PÃ¡l Jedlovszky

List of Publications by Year
in descending order

151 papers	4,180 citations	94269 37 h-index	168136 53 g-index
153 all docs	153 docs citations	153 times ranked	2514 citing authors

#	Article	IF	Citations
1	A new method for determining the interfacial molecules and characterizing the surface roughness in computer simulations. Application to the liquidâ€“vapor interface of water. Journal of Computational Chemistry, 2008, 29, 945-956.	1.5	181
2	Molecular Aggregates in Aqueous Solutions of Bile Acid Salts. Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 9886-9896.	1.2	132
3	New insight into the orientational order of water molecules at the water/1,2-dichloroethane interface: A Monte Carlo simulation study. Journal of Chemical Physics, 2002, 117, 2271-2280.	1.2	113
4	Full description of the orientational statistics of molecules near to interfaces. Water at the interface with CCl4. Physical Chemistry Chemical Physics, 2004, 6, 1874-1879.	1.3	112
5	Calculation of the Free Energy Profile of H2O, O2, CO, CO2, NO, and CHCl3in a Lipid Bilayer with a Cavity Insertion Variant of the Widom Method. Journal of the American Chemical Society, 2000, 122, 5125-5131.	6.6	101
6	A Critical Assessment of Methods for the Intrinsic Analysis of Liquid Interfaces. 1. Surface Site Distributions. Journal of Physical Chemistry C, 2010, 114, 11169-11179.	1.5	89
7	Morphology of Voids in Molecular Systems. A Voronoiâ^'Delaunay Analysis of a Simulated DMPC Membrane. Journal of Physical Chemistry B, 2004, 108, 19056-19067.	1.2	81
8	Effect of Cholesterol on the Properties of Phospholipid Membranes. 1. Structural Features. Journal of Physical Chemistry B, 2003, 107, 5311-5321.	1.2	72
9	Determination of the Adsorption Isotherm of Methanol on the Surface of Ice. An Experimental and Grand Canonical Monte Carlo Simulation Study. Journal of the American Chemical Society, 2006, 128, 15300-15309.	6.6	72
10	The generalized identification of truly interfacial molecules (ITIM) algorithm for nonplanar interfaces. Journal of Chemical Physics, 2013, 138, 044110.	1.2	70
11	Properties of Free Surface of Waterâ^'Methanol Mixtures. Analysis of the Truly Interfacial Molecular Layer in Computer Simulation. Journal of Physical Chemistry B, 2008, 112, 5428-5438.	1.2	69
12	A Critical Assessment of Methods for the Intrinsic Analysis of Liquid Interfaces: 2. Density Profiles. Journal of Physical Chemistry C, 2010, 114, 18656-18663.	1.5	64
13	Liquidâ€“vapor and liquidâ€“liquid phase equilibria of the Brodholtâ€“Sampoliâ€“Vallauri polarizable water model. Journal of Chemical Physics, 2005, 122, 081101.	1.2	62
14	Pytim: A python package for the interfacial analysis of molecular simulations. Journal of Computational Chemistry, 2018, 39, 2118-2125.	1.5	61
15	Adsorption Isotherm of Formic Acid on the Surface of Ice, as Seen from Experiments and Grand Canonical Monte Carlo Simulation. Journal of Physical Chemistry C, 2008, 112, 8976-8987.	1.5	51
16	Voronoi polyhedra analysis of the local structure of water from ambient to supercritical conditions. Journal of Chemical Physics, 1999, 111, 5975-5985.	1.2	50
17	Molecular level structure of the liquid/liquid interface. Molecular dynamics simulation and ITIM analysis of the water-CCl4 system. Physical Chemistry Chemical Physics, 2008, 10, 4754.	1.3	50
18	Water in Contact with Magnetite Nanoparticles, as Seen from Experiments and Computer Simulations. Langmuir, 2009, 25, 13007-13014.	1.6	50

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19	Grand canonical ensemble Monte Carlo simulation of a lipid bilayer using extension biased rotations. Journal of Chemical Physics, 1999, 111, 10770-10773.	1.2	49
