

# Patrice Malfreyt

## List of Publications by Year in descending order

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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	Computer modelling of the surface tension of the gas-liquid and liquid-liquid interface. <i>Chemical Society Reviews</i> , 2016, 45, 1387-1409.	18.7	167
2	Molecular simulations of the $n$ -alkane liquid-vapor interface: Interfacial properties and their long range corrections. <i>Physical Review E</i> , 2007, 75, 051602.	0.8	97
3	Dissipative Particle Dynamics Simulations of Grafted Polymer Chains between Two Walls. <i>Langmuir</i> , 2000, 16, 4732-4740.	1.6	96
4	Surface tension of water and acid gases from Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2008, 128, 154716.	1.2	84
5	Mesoscale modeling of the water liquid-vapor interface: A surface tension calculation. <i>Physical Review E</i> , 2011, 83, 051601.	0.8	83
6	Calculation of the surface tension from Monte Carlo simulations: Does the model impact on the finite-size effects?. <i>Journal of Chemical Physics</i> , 2009, 130, 184710.	1.2	82
7	Surface tension of water-alcohol mixtures from Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2011, 134, 044709.	1.2	81
8	Mesoscopic simulation of entanglements using dissipative particle dynamics: Application to polymer brushes. <i>Journal of Chemical Physics</i> , 2008, 129, 034902.	1.2	76
9	Direct Monte Carlo simulations of the equilibrium properties of <i>n</i> -pentane liquid-vapor interface. <i>Journal of Chemical Physics</i> , 2002, 116, 8106-8117.	1.2	75
10	Dissipative particle dynamics simulation of grafted polymer brushes under shear. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 3008-3015.	1.3	74
11	Monte Carlo versus molecular dynamics simulations in heterogeneous systems: An application to the <i>n</i> -pentane liquid-vapor interface. <i>Journal of Chemical Physics</i> , 2004, 121, 12559.	1.2	71
12	Physics behind Water Transport through Nanoporous Boron Nitride and Graphene. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3371-3376.	2.1	70
13	Nonequilibrium Molecular Simulations of New Ionic Lubricants at Metallic Surfaces: Prediction of the Friction. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1600-1610.	2.3	67
14	Multiscale Modeling Approach toward the Prediction of Viscoelastic Properties of Polymers. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4570-4579.	2.3	66
15	Interactions and Ordering of Ionic Liquids at a Metal Surface. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3348-3355.	2.3	66
16	Recent advances in Many Body Dissipative Particles Dynamics simulations of liquid-vapor interfaces. <i>European Physical Journal E</i> , 2013, 36, 10.	0.7	66
17	Expressions for local contributions to the surface tension from the virial route. <i>Physical Review E</i> , 2008, 77, 031601.	0.8	64
18	Dissipative Particle Dynamics Simulations in the Grand Canonical Ensemble: Applications to Polymer Brushes. <i>ChemPhysChem</i> , 2004, 5, 457-464.	1.0	58

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19	Bulk and Liquid-Vapor Interface of Pyrrolidinium-Based Ionic Liquids: A Molecular Simulation Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 731-742.	1.2	51
20	Coarse Grained Simulations of the Electrolytes at the Water-Air Interface from Many Body Dissipative Particle Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 787-791.	2.3	50
21	Molecular Dynamics Simulations of p-Sulfonatocalix[4]arene Complexes with Inorganic and Organic Cations in Water: A Structural and Thermodynamic Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 4516-4524.	1.2	49
22	Prediction of the Temperature Dependence of the Surface Tension Of $\text{SO}_2$ , $\text{N}_2$ , $\text{O}_2$ , and Ar by Monte Carlo Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9421-9430.	1.2	49
23	Multiscale Modeling of the Polymer-Silica Surface Interaction: From Atomistic to Mesoscopic Simulations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4817-4826.	1.5	49
24	Entropy and enthalpy calculations from perturbation and integration thermodynamics methods using molecular dynamics simulations: applications to the calculation of hydration and association thermodynamic properties. <i>Molecular Physics</i> , 2006, 104, 2929-2943.	0.8	47
25	Mesoscopic Simulation of Entangled Polymer Brushes under Shear: Compression and Rheological Properties. <i>Macromolecules</i> , 2009, 42, 4310-4318.	2.2	46
26	Interactions between polymer brushes and a polymer solution: mesoscale modelling of the structural and frictional properties. <i>Soft Matter</i> , 2010, 6, 3472.	1.2	46
27	A Transferable Force Field To Predict Phase Equilibria and Surface Tension of Ethers and Glycol Ethers. <i>Journal of Physical Chemistry B</i> , 2011, 115, 10654-10664.	1.2	45
28	The compression of polymer brushes under shear: the friction coefficient as a function of compression, shear rate and the properties of the solvent. <i>Molecular Physics</i> , 2005, 103, 2675-2285.	0.8	43
29	Multiple histogram reweighting method for the surface tension calculation. <i>Journal of Chemical Physics</i> , 2008, 128, 154718.	1.2	42
30	Prediction of the Surface Tension of the Liquid-Vapor Interface of Alcohols from Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8670-8683.	1.5	42
31	Vapour-Liquid Phase Equilibria of n-alkanes by Direct Monte Carlo Simulations. <i>Molecular Simulation</i> , 2001, 27, 99-114.	0.9	41
32	Structures and Energetics of Complexes of the p-Sulfonatocalix[4]arene with Ammonium, Alkylammonium, and Tetraalkylammonium Cations in Water Using Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 5095-5104.	1.2	41
33	Coarse-Graining the Liquid-Liquid Interfaces with the MARTINI Force Field: How Is the Interfacial Tension Reproduced?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3818-3828.	2.3	40
34	Frictional forces in polyelectrolyte brushes: effects of sliding velocity, solvent quality and salt. <i>Soft Matter</i> , 2012, 8, 4635.	1.2	36
35	The gas-liquid surface tension of argon: A reconciliation between experiment and simulation. <i>Journal of Chemical Physics</i> , 2014, 140, 244710.	1.2	36
36	Quantitative Predictions of the Interfacial Tensions of Liquid-Liquid Interfaces through Atomistic and Coarse Grained Models. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1887-1899.	2.3	36

