Patrice Malfreyt

List of Publications by Year
in descending order

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Version: 2024-02-01

94 papers	2,955 citations	109137 35 h-index	174990 52 g-index
94 all docs	94 docs citations	94 times ranked	2095 citing authors

#	Article	IF	Citations
1	Predicting Mechanical Constitutive Laws of Elastomers with Mesoscale Simulations. Macromolecules, 2022, 55, 1487-1494.	2.2	0
2	Enhancing the Thermostability of Engineered Laccases in Aqueous Betaine-Based Natural Deep Eutectic Solvents. ACS Sustainable Chemistry and Engineering, 2022, 10, 572-581.	3.2	14
3	Insulin Adsorption onto PE and PVC Tubings. ACS Applied Bio Materials, 2022, 5, 2567-2575.	2.3	3
4	Molecular interactions at the metalâ€“liquid interfaces. Journal of Chemical Physics, 2022, 156, .	1.2	4
5	Drug Interactions with Plasticized PVCs. ACS Applied Polymer Materials, 2022, 4, 4538-4550.	2.0	5
6	Heterogeneity Effects in Highly Cross-Linked Polymer Networks. Polymers, 2021, 13, 757.	2.0	3
7	Assessing the derivation of time parameters from branched polymer coarse-grain model. Journal of Chemical Physics, 2021, 154, 124901.	1.2	1
8	Associated molecular liquids at the graphene monolayer interface. Journal of Chemical Physics, 2021, 154, 104504.	1.2	6
9	Understanding and Characterizing the Drug Sorption to PVC and PE Materials. ACS Applied Materials & Interfaces, 2021, 13, 18594-18603.	4.0	13
10	Strain induced crystallization of polymers at and above the crystallization temperature by coarse-grained simulations. Journal of Chemical Physics, 2021, 154, 234902.	1.2	2
11	Interfacial tension of the grapheneâ€“water solidâ€“liquid interface: how to handle the electrostatic interactions?. Molecular Physics, 2021, 119, .	0.8	2
12	Rheological properties of polymer chains at a copper oxide surface: Impact of the chain length, surface coverage, and grafted polymer shape. Physical Review E, 2021, 104, 024501.	0.8	2
13	Multi-scale modeling of the polymerâ€“filler interaction. Soft Matter, 2020, 16, 1538-1547.	1.2	10
14	A Multiscale Modelling Approach for the Design of new Polymer Materials. Computer Aided Chemical Engineering, 2020, 48, 25-30.	0.3	0
15	Freeâ€energy calculations of the hostâ€“guest association in grafted supramolecular assemblies. Journal of Computational Chemistry, 2020, 41, 2189-2196.	1.5	0
16	Grain Shape Dynamics for Molecular Simulations at the Mesoscale. Advanced Theory and Simulations, 2020, 3, 2000124.	1.3	5
17	Backbone oriented anisotropic coarse grains for efficient simulations of polymers. Journal of Chemical Physics, 2020, 153, 214901.	1.2	7
18	Molecular Description of Grafted Supramolecular Assemblies on Gold Surfaces: Effect of Grafting Points and Chain Lengths. ACS Omega, 2020, 5, 16628-16634.	1.6	2