20	Orientational Order of the Water Molecules Across a Fully Hydrated DMPC Bilayer:Â A Monte Carlo Simulation Study. Journal of Physical Chemistry B, 2001, 105, 3614-3623.	1.2	48
21	A New Five-Site Pair Potential for Formic Acid in Liquid Simulations. Journal of Physical Chemistry A, 1997, 101, 2662-2665.	1.1	46
22	Effect of Cholesterol on the Properties of Phospholipid Membranes. 3. Local Lateral Structure. Journal of Physical Chemistry B, 2004, 108, 465-472.	1.2	46
23	Free-Energy Profile of Small Solute Molecules at the Free Surfaces of Water and Ice, as Determined by Cavity Insertion Widom Calculations. Journal of Physical Chemistry C, 2007, 111, 9407-9416.	1.5	45
24	Structure of the Liquidâ^'Vapor Interface of Waterâ^'Acetonitrile Mixtures As Seen from Molecular Dynamics Simulations and Identification of Truly Interfacial Molecules Analysis. Journal of Physical Chemistry C, 2009, 113, 18173-18183.	1.5	45
25	Water adsorption on hydrophilic and hydrophobic self-assembled monolayers as proxies for atmospheric surfaces. A grand canonical Monte Carlo simulation study. Physical Chemistry Chemical Physics, 2010, 12, 4604.	1.3	45
26	Line of percolation in supercritical water. Journal of Chemical Physics, 2005, 123, 024502.	1.2	43
27	Counterion and Surface Density Dependence of the Adsorption Layer of Ionic Surfactants at the Vaporâ^'Aqueous Solution Interface:Â A Computer Simulation Study. Journal of Physical Chemistry B, 2007, 111, 1769-1774.	1.2	43
28	Self-association of urea in aqueous solutions: A Voronoi polyhedron analysis study. Journal of Chemical Physics, 2008, 129, 164512.	1.2	42
29	Hydration of apolar solutes of varying size: a systematic study. Molecular Physics, 2006, 104, 2465-2476.	0.8	41
30	Investigation of the adsorption behaviour of acetone at the surface of ice. A grand canonical Monte Carlo simulation study. Physical Chemistry Chemical Physics, 2008, 10, 6369.	1.3	41
31	Molecular Level Properties of the Waterâ^'Dichloromethane Liquid/Liquid Interface, as Seen from Molecular Dynamics Simulation and Identification of Truly Interfacial Molecules Analysis. Journal of Physical Chemistry C, 2009, 113, 19263-19276.	1.5	41
32	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
33	Structure of the Liquidâ^'Vapor Interface of Waterâ^'Methanol Mixtures as Seen from Monte Carlo Simulations. Journal of Physical Chemistry B, 2005, 109, 20493-20503.	1.2	40
34	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
35	Layer-by-layer and intrinsic analysis of molecular and thermodynamic properties across soft interfaces. Journal of Chemical Physics, 2015, 143, 114709.	1.2	40
36	Adsorption of Aromatic Hydrocarbon Molecules at the Surface of Ice, As Seen by Grand Canonical Monte Carlo Simulation. Journal of Physical Chemistry C, 2013, 117, 6719-6729.	1.5	38

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37	Properties of water/apolar interfaces as seen from Monte Carlo simulations. Journal of Molecular Liquids, 2004, 109, 99-108.	2.3	37
38	Calculation of the Adsorption Isotherm of Formaldehyde on Ice by Grand Canonical Monte Carlo Simulation. Journal of Physical Chemistry C, 2007, 111, 14170-14178.	1.5	37
39	How Is the Surface Tension of Various Liquids Distributed along the Interface Normal?. Journal of Physical Chemistry C, 2016, 120, 27468-27477.	1.5	37
40	Water adsorption isotherms on porous onionlike carbonaceous particles. Simulations with the grand canonical Monte Carlo method. Journal of Chemical Physics, 2010, 133, 144702.	1.2	36