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37	Gibbs Free Energy Perturbation Calculations: An Application to the Binding of Alkylammonium Cations by a Water-Soluble Calixarene. <i>Journal of Physical Chemistry B</i> , 2004, 108, 11744-11752.	1.2	35
38	The kinetic friction coefficient of neutral and charged polymer brushes. <i>Soft Matter</i> , 2013, 9, 2966.	1.2	34
39	Numerical evidence of the formation of a thin microscopic film of methane at the water surface: a free energy calculation. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5203.	1.3	32
40	Calculation of the surface tension and pressure components from a non-exponential perturbation method of the thermodynamic route. <i>Journal of Chemical Physics</i> , 2012, 136, 024104.	1.2	32
41	Superpermittivity of nanoconfined water. <i>Journal of Chemical Physics</i> , 2015, 142, 184706.	1.2	32
42	Prediction of structural and thermomechanical properties of polymers from multiscale simulations. <i>RSC Advances</i> , 2015, 5, 14065-14073.	1.7	30
43	Development of Coarse-Grained Models for Polymers by Trajectory Matching. <i>ACS Omega</i> , 2019, 4, 5955-5967.	1.6	30
44	Prediction of the concentration dependence of the surface tension and density of salt solutions: atomistic simulations using Drude oscillator polarizable and nonpolarizable models. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11679.	1.3	29
45	Realistic Coarse-Grain Model of <i>cis</i> -1,4-Polybutadiene: From Chemistry to Rheology. <i>Macromolecules</i> , 2019, 52, 2736-2747.	2.2	27
46	Development of DPD coarse-grained models: From bulk to interfacial properties. <i>Journal of Chemical Physics</i> , 2016, 145, 054107.	1.2	26
47	Calculation of the interfacial tension of the graphene-water interaction by molecular simulations. <i>Journal of Chemical Physics</i> , 2019, 150, 014703.	1.2	26
48	Controlling the Long-Range Corrections in Atomistic Monte Carlo Simulations of Two-Phase Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4573-4585.	2.3	24
49	Local pressure components and surface tension of spherical interfaces. Thermodynamic versus mechanical definitions. I. A mesoscale modeling of droplets. <i>Journal of Chemical Physics</i> , 2011, 135, 104105.	1.2	23
50	Calculation of a solid/liquid surface tension: A methodological study. <i>Journal of Chemical Physics</i> , 2018, 148, 034702.	1.2	21
51	Coarse-grained modeling of the oil-water surfactant interface through the local definition of the pressure tensor and interfacial tension. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	19
52	Calculation of the surface tension of water: 40 years of molecular simulations. <i>Molecular Simulation</i> , 2019, 45, 295-303.	0.9	19
53	Atomistic Descriptions of the <i>cis</i> -1,4-Polybutadiene/Silica Interfaces. <i>ACS Applied Polymer Materials</i> , 2019, 1, 969-981.	2.0	18
54	Free Energy Calculations in Electroactive Self-Assembled Monolayers (SAMs): Impact of the Chain Length on the Redox Reaction. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11678-11687.	1.2	14