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19	Calculation of the surface tension of water: 40 years of molecular simulations. Molecular Simulation, 2019, 45, 295-303.	0.9	19
20	Development of a coarse-grain model for the description of the metal oxide-polymer interface from a bottom-up approach. Journal of Chemical Physics, 2019, 151, 064703.	1.2	9
21	Thermodynamics of Supramolecular Associations with Macrocyclic Water-Soluble Hosts. ACS Omega, 2019, 4, 16899-16905.	1.6	4
22	Atomistic Descriptions of the cis-1,4-Polybutadiene/Silica Interfaces. ACS Applied Polymer Materials, 2019, 1, 969-981.	2.0	18
23	Realistic Coarse-Grain Model of cis-1,4-Polybutadiene: From Chemistry to Rheology. Macromolecules, 2019, 52, 2736-2747.	2.2	27
24	Development of Coarse-Grained Models for Polymers by Trajectory Matching. ACS Omega, 2019, 4, 5955-5967.	1.6	30
25	The pair distribution function in the planar gasâ€“liquid interface: Application to the calculation of the surface tension. Journal of Chemical Physics, 2019, 151, 204702.	1.2	3
26	Anisotropic surface stresses of a solid/fluid interface: Molecular dynamics calculations for the copper/methane interface. Journal of Chemical Physics, 2019, 151, 244703.	1.2	8
27	Calculation of the interfacial tension of the graphene-water interaction by molecular simulations. Journal of Chemical Physics, 2019, 150, 014703.	1.2	26
28	Size-effects on the surface tension near the critical point: Monte Carlo simulations of the Lennard-Jones fluid. Chemical Physics Letters, 2018, 694, 60-64.	1.2	8
29	Calculations of potential of mean force: application to ion-pairs and hostâ€“guest systems. Molecular Physics, 2018, 116, 1998-2008.	0.8	2
30	How Does the Surface Tension Depend on the Surface Area with Coarse-Grained Models?. Journal of Chemical Theory and Computation, 2018, 14, 2644-2651.	2.3	14
31	Calculation of a solid/liquid surface tension: A methodological study. Journal of Chemical Physics, 2018, 148, 034702.	1.2	21
32	Radial-based tail methods for Monte Carlo simulations of cylindrical interfaces. Journal of Chemical Physics, 2018, 148, 094702.	1.2	2
33	Associations of Water-Soluble Macrocyclic Hosts with 4-Aminoazobenzene: Impact of pH. Journal of Physical Chemistry B, 2018, 122, 11953-11961.	1.2	9
34	Coarse-grained modeling of the oilâ€“waterâ€“surfactant interface through the local definition of the pressure tensor and interfacial tension. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	19
35	Test-area surface tension calculation of the graphene-methane interface: Fluctuations and commensurability. Journal of Chemical Physics, 2017, 146, 214112.	1.2	14
36	Development of DPD coarse-grained models: From bulk to interfacial properties. Journal of Chemical Physics, 2016, 145, 054107.	1.2	26

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37	Can we approach the gasâ€“liquid critical point using slab simulations of two coexisting phases?. Journal of Chemical Physics, 2016, 145, 124702.	1.2	5
38	Physics behind Water Transport through Nanoporous Boron Nitride and Graphene. Journal of Physical Chemistry Letters, 2016, 7, 3371-3376.	2.1	70
39	Computer modelling of the surface tension of the gasâ€“liquid and liquidâ€“liquid interface. Chemical Society Reviews, 2016, 45, 1387-1409.	18.7	167
40	Response to â€œComment on â€˜The gas-liquid surface tension of argon: A reconciliation between experiment and simulationâ€â€™ [J. Chem. Phys. 142, 107101 (2015)]. Journal of Chemical Physics, 2015, 142, 107102.	1.2	12
41	Multiscale Modeling of the Polymerâ€“Silica Surface Interaction: From Atomistic to Mesoscopic Simulations. Journal of Physical Chemistry C, 2015, 119, 4817-4826.	1.5	49
42	Prediction of structural and thermomechanical properties of polymers from multiscale simulations. RSC Advances, 2015, 5, 14065-14073.	1.7	30
43	Coarse-Graining the Liquidâ€“Liquid Interfaces with the MARTINI Force Field: How Is the Interfacial Tension Reproduced?. Journal of Chemical Theory and Computation, 2015, 11, 3818-3828.	2.3	40
44	Superpermittivity of nanoconfined water. Journal of Chemical Physics, 2015, 142, 184706.	1.2	32
45	Controlling the Long-Range Corrections in Atomistic Monte Carlo Simulations of Two-Phase Systems. Journal of Chemical Theory and Computation, 2015, 11, 4573-4585.	2.3	24
46	The gas-liquid surface tension of argon: A reconciliation between experiment and simulation. Journal of Chemical Physics, 2014, 140, 244710.	1.2	36
47	How does the dehydration change the hostâ€“guest association under homogeneous and heterogeneous conditions?. Physical Chemistry Chemical Physics, 2014, 16, 8667-8674.	1.3	4
48	Hostâ€“Guest Complexation in the Ferrocenyl Alkanethiolsâ€“Thio Î²-Cyclodextrin Mixed Self-Assembled Monolayers. Journal of Physical Chemistry C, 2014, 118, 3102-3109.	1.5	8
49	Bulk and Liquidâ€“Vapor Interface of Pyrrolidinium-Based Ionic Liquids: A Molecular Simulation Study. Journal of Physical Chemistry B, 2014, 118, 731-742.	1.2	51
50	Quantitative Predictions of the Interfacial Tensions of Liquidâ€“Liquid Interfaces through Atomistic and Coarse Grained Models. Journal of Chemical Theory and Computation, 2014, 10, 1887-1899.	2.3	36
51	Recent advances in Many Body Dissipative Particles Dynamics simulations of liquid-vapor interfaces. European Physical Journal E, 2013, 36, 10.	0.7	66
52	Nonequilibrium Molecular Simulations of New Ionic Lubricants at Metallic Surfaces: Prediction of the Friction. Journal of Chemical Theory and Computation, 2013, 9, 1600-1610.	2.3	67
53	The kinetic friction coefficient of neutral and charged polymer brushes. Soft Matter, 2013, 9, 2966.	1.2	34
54	Prediction of the concentration dependence of the surface tension and density of salt solutions: atomistic simulations using Drude oscillator polarizable and nonpolarizable models. Physical Chemistry Chemical Physics, 2013, 15, 11679.	1.3	29

