. Theory Comput., 11, pp. 683-693, (2015)

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