Marcello Sega

List of Publications by Year
in descending order

85 papers	2,037 citations	218677 26 h-index	276875 41 g-index
87 all docs	87 docs citations	87 times ranked	2008 citing authors

#	Article	IF	Citations
1	Dominant Pathways in Protein Folding. Physical Review Letters, 2006, 97, 108101.	7.8	143
2	Molecular Aggregates in Aqueous Solutions of Bile Acid Salts. Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 9886-9896.	2.6	132
3	Morphology of Bile Salt Micelles as Studied by Computer Simulation Methods. Langmuir, 2007, 23, 12322-12328.	3.5	84
4	An iterative, fast, linear-scaling method for computing induced charges on arbitrary dielectric boundaries. Journal of Chemical Physics, 2010, 132, 154112.	3.0	76
5	The generalized identification of truly interfacial molecules (ITIM) algorithm for nonplanar interfaces. Journal of Chemical Physics, 2013, 138, 044110.	3.0	70
6	Quantitative Protein Dynamics from Dominant Folding Pathways. Physical Review Letters, 2007, 99, 118102.	7.8	67
7	Electrophoretic mobility and charge inversion of a colloidal particle studied by single-colloid electrophoresis and molecular dynamics simulations. Physical Review E, 2013, 87, 022302.	2.1	64
8	Pytim: A python package for the interfacial analysis of molecular simulations. Journal of Computational Chemistry, 2018, 39, 2118-2125.	3.3	61
9	Mesoscale structures at complex fluidâ€“fluid interfaces: a novel lattice Boltzmann/molecular dynamics coupling. Soft Matter, 2013, 9, 10092.	2.7	51
10	Mesoscopic simulations of the counterion-induced electro-osmotic flow: A comparative study. Journal of Chemical Physics, 2009, 130, 244702.	3.0	48
11	Puckering free energy of pyranoses: A NMR and metadynamics-umbrella sampling investigation. Journal of Chemical Physics, 2010, 133, 095104.	3.0	47
12	Dielectric and Terahertz Spectroscopy of Polarizable and Nonpolarizable Water Models: A Comparative Study. Journal of Physical Chemistry A, 2015, 119, 1539-1547.	2.5	47
13	Layer-by-layer and intrinsic analysis of molecular and thermodynamic properties across soft interfaces. Journal of Chemical Physics, 2015, 143, 114709.	3.0	40
14	Kinetic dielectric decrement revisited: phenomenology of finite ion concentrations. Physical Chemistry Chemical Physics, 2015, 17, 130-133.	2.8	40
15	Long-Range Dispersion Effects on the Water/Vapor Interface Simulated Using the Most Common Models. Journal of Physical Chemistry B, 2017, 121, 3798-3803.	2.6	40
16	How Is the Surface Tension of Various Liquids Distributed along the Interface Normal?. Journal of Physical Chemistry C, 2016, 120, 27468-27477.	3.1	37
17	Diffusion of water in confined geometry: The case of a multilamellar bilayer. Physical Review E, 2005, 72, 041201.	2.1	35
18	Dominant reaction pathways in high-dimensional systems. Journal of Chemical Physics, 2009, 130, 064106.	3.0	35