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55	Why is the association of supramolecular assemblies different under homogeneous and heterogeneous conditions?. Physical Chemistry Chemical Physics, 2012, 14, 10122.	1.3	9
56	Multiscale Modeling Approach toward the Prediction of Viscoelastic Properties of Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4570-4579.	2.3	66
57	Energetic Competition Effects on Thermodynamic Properties of Association between Î²-CD and Fc Group: A Potential of Mean Force Approach. Journal of Physical Chemistry C, 2012, 116, 22350-22358.	1.5	14
58	Frictional forces in polyelectrolyte brushes: effects of sliding velocity, solvent quality and salt. Soft Matter, 2012, 8, 4635.	1.2	36
59	Calculation of the surface tension and pressure components from a non-exponential perturbation method of the thermodynamic route. Journal of Chemical Physics, 2012, 136, 024104.	1.2	32
60	Interactions and Ordering of Ionic Liquids at a Metal Surface. Journal of Chemical Theory and Computation, 2012, 8, 3348-3355.	2.3	66
61	Coarse Grained Simulations of the Electrolytes at the Waterâ€“Air Interface from Many Body Dissipative Particle Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 787-791.	2.3	50
62	Free Energy Calculations in Electroactive Self-Assembled Monolayers (SAMs): Impact of the Chain Length on the Redox Reaction. Journal of Physical Chemistry B, 2011, 115, 11678-11687.	1.2	14
63	Local pressure components and surface tension of spherical interfaces. Thermodynamic versus mechanical definitions. I. A mesoscale modeling of droplets. Journal of Chemical Physics, 2011, 135, 104105.	1.2	23
64	Prediction of the Temperature Dependence of the Surface Tension Of SO₂, N₂, O₂, and Ar by Monte Carlo Molecular Simulations. Journal of Physical Chemistry B, 2011, 115, 9421-9430.	1.2	49
65	Surface tension of waterâ€“alcohol mixtures from Monte Carlo simulations. Journal of Chemical Physics, 2011, 134, 044709.	1.2	81
66	A Transferable Force Field To Predict Phase Equilibria and Surface Tension of Ethers and Glycol Ethers. Journal of Physical Chemistry B, 2011, 115, 10654-10664.	1.2	45
67	Prediction of the Surface Tension of the Liquidâ^'Vapor Interface of Alcohols from Monte Carlo Simulations. Journal of Physical Chemistry C, 2011, 115, 8670-8683.	1.5	42
68	Mesoscale modeling of the water liquid-vapor interface: A surface tension calculation. Physical Review E, 2011, 83, 051601.	0.8	83
69	Interactions between polymer brushes and a polymer solution: mesoscale modelling of the structural and frictional properties. Soft Matter, 2010, 6, 3472.	1.2	46
70	Numerical evidence of the formation of a thin microscopic film of methane at the water surface: a free energy calculation. Physical Chemistry Chemical Physics, 2010, 12, 5203.	1.3	32
71	Mesoscopic Simulation of Entangled Polymer Brushes under Shear: Compression and Rheological Properties. Macromolecules, 2009, 42, 4310-4318.	2.2	46
72	Calculation of the surface tension from Monte Carlo simulations: Does the model impact on the finite-size effects?. Journal of Chemical Physics, 2009, 130, 184710.	1.2	82