41	Lateral Dynamics of Surfactants at the Free Water Surface: A Computer Simulation Study. Langmuir, 2012, 28, 14944-14953.	1.6	35
42	The local structure of various hydrogen bonded liquids: Voronoi polyhedra analysis of water, methanol, and HF. Journal of Chemical Physics, 2000, 113, 9113-9121.	1.2	34
43	Competitive Adsorption of Surfactants and Polymers at the Free Water Surface. A Computer Simulation Study of the Sodium Dodecyl Sulfateâˆ'Poly(ethylene oxide) System. Journal of Physical Chemistry B, 2011, 115, 933-944.	1.2	34
44	Floating Patches of HCN at the Surface of Their Aqueous Solutions â€" Can They Make â€œHCN Worldâ€• Plausible?. Journal of Physical Chemistry C, 2014, 118, 21469-21482.	1.5	34
45	Effect of Cholesterol on the Properties of Phospholipid Membranes. 4. Interatomic Voids. Journal of Physical Chemistry B, 2005, 109, 16490-16502.	1.2	33
46	Temperature and Pressure Dependence of the Properties of the Liquidâˆ'Liquid Interface. A Computer Simulation and Identification of the Truly Interfacial Molecules Investigation of the Waterâˆ'Benzene System. Journal of Physical Chemistry C, 2010, 114, 21681-21693.	1.5	33
47	Structural and thermodynamic properties of different phases of supercooled liquid water. Journal of Chemical Physics, 2008, 128, 244503.	1.2	31
48	Properties of the Liquidâˆ'Vapor Interface of Waterâˆ'Dimethyl Sulfoxide Mixtures. A Molecular Dynamics Simulation and ITIM Analysis Study. Journal of Physical Chemistry C, 2010, 114, 12207-12220.	1.5	31
49	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
50	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
51	Contribution of Different Molecules and Moieties to the Surface Tension in Aqueous Surfactant Solutions. Journal of Physical Chemistry C, 2019, 123, 16660-16670.	1.5	31
52	A Comprehensive Liquid Simulation Study of Neat Formic Acid. Journal of Physical Chemistry B, 2000, 104, 8287-8294.	1.2	30
53	Adsorption of 1-octanol at the free water surface as studied by Monte Carlo simulation. Journal of Chemical Physics, 2004, 120, 11839-11851.	1.2	30
54	Can existing models qualitatively describe the mixing behavior of acetone with water?. Journal of Chemical Physics, 2009, 130, 124516.	1.2	30

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55	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
56	Local Structure in Terms of Nearest-Neighbor Approach in 1-Butyl-3-methylimidazolium-Based Ionic Liquids: MD Simulations. Journal of Physical Chemistry B, 2016, 120, 5029-5041.	1.2	30
57	Adsorption of Benzaldehyde at the Surface of Ice, Studied by Experimental Method and Computer Simulation. Langmuir, 2010, 26, 9596-9606.	1.6	29
58	Computer simulation study of liquid CH2F2 with a new effective pair potential model. Journal of Chemical Physics, 1999, 110, 2991-3002.	1.2	27
59	Modeling of Mixing Acetone and Water: How Can Their Full Miscibility Be Reproduced in Computer Simulations?. Journal of Physical Chemistry B, 2012, 116, 5977-5984.	1.2	27
60	Anesthetic molecules embedded in a lipid membrane: a computer simulation study. Physical Chemistry Chemical Physics, 2012, 14, 12956.	1.3	27
61	Adsorption of apolar molecules at the water liquidâ€“vapor interface: A Monte Carlo simulations study of the water-n-octane system. Journal of Chemical Physics, 2003, 119, 1731-1740.	1.2	26
62	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
63	Microscopic Origin of the Surface Tension Anomaly of Water. Langmuir, 2014, 30, 2969-2972.	1.6	26
64	Adsorption of Acetaldehyde on Ice As Seen from Computer Simulation and Infrared Spectroscopy Measurements. Langmuir, 2012, 28, 4198-4207.	1.6	25