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19	Efficient Handling of Gaussian Charge Distributions: An Application to Polarizable Molecular Models. Journal of Chemical Theory and Computation, 2014, 10, 5513-5519.	5.3	33
20	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.	2.6	31
21	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.	2.8	31
22	Contribution of Different Molecules and Moieties to the Surface Tension in Aqueous Surfactant Solutions. Journal of Physical Chemistry C, 2019, 123, 16660-16670.	3.1	31
23	Conformation and Dynamics of Poly(N-isopropyl acrylamide) Trimers in Water: A Molecular Dynamics and Metadynamics Simulation Study. Journal of Physical Chemistry B, 2011, 115, 5827-5839.	2.6	30
24	Regularization of the slip length divergence in water nanoflows by inhomogeneities at the Angstrom scale. Soft Matter, 2013, 9, 8526.	2.7	30
25	Anesthetic molecules embedded in a lipid membrane: a computer simulation study. Physical Chemistry Chemical Physics, 2012, 14, 12956.	2.8	27
26	Ensemble inequivalence in single-molecule experiments. Physical Review E, 2009, 79, 051118.	2.1	26
27	Microscopic Origin of the Surface Tension Anomaly of Water. Langmuir, 2014, 30, 2969-2972.	3.5	26
28	On the calculation of puckering free energy surfaces. Journal of Chemical Physics, 2009, 130, 225102.	3.0	25
29	Communication: Kinetic and pairing contributions in the dielectric spectra of electrolyte solutions. Journal of Chemical Physics, 2014, 140, 211101.	3.0	25
30	Molecular Dynamics Simulation of a GM3 Ganglioside Bilayer. Journal of Physical Chemistry B, 2004, 108, 20322-20330.	2.6	24
31	Counterion Binding in the Aqueous Solutions of Bile Acid Salts, as Studied by Computer Simulation Methods. Langmuir, 2008, 24, 10729-10736.	3.5	24
32	Pickett angles and Cremerâ€“Pople coordinates as collective variables for the enhanced sampling of six-membered ring conformations. Molecular Physics, 2011, 109, 141-148.	1.7	24
33	Pressure Profile Calculation with Mesh Ewald Methods. Journal of Chemical Theory and Computation, 2016, 12, 4509-4515.	5.3	24
34	Ab initio structure and thermodynamics of the RPBE-D3 water/vapor interface by neural-network molecular dynamics. Journal of Chemical Physics, 2020, 153, 144710.	3.0	24
35	Free volume properties of a linear soft polymer: A computer simulation study. Journal of Chemical Physics, 2004, 121, 2422-2427.	3.0	21
36	GM1 Ganglioside Embedded in a Hydrated DOPC Membrane: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2009, 113, 4876-4886.	2.6	21

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37	An atomistic study of a poly(styrene sulfonate)/poly(diallyldimethylammonium) bilayer: the role of surface properties and charge reversal. Physical Chemistry Chemical Physics, 2011, 13, 16336.	2.8	21
38	Applying to DNA translocation: Effect of dielectric boundaries. Computer Physics Communications, 2011, 182, 33-35.	7.5	19
39	Computing the Electrophoretic Mobility of Large Spherical Colloids by Combining Explicit Ion Simulations with the Standard Electrokinetic Model. Langmuir, 2014, 30, 1758-1767.	3.5	18
40	Extended friction elucidates the breakdown of fast water transport in graphene oxide membranes. Europhysics Letters, 2016, 116, 54002.	2.0	17
41	Lateral Pressure Profile and Free Volume Properties in Phospholipid Membranes Containing Anesthetics. Journal of Physical Chemistry B, 2017, 121, 2814-2824.	2.6	17
42	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.	3.0	16
43	Nonzero Ideal Gas Contribution to the Surface Tension of Water. Journal of Physical Chemistry Letters, 2017, 8, 2608-2612.	4.6	16
44	Intrinsic Structure of the Interface of Partially Miscible Fluids: An Application to Ionic Liquids. Journal of Physical Chemistry C, 2015, 119, 28448-28461.	3.1	15
45	Short-Range Structure of a GM3 Ganglioside Membrane:â€‰ Comparison between Experimental WAXS and Computer Simulation Results. Journal of Physical Chemistry B, 2007, 111, 10965-10969.	2.6	14
46	Dominant folding pathways of a peptide chain from ab initio quantum-mechanical simulations. Journal of Chemical Physics, 2011, 134, 024501.	3.0	13
47	Properties of water in the interfacial region of a polyelectrolyte bilayer adsorbed onto a substrate studied by computer simulations. Physical Chemistry Chemical Physics, 2012, 14, 11425.	2.8	13
48	On the collective network of ionic liquid/water mixtures. IV. Kinetic and rotational depolarization. Journal of Chemical Physics, 2014, 140, 204505.	3.0	13
49	Layer-by-Layer Formation of Oligoelectrolyte Multilayers: A Combined Experimental and Computational Study. Soft Materials, 2014, 12, S14-S21.	1.7	13
50	Effect of general anesthetics on the properties of lipid membranes of various compositions. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 594-609.	2.6	13
51	Effects of dielectric mismatch and chain flexibility on the translocation barriers of charged macromolecules through solid state nanopores. Soft Matter, 2012, 8, 9480.	2.7	12
52	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.	2.6	12
53	Capillaryâ€bridge forces between solid particles: Insights from lattice Boltzmann simulations. AICHE Journal, 2021, 67, e17350.	3.6	12
54	On the Calculation of the Dielectric Properties of Liquid Ionic Systems. NATO Science for Peace and Security Series B: Physics and Biophysics, 2013, , 103-122.	0.3	12