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73	Expressions for local contributions to the surface tension from the virial route. Physical Review E, 2008, 77, 031601.	0.8	64
74	Surface tension of water and acid gases from Monte Carlo simulations. Journal of Chemical Physics, 2008, 128, 154716.	1.2	84
75	Multiple histogram reweighting method for the surface tension calculation. Journal of Chemical Physics, 2008, 128, 154718.	1.2	42
76	Mesoscopic simulation of entanglements using dissipative particle dynamics: Application to polymer brushes. Journal of Chemical Physics, 2008, 129, 034902.	1.2	76
77	Molecular simulations of grafted metal-chelating monolayers: methodology, structure and energy. Molecular Physics, 2008, 106, 1397-1411.	0.8	11
78	Molecular simulations of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-alkane liquid-vapor interface: Interfacial properties and their long range corrections. Physical Review E, 2007, 75, 051602.	0.8	97
79	Computational and Experimental Investigations of Supramolecular Assemblies of p-Sulfonatocalix[4]arene Organized by Weak Forces. Journal of Physical Chemistry B, 2007, 111, 11478-11485.	1.2	9
80	Methodology for the Calculation of the Potential of Mean Force for a Cationâ€“Ï€ Complex in Water. ChemPhysChem, 2007, 8, 1648-1656.	1.0	8
81	Entropy and enthalpy calculations from perturbation and integration thermodynamics methods using molecular dynamics simulations: applications to the calculation of hydration and association thermodynamic properties. Molecular Physics, 2006, 104, 2929-2943.	0.8	47
82	Calculation of the absolute thermodynamic properties of association of host-guest systems from the intermolecular potential of mean force. Journal of Chemical Physics, 2006, 125, 224503.	1.2	11
83	The compression of polymer brushes under shear: the friction coefficient as a function of compression, shear rate and the properties of the solvent. Molecular Physics, 2005, 103, 2675-2285.	0.8	43
84	Monte Carlo versus molecular dynamics simulations in heterogeneous systems: An application to the n-pentane liquid-vapor interface. Journal of Chemical Physics, 2004, 121, 12559.	1.2	71
85	Dissipative Particle Dynamics Simulations in the Grand Canonical Ensemble: Applications to Polymer Brushes. ChemPhysChem, 2004, 5, 457-464.	1.0	58
86	Structures and Energetics of Complexes of the p-Sulfonatocalix[4]arene with Ammonium, Alkylammonium, and Tetraalkylammonium Cations in Water Using Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 5095-5104.	1.2	41
87	Gibbs Free Energy Perturbation Calculations:â€‰ An Application to the Binding of Alkylammonium Cations by a Water-Soluble Calixarene. Journal of Physical Chemistry B, 2004, 108, 11744-11752.	1.2	35
88	Molecular Dynamics Simulations ofp-Sulfonatocalix[4]arene Complexes with Inorganic and Organic Cations in Water:Â A Structural and Thermodynamic Study. Journal of Physical Chemistry B, 2002, 106, 4516-4524.	1.2	49
89	Dissipative particle dynamics simulation of grafted polymer brushes under shear. Physical Chemistry Chemical Physics, 2002, 4, 3008-3015.	1.3	74
90	Direct Monte Carlo simulations of the equilibrium properties ofn-pentane liquidâ€“vapor interface. Journal of Chemical Physics, 2002, 116, 8106-8117.	1.2	75

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91	Vapour-Liquid Phase Equilibria of n-alkanes by Direct Monte Carlo Simulations. Molecular Simulation, 2001, 27, 99-114.	0.9	41
92	Dissipative Particle Dynamics Simulations of Grafted Polymer Chains between Two Walls. Langmuir, 2000, 16, 4732-4740.	1.6	96
93	Cloud Microorganisms, an Interesting Source of Biosurfactants. , 0, , .		6
94	Investigation of the Complexation between 4-Aminoazobenzene and Cucurbit[7]uril through a Combined Spectroscopic, Nuclear Magnetic Resonance, and Molecular Simulation Studies. ACS Omega, 0, , .	1.6	3