65	Thermodynamics of Mixing Water with Dimethyl Sulfoxide, as Seen from Computer Simulations. Journal of Physical Chemistry B, 2014, 118, 8724-8733.	1.2	25
66	Hydration free energy difference of acetone, acetamide, and urea. Journal of Chemical Physics, 2008, 129, 164501.	1.2	24
67	Surface Hydrophilicity-Dependent Water Adsorption on Mixed Self-Assembled Monolayers of C₇â€“CH₃ and C₇â€“COOH Residues. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2011, 115, 19165-19177.	1.5	24
68	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
69	Detailed insight into the hydrogen bonding interactions in acetoneâ€“methanol mixtures. A molecular dynamics simulation and Voronoi polyhedra analysis study. Physical Chemistry Chemical Physics, 2012, 14, 5979.	1.3	24
70	Free Energy of Mixing of Acetone and Methanol: A Computer Simulation Investigation. Journal of Physical Chemistry B, 2013, 117, 16157-16164.	1.2	24
71	Molecular Dynamics Simulations of the Interaction between Water Molecules and Aggregates of Acetic or Propionic Acid Molecules. Journal of Physical Chemistry B, 2015, 119, 15662-15674.	1.2	24
72	The local environment of the molecules in waterâ€“DMSO mixtures, as seen from computer simulations and Voronoi polyhedra analysis. Physical Chemistry Chemical Physics, 2015, 17, 3470-3481.	1.3	24

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73	Pressure Profile Calculation with Mesh Ewald Methods. Journal of Chemical Theory and Computation, 2016, 12, 4509-4515.	2.3	24
74	The hydrogen bonding structure of water in the vicinity of apolar interfaces: a computer simulation study. Journal of Physics Condensed Matter, 2004, 16, S5389-S5402.	0.7	22
75	Adsorption of HCN at the Surface of Ice: A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2014, 118, 3599-3609.	1.5	22
76	Free volume properties of a linear soft polymer: A computer simulation study. Journal of Chemical Physics, 2004, 121, 2422-2427.	1.2	21
77	GM1 Ganglioside Embedded in a Hydrated DOPC Membrane: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2009, 113, 4876-4886.	1.2	21
78	Dynamics of the Water Molecules at the Intrinsic Liquid Surface As Seen from Molecular Dynamics Simulation and Identification of Truly Interfacial Molecules Analysis. Journal of Physical Chemistry C, 2016, 120, 8578-8588.	1.5	21
79	Properties of the Liquidâ€“Vapor Interface of Acetoneâ€“Water Mixtures. A Computer Simulation and ITIM Analysis Study. Journal of Physical Chemistry C, 2015, 119, 12473-12487.	1.5	20
80	Ammonia Clathrate Hydrate As Seen from Grand Canonical Monte Carlo Simulations. ACS Earth and Space Chemistry, 2018, 2, 521-531.	1.2	20
81	Temperature dependence of thermodynamic properties of a polarizable potential model of water. Molecular Physics, 1999, 97, 1157-1163.	0.8	19
82	Adsorption of Fluorinated Methane Derivatives at the Surface of Ice under Tropospheric Conditions, As Seen from Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry C, 2016, 120, 17386-17399.	1.5	19
83	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
84	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
85	Assessment of the potential models of acetone/CO2 and ethanol/CO2 mixtures by computer simulation and thermodynamic integration in liquid and supercritical states. Physical Chemistry Chemical Physics, 2011, 13, 16272.	1.3	17
86	Molecular dynamics simulations of the water adsorption around malonic acid aerosol models. Physical Chemistry Chemical Physics, 2013, 15, 10942.	1.3	17
87	Lateral Pressure Profile and Free Volume Properties in Phospholipid Membranes Containing Anesthetics. Journal of Physical Chemistry B, 2017, 121, 2814-2824.	1.2	17
