Florian Mller-Plathe

List of Publications by Citations

90 papers	6,607 citations	35 h-index	81 g-index
100 ext. papers	7,307 ext. citations	4.5 avg, IF	6.38 L-index

#	Paper	IF	Citations
90	A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity. *Journal of Chemical Physics*, **1997**, 106, 6082-6085	3.9	1033
89	Deriving effective mesoscale potentials from atomistic simulations. *Journal of Computational Chemistry*, **2003**, 24, 1624-36	3.5	917
88	Coarse-graining in polymer simulation: from the atomistic to the mesoscopic scale and back. *ChemPhysChem*, **2002**, 3, 755-69	3.2	681
87	Reversing the perturbation in nonequilibrium molecular dynamics: an easy way to calculate the shear viscosity of fluids. *Physical Review E*, **1999**, 59, 4894-8	2.4	300
86	Are there stable ion-pairs in room-temperature ionic liquids? Molecular dynamics simulations of 1-n-butyl-3-methylimidazolium hexafluorophosphate. *Journal of the American Chemical Society*, **2009**, 131, 15825-33	16.4	245
85	Mapping atomistic simulations to mesoscopic models: a systematic coarse-graining procedure for vinyl polymer chains. *Journal of Physical Chemistry B*, **2005**, 109, 18609-19	3.4	213
84	Mapping Atomistic to Coarse-Grained Polymer Models Using Automatic Simplex Optimization To Fit Structural Properties. *Macromolecules*, **2001**, 34, 2335-2345	5.5	176
83	Temperature-Transferable Coarse-Grained Potentials for Ethylbenzene, Polystyrene, and Their Mixtures. *Macromolecules*, **2008**, 41, 9919-9929	5.5	174
82	Transferability of coarse-grained force fields: the polymer case. *Journal of Chemical Physics*, **2008**, 128, 064904	3.9	171
81	Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts:□Structure, Thermodynamic Properties, Chain Conformation, and Entanglements. *Macromolecules*, **2007**, 40, 3876-3885	5.5	165
80	YASP: A molecular simulation package. *Computer Physics Communications*, **1993**, 78, 77-94	4.2	163
79	Force field parametrization by weak coupling. Re-engineering SPC water. *Chemical Physics Letters*, **1995**, 232, 429-436	2.5	143
78	Interphase Structure in Silica□Polystyrene Nanocomposites: A Coarse-Grained Molecular Dynamics Study. *Macromolecules*, **2012**, 45, 572-584	5.5	140
77	Thermal conductivities of molecular liquids by reverse nonequilibrium molecular dynamics. *Journal of Physical Chemistry B*, **2005**, 109, 15060-7	3.4	136
76	The thermal conductivity and thermal rectification of carbon nanotubes studied using reverse non-equilibrium molecular dynamics simulations. *Nanotechnology*, **2009**, 20, 115704	3.4	124
75	Interface and Interphase Dynamics of Polystyrene Chains near Grafted and Ungrafted Silica Nanoparticles. *Macromolecules*, **2012**, 45, 171-179	5.5	121
74	Molecular Dynamics Simulation of a Silica Nanoparticle in Oligomeric Poly(methyl methacrylate): A Model System for Studying the Interphase Thickness in a Polymer□Nanocomposite via Different Properties. *Macromolecules*, **2013**, 46, 8680-8692	5.5	91