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55	Molecular dynamics simulation of GM1 gangliosides embedded in a phospholipid membrane. Journal of Molecular Liquids, 2006, 129, 86-91.	4.9	11
56	Inhomogeneity effects on the structure and dynamics of water at the surface of a membrane: A computer simulation study. Journal of Chemical Physics, 2007, 126, 125103.	3.0	11
57	Microscopic Structure of Phospholipid Bilayers:Â Comparison between Molecular Dynamics Simulations and Wide-Angle X-ray Spectra. Journal of Physical Chemistry B, 2007, 111, 2484-2489.	2.6	11
58	The role of a small-scale cutoff in determining molecular layers at fluid interfaces. Physical Chemistry Chemical Physics, 2016, 18, 23354-23357.	2.8	11
59	Phase and interface determination in computer simulations of liquid mixtures with high partial miscibility. Physical Chemistry Chemical Physics, 2017, 19, 18968-18974.	2.8	11
60	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.	2.6	10
61	The importance of chemical potential in the determination of water slip in nanochannels. European Physical Journal E, 2015, 38, 127.	1.6	8
62	ForConX: A forcefield conversion tool based on XML. Journal of Computational Chemistry, 2017, 38, 629-638.	3.3	8
63	Contribution of the two liquid phases to the interfacial tension at various water-organic liquid-liquid interfaces. Journal of Molecular Liquids, 2020, 306, 112872.	4.9	8
64	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.	2.1	8
65	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.	3.1	7
66	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.	3.1	7
67	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.	2.6	7
68	Single-Particle Dynamics at the Intrinsic Surface of Aqueous Alkali Halide Solutions. Journal of Physical Chemistry B, 2021, 125, 665-679.	2.6	6
69	Early Detection of Agglomeration in Fluidized Beds by Means of Frequency Analysis of Pressure Fluctuations. Energy & Fuels, 2022, 36, 4924-4932.	5.1	6
70	Atomistic simulation of PDADMAC/PSS oligoelectrolyte multilayers: overall comparison of tri- and tetra-layer systems. Soft Matter, 2019, 15, 9437-9451.	2.7	5
71	Capillary interactions between soft capsules protruding through thin fluid films. Soft Matter, 2020, 16, 10910-10920.	2.7	5
72	PDADMAC/PSS Oligoelectrolyte Multilayers: Internal Structure and Hydration Properties at Early Growth Stages from Atomistic Simulations. Molecules, 2020, 25, 1848.	3.8	5

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73	AÂTwo-step Aggregation Scheme of Bile Acid Salts, as Seen From Computer Simulations. , 2008, , 181-187.		4
74	Electrokinetic droplet transport from electroosmosis to electrophoresis. Soft Matter, 2018, 14, 9571-9576.	2.7	4
75	Phase stability of the ice XVII-based CO2 chiral hydrate from molecular dynamics simulations. Journal of Chemical Physics, 2019, 151, 104502.	3.0	3
76	Weak scaling of the contact distance between two fluctuating interfaces with system size. Physical Review E, 2020, 102, 062801.	2.1	3
77	Monolayer Structures of Supramolecular Antagonistic Salt Aggregates. Journal of Physical Chemistry B, 2021, 125, 2351-2359.	2.6	3
78	Lattice Boltzmann simulations of drying suspensions of soft particles. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200399.	3.4	3
79	Liquid film rupture beyond the thin-film equation: A multi-component lattice Boltzmann study. Physics of Fluids, 2022, 34, .	4.0	3
80	On the calculation of the surface entropy in computer simulation. Journal of Molecular Liquids, 2018, 262, 58-62.	4.9	2
81	The impact of tensorial temperature on equilibrium thermodynamics. Physical Chemistry Chemical Physics, 2018, 20, 16910-16912.	2.8	2
82	Capillary Interactions, Aggregate Formation, and the Rheology of Particle-Laden Flows: A Lattice Boltzmann Study. Industrial & Engineering Chemistry Research, 2022, 61, 1863-1870.	3.7	2
83	Atomistic Simulation of Oligoelectrolyte Multilayers Growth. , 2016, , 215-228.		1
84	A simple approximation for the distribution of ions between charged plates in the weak coupling regime. Journal of Molecular Liquids, 2018, 271, 301-304.	4.9	1
85	Stochastic dynamics and dominant protein folding pathways. Philosophical Magazine, 2008, 88, 4093-4099.	1.6	0