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55	Energetic Competition Effects on Thermodynamic Properties of Association between $\beta$ -CD and Fc Group: A Potential of Mean Force Approach. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22350-22358.	1.5	14
56	Test-area surface tension calculation of the graphene-methane interface: Fluctuations and commensurability. <i>Journal of Chemical Physics</i> , 2017, 146, 214112.	1.2	14
57	How Does the Surface Tension Depend on the Surface Area with Coarse-Grained Models?. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2644-2651.	2.3	14
58	Enhancing the Thermostability of Engineered Laccases in Aqueous Betaine-Based Natural Deep Eutectic Solvents. <i>ACS Sustainable Chemistry and Engineering</i> , 2022, 10, 572-581.	3.2	14
59	Understanding and Characterizing the Drug Sorption to PVC and PE Materials. <i>ACS Applied Materials &amp; Interfaces</i> , 2021, 13, 18594-18603.	4.0	13
60	Response to "Comment on "The gas-liquid surface tension of argon: A reconciliation between experiment and simulation" [J. Chem. Phys. 142, 107101 (2015)]. <i>Journal of Chemical Physics</i> , 2015, 142, 107102.	1.2	12
61	Calculation of the absolute thermodynamic properties of association of host-guest systems from the intermolecular potential of mean force. <i>Journal of Chemical Physics</i> , 2006, 125, 224503.	1.2	11
62	Molecular simulations of grafted metal-chelating monolayers: methodology, structure and energy. <i>Molecular Physics</i> , 2008, 106, 1397-1411.	0.8	11
63	Multi-scale modeling of the polymer-filler interaction. <i>Soft Matter</i> , 2020, 16, 1538-1547.	1.2	10
64	Computational and Experimental Investigations of Supramolecular Assemblies of <i>p</i> -Sulfonatocalix[4]arene Organized by Weak Forces. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11478-11485.	1.2	9
65	Why is the association of supramolecular assemblies different under homogeneous and heterogeneous conditions?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10122.	1.3	9
66	Associations of Water-Soluble Macrocyclic Hosts with 4-Aminoazobenzene: Impact of pH. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11953-11961.	1.2	9
67	Development of a coarse-grain model for the description of the metal oxide-polymer interface from a bottom-up approach. <i>Journal of Chemical Physics</i> , 2019, 151, 064703.	1.2	9
68	Methodology for the Calculation of the Potential of Mean Force for a Cation- $\beta$ CD Complex in Water. <i>ChemPhysChem</i> , 2007, 8, 1648-1656.	1.0	8
69	Host-Guest Complexation in the Ferrocenyl Alkanethiols-Thio $\beta$ -Cyclodextrin Mixed Self-Assembled Monolayers. <i>Journal of Physical Chemistry C</i> , 2014, 118, 3102-3109.	1.5	8
70	Size-effects on the surface tension near the critical point: Monte Carlo simulations of the Lennard-Jones fluid. <i>Chemical Physics Letters</i> , 2018, 694, 60-64.	1.2	8
71	Anisotropic surface stresses of a solid/fluid interface: Molecular dynamics calculations for the copper/methane interface. <i>Journal of Chemical Physics</i> , 2019, 151, 244703.	1.2	8
72	Backbone oriented anisotropic coarse grains for efficient simulations of polymers. <i>Journal of Chemical Physics</i> , 2020, 153, 214901.	1.2	7

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73	Cloud Microorganisms, an Interesting Source of Biosurfactants. , 0, , .		6
74	Associated molecular liquids at the graphene monolayer interface. Journal of Chemical Physics, 2021, 154, 104504.	1.2	6
75	Can we approach the gas-liquid critical point using slab simulations of two coexisting phases?. Journal of Chemical Physics, 2016, 145, 124702.	1.2	5
76	Grain Shape Dynamics for Molecular Simulations at the Mesoscale. Advanced Theory and Simulations, 2020, 3, 2000124.	1.3	5
77	Drug Interactions with Plasticized PVCs. ACS Applied Polymer Materials, 2022, 4, 4538-4550.	2.0	5
78	How does the dehydration change the host-guest association under homogeneous and heterogeneous conditions?. Physical Chemistry Chemical Physics, 2014, 16, 8667-8674.	1.3	4
79	Thermodynamics of Supramolecular Associations with Macrocyclic Water-Soluble Hosts. ACS Omega, 2019, 4, 16899-16905.	1.6	4
80	Molecular interactions at the metal-liquid interfaces. Journal of Chemical Physics, 2022, 156, .	1.2	4
81	The pair distribution function in the planar gas-liquid interface: Application to the calculation of the surface tension. Journal of Chemical Physics, 2019, 151, 204702.	1.2	3
82	Heterogeneity Effects in Highly Cross-Linked Polymer Networks. Polymers, 2021, 13, 757.	2.0	3
83	Insulin Adsorption onto PE and PVC Tubings. ACS Applied Bio Materials, 2022, 5, 2567-2575.	2.3	3
84	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
85	Calculations of potential of mean force: application to ion-pairs and host-guest systems. Molecular Physics, 2018, 116, 1998-2008.	0.8	2
86	Radial-based tail methods for Monte Carlo simulations of cylindrical interfaces. Journal of Chemical Physics, 2018, 148, 094702.	1.2	2
87	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
88	Interfacial tension of the graphene-water solid-liquid interface: how to handle the electrostatic interactions?. Molecular Physics, 2021, 119, .	0.8	2
89	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
90	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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91	Assessing the derivation of time parameters from branched polymer coarse-grain model. Journal of Chemical Physics, 2021, 154, 124901.	1.2	1
92	A Multiscale Modelling Approach for the Design of new Polymer Materials. Computer Aided Chemical Engineering, 2020, 48, 25-30.	0.3	0
93	Free energy calculations of the host-guest association in grafted supramolecular assemblies. Journal of Computational Chemistry, 2020, 41, 2189-2196.	1.5	0
94	Predicting Mechanical Constitutive Laws of Elastomers with Mesoscale Simulations. Macromolecules, 2022, 55, 1487-1494.	2.2	0