88	Two-dimensional percolation at the free water surface and its relation with the surface tension anomaly of water. Journal of Chemical Physics, 2014, 141, 054707.	1.2	16
89	Nonzero Ideal Gas Contribution to the Surface Tension of Water. Journal of Physical Chemistry Letters, 2017, 8, 2608-2612.	2.1	16
90	Orientational order of the water molecules at the vicinity of the waterâ€“benzene interface in a broad range of thermodynamic states, as seen from Monte Carlo simulations. Faraday Discussions, 2005, 129, 35-46.	1.6	15

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91	Properties of the liquidâ€“vapor interface of acetoneâ€“methanol mixtures, as seen from computer simulation and ITIM surface analysis. Physical Chemistry Chemical Physics, 2015, 17, 8913-8926.	1.3	15
92	Distance Angle Descriptors of the Interionic and Ionâ€“Solvent Interactions in Imidazolium-Based Ionic Liquid Mixtures with Aprotic Solvents: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2019, 123, 6065-6075.	1.2	15
93	Molecular Dynamics Simulation of the Adsorption of Oxalic Acid on an Ice Surface. ChemPhysChem, 2010, 11, 3971-3979.	1.0	14
94	Adsorption of Methylene Fluoride and Methylene Chloride at the Surface of Ice under Tropospheric Conditions: A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2015, 119, 17243-17252.	1.5	14
95	Adsorption of Methylamine on Amorphous Ice under Interstellar Conditions. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry A, 2018, 122, 3398-3412.	1.1	14
96	Adsorption of Formamide at the Surface of Amorphous and Crystalline Ices under Interstellar and Tropospheric Conditions. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry A, 2019, 123, 2935-2948.	1.1	14
97	Structure of the nonionic surfactant triethoxy monooctylether C8E3 adsorbed at the free water surface, as seen from surface tension measurements and Monte Carlo simulations. Journal of Chemical Physics, 2005, 122, 124704.	1.2	13
98	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
99	Local structure of dilute aqueous DMSO solutions, as seen from molecular dynamics simulations. Journal of Chemical Physics, 2017, 146, 234507.	1.2	13
100	Analysis of Mixed Formic and Acetic Acid Aggregates Interacting With Water: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2017, 121, 13863-13875.	1.5	13
101	Miscibility and Thermodynamics of Mixing of Different Models of Formamide and Water in Computer Simulation. Journal of Physical Chemistry B, 2017, 121, 7147-7155.	1.2	13
102	Effect of general anesthetics on the properties of lipid membranes of various compositions. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 594-609.	1.4	13
103	Temperature of maximum density line of a polarizable water model. Physical Review E, 2003, 67, 011201.	0.8	12
104	Surface properties of the polarizable Baranyai-Kiss water model. Journal of Chemical Physics, 2012, 136, 114706.	1.2	12
105	Adsorption of H2O2 at the surface of Ih ice, as seen from grand canonical Monte Carlo simulations. Chemical Physics Letters, 2014, 600, 73-78.	1.2	12
106	Adsorption of Methylamine at the Surface of Ice. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2016, 120, 23480-23489.	1.5	12
107	Single Particle Dynamics at the Intrinsic Surface of Various Apolar, Aprotic Dipolar, and Hydrogen Bonding Liquids As Seen from Computer Simulations. Journal of Physical Chemistry B, 2017, 121, 5582-5594.	1.2	12
108	Adsorption of Hydroxyacetone on Pure Ice Surfaces. ChemPhysChem, 2010, 11, 3921-3927.	1.0	11

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109	Structure of coexisting liquid phases of supercooled water: Analogy with ice polymorphs. Journal of Chemical Physics, 2007, 126, 241103.	1.2	10
