MÃ¡ria Darvas

List of Publications by Year
in descending order

27 papers	557 citations	516561 16 h-index	610775 24 g-index
27 all docs	27 docs citations	27 times ranked	521 citing authors

#	Article	IF	Citations
1	Molecular simulations of interfacial systems: challenges, applications and future perspectives. Molecular Simulation, 2023, 49, 1229-1266.	0.9	14
2	Computer Simulation of the Surface of Aqueous Ionic and Surfactant Solutions. Journal of Physical Chemistry B, 2022, 126, 751-765.	1.2	8
3	Atmospheric particulate matter characterization by Fourier transform infrared spectroscopy: a review of statistical calibration strategies for carbonaceous aerosol quantification in US measurement networks. Atmospheric Measurement Techniques, 2019, 12, 525-567.	1.2	17
4	Molecular Structure Inhibiting Synergism in Charged Surfactant Mixtures: An Atomistic Molecular Dynamics Simulation Study. Langmuir, 2017, 33, 14093-14104.	1.6	13
5	The effect of anaesthetics on the properties of a lipid membrane in the biologically relevant phase: a computer simulation study. Physical Chemistry Chemical Physics, 2015, 17, 14750-14760.	1.3	31
6	Calculation of the intrinsic solvation free energy profile of methane across a liquid/liquid interface in computer simulations. Journal of Molecular Liquids, 2014, 189, 39-43.	2.3	13
7	Reprint of â€œRole of the fluidity of a liquid phase in determining the surface properties of the opposite phaseâ€• Journal of Molecular Liquids, 2014, 189, 122-128.	2.3	2
8	Immersion Depth of Surfactants at the Free Water Surface: A Computer Simulation and ITIM Analysis Study. Journal of Physical Chemistry B, 2013, 117, 8733-8746.	1.2	41
9	Calculation of the Intrinsic Solvation Free Energy Profile of an Ionic Penetrant Across a Liquidâ€“Liquid Interface with Computer Simulations. Journal of Physical Chemistry B, 2013, 117, 16148-16156.	1.2	31
10	Molecular dynamics simulations of the water adsorption around malonic acid aerosol models. Physical Chemistry Chemical Physics, 2013, 15, 10942.	1.3	17
11	Role of the fluidity of a liquid phase in determining the surface properties of the opposite phase at the liquidâ€“liquid interface. Journal of Molecular Liquids, 2013, 186, 7.	2.3	1
12	Surface properties of the polarizable Baranyai-Kiss water model. Journal of Chemical Physics, 2012, 136, 114706.	1.2	12
13	Anesthetic molecules embedded in a lipid membrane: a computer simulation study. Physical Chemistry Chemical Physics, 2012, 14, 12956.	1.3	27
14	Adsorption of Acetaldehyde on Ice As Seen from Computer Simulation and Infrared Spectroscopy Measurements. Langmuir, 2012, 28, 4198-4207.	1.6	25
15	Temperature dependence of the lateral hydrogen bonded clusters of molecules at the free water surface. Journal of Molecular Liquids, 2012, 176, 33-38.	2.3	9
16	Lateral Dynamics of Surfactants at the Free Water Surface: A Computer Simulation Study. Langmuir, 2012, 28, 14944-14953.	1.6	35
17	Solvation Free Energy Profile of the SCN^{â€“} Ion across the Waterâ€“1,2-Dichloroethane Liquid/Liquid Interface. A Computer Simulation Study. Journal of Physical Chemistry C, 2011, 115, 11140-11146.	1.5	15
18	Competitive Adsorption of Surfactants and Polymers at the Free Water Surface. A Computer Simulation Study of the Sodium Dodecyl Sulfateâ^'Poly(ethylene oxide) System. Journal of Physical Chemistry B, 2011, 115, 933-944.	1.2	34

#	Article	IF	Citations
19	Water adsorption around oxalic acid aggregates: a molecular dynamics simulation of water nucleation on organic aerosols. Physical Chemistry Chemical Physics, 2011, 13, 19830.	1.3	24
20	Molecular Dynamics Simulation of the Adsorption of Oxalic Acid on an Ice Surface. ChemPhysChem, 2010, 11, 3971-3979.	1.0	14
21	Adsorption of Hydroxyacetone on Pure Ice Surfaces. ChemPhysChem, 2010, 11, 3921-3927.	1.0	11
22	Computer simulation and ITIM analysis of the surface of waterâ€“methanol mixtures containing traces of water. Journal of Molecular Liquids, 2010, 153, 88-93.	2.3	26
23	Molecular dynamics simulation and identification of the truly interfacial molecules (ITIM) analysis of the liquid-vapor interface of dimethyl sulfoxide. Journal of Chemical Physics, 2010, 132, 134701.	1.2	30
24	Molecular level properties of the free water surface and different organic liquid/water interfaces, as seen from ITIM analysis of computer simulation results. Journal of Physics Condensed Matter, 2010, 22, 284112.	0.7	40
25	Adsorption of Poly(ethylene oxide) at the Free Water Surface. A Computer Simulation Study. Journal of Physical Chemistry B, 2010, 114, 10995-11001.	1.2	18
26	Properties of the Liquidâ^'Vapor Interface of Waterâ^'Dimethyl Sulfoxide Mixtures. A Molecular Dynamics Simulation and ITIM Analysis Study. Journal of Physical Chemistry C, 2010, 114, 12207-12220.	1.5	31
27	Free Energy of Mixing of Pyridine and Its Methyl-Substituted Derivatives with Water, As Seen from Computer Simulations. Journal of Physical Chemistry B, 2009, 113, 7615-7620.	1.2	18