Hector DomÃ-nguez

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Self-Aggregation of the SDS Surfactant at a Solidâ^'Liquid Interface. Journal of Physical Chemistry B, 2007, 111, 4054-4059.	2.6	79
2	Systematic Procedure To Parametrize Force Fields for Molecular Fluids. Journal of Chemical Theory and Computation, 2015, 11, 683-693.	5.3	43
3	Mixtures of Sodium Dodecyl Sulfate/Dodecanol at the Air/Water Interface by Computer Simulations. Langmuir, 2005, 21, 7257-7262.	3.5	42
4	Computational studies on the behavior of Sodium Dodecyl Sulfate (SDS) at TiO2(rutile)/water interfaces. Journal of Colloid and Interface Science, 2011, 364, 417-427.	9.4	32
5	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 and Surfaces A: Physicochemical and Engineering Aspects, 2020, 603, 125284.	4.7	31
6	Structural Transition of the Sodium Dodecyl Sulfate (SDS) Surfactant Induced by Changes in Surfactant Concentrations. Journal of Physical Chemistry B, 2011, 115, 12422-12428.	2.6	29
7	Structure of the Sodium Dodecyl Sulfate Surfactant on a Solid Surface in Different NaCl Solutions. Langmuir, 2009, 25, 9006-9011.	3.5	21
8	Adsorption of phenol molecules by sodium dodecyl sulfate (SDS) surfactants deposited on solid surfaces: A computer simulation study. Journal of Molecular Graphics and Modelling, 2016, 65, 108-112.	2.4	19
9	Structural and interfacial properties of the CO2-in-water foams prepared with sodium dodecyl sulfate (SDS): A molecular dynamics simulation study. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 578, 123615.	4.7	18
10	A simulation study of self-assembly behaviors and micellization properties of mixed ionic surfactants. Journal of Molecular Liquids, 2021, 336, 116003.	4.9	18
11	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. Journal of Physical Chemistry B, 2006, 110, 13151-13157.	2.6	16
12	New Force Field Parameters for the Sodium Dodecyl Sulfate and Alpha Olefin Sulfonate Anionic Surfactants. Journal of Physical Chemistry B, 2018, 122, 4558-4565.	2.6	16
13	Structure of the SDS/1-dodecanol surfactant mixture on a graphite surface: A computer simulation study. Journal of Colloid and Interface Science, 2010, 345, 293-301.	9.4	15
14	Structural changes of a sodium dodecyl sulfate (SDS) micelle induced by alcohol molecules. Journal of Molecular Modeling, 2016, 22, 33.	1.8	15
15	Influence of solvent permittivity and divalent salt on micellization behavior of sodium dodecyl sulfate: Conductivity measurements and simulation study. Journal of Molecular Liquids, 2022, 349, 118186.	4.9	14
16	Computer simulations of surfactant monolayers at solid walls. Journal of Colloid and Interface Science, 2006, 297, 370-373.	9.4	13
17	Desorption of decane molecules from a graphite surface produced by sodium alpha olefin sulphate/betaine surfactant mixtures: A computer simulation study. Journal of Molecular Liquids, 2014, 200, 465-473.	4.9	12
18	Surface tension calculations of the cationic (CTAB) and the zwitterionic (SB3-12) surfactants using new force field models: a computational study. Molecular Physics, 2019, 117, 3632-3641.	1.7	11

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19	Prediction of experimental properties of CO2: improving actual force fields. Journal of Molecular Modeling, 2019, 25, 146.	1.8	11
20	Modelling and understanding of the vapour–liquid and liquid–liquid interfacial properties for the binary mixture of n-heptane and perfluoro-n-hexane. Journal of Molecular Liquids, 2013, 185, 36-43.	4.9	9
21	Conductance Study of Aerosol-OT in Binary Mixed Solvents of Short-Chain Alcohol–Water Systems at Various Temperatures. Journal of Chemical & Engineering Data, 2021, 66, 65-78.	1.9	8
22	Interaction of the interleukin 8 protein with a sodium dodecyl sulfate micelle: A computer simulation study. Journal of Molecular Modeling, 2017, 23, 210.	1.8	7
23	Carbon dioxide adsorption on a modified zeolite with sodium dodecyl sulfate surfactants: A molecular dynamics study. Journal of Molecular Graphics and Modelling, 2019, 92, 243-248.	2.4	7
24	Decane structure on a graphite surface with sodium dodecyl sulfate and betaine surfactant mixtures: A molecular dynamics study. Chemical Physics, 2020, 539, 110945.	1.9	4
25	Molecular dynamics simulations to study the solvent influence on protein structure. Chemical Physics Letters, 2016, 651, 92-96.	2.6	3
26	Surfactant molecules to promote removal of cadmium ions from solid surfaces: A complementary experimental-simulational study. Chemical Physics, 2017, 485-486, 13-21.	1.9	3
27	Carbon Dioxide Confined between Two Charged Single Layers of Graphene: Molecular Dynamics Studies. Journal of Physical Chemistry C, 2019, 123, 23705-23710.	3.1	3
28	Lead and mercury removal from aqueous solution using Sodium Dodecyl Sulfate micelles: A molecular dynamics study. Chemical Physics Letters, 2021, 767, 138340.	2.6	3
29	The non-ideal behaviour of the interfacial tension of the n-heptane+perfluoro-n-hexane mixture: A computational study. Chemical Physics Letters, 2015, 627, 77-81.	2.6	2
30	Gas sorption in solid surfaces: a computational study using rigid and Einstein-solid models. Physical Chemistry Chemical Physics, 2015, 17, 27894-27899.	2.8	1
31	Electric Fields Applied to Surfactant Molecules for Enhancing Removal of Hydrocarbons from a Solid Surface: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2022, 126, 11761-11768.	3.1	0