110	Relation between the Surface Tension and Roughness of the Intrinsic Liquid Surface. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2013, 68, 123-129.	0.7	10
111	Thermodynamics of Mixing Primary Alkanolamines with Water. Journal of Physical Chemistry B, 2018, 122, 6251-6259.	1.2	10
112	Investigation of the Liquidâ€“Vapor Interface of Waterâ€“Formamide Mixtures by Computer Simulation and Intrinsic Surface Analysis. Journal of Physical Chemistry C, 2018, 122, 19639-19651.	1.5	10
113	Surface Affinity of Alkali and Halide Ions in Their Aqueous Solution: Insight from Intrinsic Density Analysis. Journal of Physical Chemistry B, 2020, 124, 9884-9897.	1.2	10
114	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
115	Structure of the adsorption layer of various ionic and non-ionic surfactants at the free water surface, as seen from computer simulation and ITIM analysis. Journal of Molecular Liquids, 2015, 205, 9-15.	2.3	9
116	Vapour-liquid equilibrium of acetone-CO2 mixtures of different compositions at the vicinity of the critical point. Journal of CO2 Utilization, 2019, 34, 465-471.	3.3	9
117	Investigation of the liquid-vapour interface of aqueous methylamine solutions by computer simulation methods. Journal of Molecular Liquids, 2019, 288, 110978.	2.3	9
118	Computer Simulation Investigation of the Adsorption of Cyanamide on Amorphous Ice at Low Temperatures. Journal of Physical Chemistry C, 2020, 124, 10615-10626.	1.5	9
119	Properties of the intrinsic surface of liquid acetone, as seen from computer simulations. Molecular Physics, 2015, 113, 985-996.	0.8	8
120	Adsorption of Chlorinated Methane Derivatives at the Ice Surface: A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2017, 121, 7782-7793.	1.5	8
121	Molecular-scale simulations of organic compounds on ice: application to atmospheric and interstellar sciences. Molecular Simulation, 2019, 45, 403-416.	0.9	8
122	Contribution of the two liquid phases to the interfacial tension at various water-organic liquid-liquid interfaces. Journal of Molecular Liquids, 2020, 306, 112872.	2.3	8
123	Role of the Counterions in the Surface Tension of Aqueous Surfactant Solutions. A Computer Simulation Study of Alkali Dodecyl Sulfate Systems. Colloids and Interfaces, 2020, 4, 15.	0.9	8
124	Computer Simulation of the Surface of Aqueous Ionic and Surfactant Solutions. Journal of Physical Chemistry B, 2022, 126, 751-765.	1.2	8
125	Relation between the Liquid Spinodal Pressure and the Lateral Pressure Profile at the Liquidâ€“Vapor Interface. Journal of Physical Chemistry C, 2017, 121, 12214-12219.	1.5	7
126	Single Particle Dynamics at the Liquidâ€“Liquid Interface. Molecular Dynamics Simulation Study of the Water-CCl‹sub›4‹/sub› System. Journal of Physical Chemistry C, 2020, 124, 2039-2049.	1.5	7

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127	Adsorption of Propylene Oxide on Amorphous Ice under Interstellar Conditions. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2020, 124, 16402-16414.	1.5	7
128	Contribution of Different Molecules and Moieties to the Surface Tension in Aqueous Surfactant Solutions. II: Role of the Size and Charge Sign of the Counterions. Journal of Physical Chemistry B, 2021, 125, 9005-9018.	1.2	7
129	Collective dynamics of supercooled water close to the liquidâ€“liquid coexistence lines. Physical Chemistry Chemical Physics, 2011, 13, 19823.	1.3	6
130	Voronoi Polyhedra as a Tool for the Characterization of Inhomogeneous Distribution in 1-Butyl-3-methylimidazolium Cation-Based Ionic Liquids. Journal of Physical Chemistry B, 2020, 124, 10419-10434.	1.2	6
131	Single-Particle Dynamics at the Intrinsic Surface of Aqueous Alkali Halide Solutions. Journal of Physical Chemistry B, 2021, 125, 665-679.	1.2	6
132	Calculation of the Free Energy of Mixing as a Tool for Assessing and Improving Potential Models: The Case of the N,N-Dimethylformamideâ€“Water System. Journal of Physical Chemistry B, 2021, 125, 4819-4830.	1.2	6
133	Adsorption of C2â€“C5 alcohols on ice: A grand canonical Monte Carlo simulation study. Journal of Chemical Physics, 2022, 156, .	1.2	6
134	Statistical Thermodynamics Through Computer Simulation to Characterize Phospholipid Interactions in Membranes. Methods in Molecular Biology, 2007, 400, 127-144.	0.4	5
135	Adsorption of Octyl Cyanide at the Free Water Surface as Studied by Monte Carlo Simulation. Journal of Physical Chemistry B, 2007, 111, 5885-5895.	1.2	5
136	Dynamical properties of supercooled water close to the liquidâ€“liquid coexistence lines, and their relation to those at ambient conditions. Journal of Physics Condensed Matter, 2010, 22, 284105.	0.7	5
137	Local lateral environment of the molecules at the surface of DMSO-water mixtures. Journal of Physics Condensed Matter, 2016, 28, 404002.	0.7	5
138	Effect of the alkyl chain and composition on the thermodynamics of mixing of small alcohols and water. Journal of Molecular Liquids, 2021, 338, 116777.	2.3	5
139	Response to â€œComment on â€˜Can existing models qualitatively describe the mixing behavior of acetone-water mixtures?â€™â€• Journal of Chemical Physics, 2009, 131, 157102.	1.2	4
140	Dependence of the adsorption of halogenated methane derivatives at the ice surface on their chemical structure. Journal of Molecular Liquids, 2017, 245, 17-26.	2.3	4
141	Thermodynamics of mixing methanol with supercritical CO₂ as seen from computer simulations and thermodynamic integration. Physical Chemistry Chemical Physics, 2020, 22, 11652-11662.	1.3	4
142	Simulations of Membranes Containing General Anesthetics. , 2019, , 177-198.		4
143	Multiscale Modeling of Interfacial Oxidation Mechanism at Air/Organic Interface: Reactions of CH₂â•CH-Terminated Self-Assembled Monolayer with OH^{â€¢}, O₃, and HO₂^{â€¢}. Journal of Physical Chemistry C, 2018, 122, 9886-9898.	1.5	3
144	Adsorption of acetamide on crystalline and amorphous ice under atmospheric conditions. A grand canonical Monte Carlo simulation study. Journal of Molecular Liquids, 2022, 354, 118870.	2.3	3

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145	Computer simulation investigation of the adsorption of acetamide on low density amorphous ice. An astrochemical perspective. Journal of Chemical Physics, 2022, 156, 184703.	1.2	3
146	The anisotropic virial-biased sampling for Monte Carlo simulations in the isothermalâ€"isobaric ensemble. Molecular Physics, 1999, 96, 293-296.	0.8	2
147	On the calculation of the surface entropy in computer simulation. Journal of Molecular Liquids, 2018, 262, 58-62.	2.3	2
148	The impact of tensorial temperature on equilibrium thermodynamics. Physical Chemistry Chemical Physics, 2018, 20, 16910-16912.	1.3	2
149	Description of the Interfacial Behavior of Benzonitrile at Icy Surfaces by Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry A, 2022, 126, 1221-1232.	1.1	2
150	Structure and single particle dynamics of the vapour-liquid interface of acetone-CO2 mixtures. Journal of Molecular Liquids, 2021, 334, 116091.	2.3	1
151	Local Structure in Mixtures of Ionic Liquid with Molecular Solvent: Vibration Spectroscopy, NMR and Molecular Dynamics Simulation. Physical Chemistry in Action, 2021, , 289-334.	0.1	1