73	How good are coarse-grained polymer models? A comparison for atactic polystyrene. *ChemPhysChem*, **2012**, 13, 3428-39	3.2	85
72	How Thick is the Interphase in an Ultrathin Polymer Film? Coarse-Grained Molecular Dynamics Simulations of Polyamide-6,6 on Graphene. *Journal of Physical Chemistry C*, **2013**, 117, 5249-5257	3.8	63
71	Recovering the reptation dynamics of polymer melts in dissipative particle dynamics simulations via slip-springs. *Journal of Chemical Physics*, **2013**, 138, 104907	3.9	63
70	Molecular Dynamics Simulation of Sorption of Gases in Polystyrene. *Macromolecules*, **2007**, 40, 6413-6421	3.5	60
69	Mechanical behavior and interphase structure in a silica-polystyrene nanocomposite under uniaxial deformation. *Nanotechnology*, **2012**, 23, 305702	3.4	58
68	Parallelizing a molecular dynamics algorithm on a multiprocessor workstation using OpenMP. *Journal of Chemical Information and Modeling*, **2005**, 45, 1943-52	6.1	55
67	Molecular dynamics simulation in the grand canonical ensemble. *Journal of Computational Chemistry*, **2007**, 28, 1763-73	3.5	53
66	Pinning of the Contact Line during Evaporation on Heterogeneous Surfaces: Slowdown or Temporary Immobilization? Insights from a Nanoscale Study. *Langmuir*, **2015**, 31, 7544-52	4	50
65	Nonequilibrium molecular dynamics calculation of the thermal conductivity of amorphous polyamide-6,6. *Journal of Physical Chemistry B*, **2007**, 111, 11516-23	3.4	47
64	Shear viscosity of the ionic liquid 1-n-butyl 3-methylimidazolium hexafluorophosphate [bmim][pf6] computed by reverse nonequilibrium molecular dynamics. *Journal of Physical Chemistry B*, **2008**, 112, 8129-33	3.4	44
63	Increasing the Thermal Conductivity of Graphene-Polyamide-6,6 Nanocomposites by Surface-Grafted Polymer Chains: Calculation with Molecular Dynamics and Effective-Medium Approximation. *Journal of Physical Chemistry B*, **2016**, 120, 1336-46	3.4	42
62	Temperature dependence of coarse-grained potentials for liquid hexane. *Physical Chemistry Chemical Physics*, **2011**, 13, 2894-902	3.6	42
61	Effective control of the transport coefficients of a coarse-grained liquid and polymer models using the dissipative particle dynamics and Lowe-Andersen equations of motion. *Physical Chemistry Chemical Physics*, **2009**, 11, 1962-9	3.6	41
60	Cyclohexane□Benzene Mixtures:□Thermodynamics and Structure from Atomistic Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 7415-7423	3.4	39
59	A kinetic chain growth algorithm in coarse-grained simulations. *Journal of Computational Chemistry*, **2016**, 37, 2634-2646	3.5	36
58	Influence of contact-line curvature on the evaporation of nanodroplets from solid substrates. *Physical Review Letters*, **2014**, 113, 046101	7.4	35
57	Reactive molecular dynamics with material-specific coarse-grained potentials: growth of polystyrene chains from styrene monomers. *Journal of Physical Chemistry B*, **2010**, 114, 13656-66	3.4	35
56	Thermal Transport at Solid-Liquid Interfaces: High Pressure Facilitates Heat Flow through Nonlocal Liquid Structuring. *Journal of Physical Chemistry Letters*, **2017**, 8, 1946-1951	6.4	34

55	Sorption and diffusion of carbon dioxide and nitrogen in poly(methyl methacrylate). *Journal of Chemical Physics*, **2013**, 139, 124902	3.9	33
54	Molecular Dynamics Calculations of the Thermal Conductivity of Molecular Liquids, Polymers, and Carbon Nanotubes. *Soft Materials*, **2012**, 10, 42-80	1.7	32
53	Anisotropy of the thermal conductivity of stretched amorphous polystyrene in supercritical carbon dioxide studied by reverse nonequilibrium molecular dynamics simulations. *Journal of Physical Chemistry B*, **2009**, 113, 14596-603	3.4	30
52	Thermal conductivity of carbon nanotube-polyamide-6,6 nanocomposites: reverse non-equilibrium molecular dynamics simulations. *Journal of Chemical Physics*, **2011**, 135, 184905	3.9	28
51	Molecular structure and multi-body potential of mean force in silica-polystyrene nanocomposites. *Nanoscale*, **2018**, 10, 21656-21670	7.7	28
50	A Multichain Slip-Spring Dissipative Particle Dynamics Simulation Method for Entangled Polymer Solutions. *Macromolecules*, **2016**, 49, 9186-9191	5.5	23
49	Nonperiodic stochastic boundary conditions for molecular dynamics simulations of materials embedded into a continuum mechanics domain. *Journal of Chemical Physics*, **2011**, 134, 154108	3.9	22
48	Molecular Dynamics Study on the Thermal Conductivity of the End-grafted Carbon Nanotubes Filled Polyamide-6.6 Nanocomposites. *Journal of Physical Chemistry C*, **2018**, 122, 1412-1421	3.8	21
47	Polymeric Flower-Like Microparticles from Self-Assembled Cellulose Stearoyl Esters. *ACS Macro Letters*, **2015**, 4, 214-219	6.6	21
46	Reptation and constraint release dynamics in bidisperse polymer melts. *Journal of Chemical Physics*, **2014**, 141, 194904	3.9	20
45	Water permeability of poly(ethylene terephthalate): a grand canonical ensemble molecular dynamics simulation study. *Journal of Chemical Physics*, **2009**, 131, 234904	3.9	20
44	Loss of Molecular Roughness upon Coarse-Graining Predicts the Artificially Accelerated Mobility of Coarse-Grained Molecular Simulation Models. *Journal of Chemical Theory and Computation*, **2020**, 16, 1411-1419	6.4	20
43	A Local Order Parameter-Based Method for Simulation of Free Energy Barriers in Crystal Nucleation. *Journal of Chemical Theory and Computation*, **2017**, 13, 1307-1316	6.4	19
42	Gaussian Charge Distributions for Incorporation of Electrostatic Interactions in Dissipative Particle Dynamics: Application to Self-Assembly of Surfactants. *Journal of Chemical Theory and Computation* , **2019**, 15, 4197-4207	6.4	19
41	Molecular Mobility in Cyclic Hydrocarbons: A Simulation Study. *Journal of Physical Chemistry B*, **1999**, 103, 9731-9737	3.4	19
40	Local bond order parameters for accurate determination of crystal structures in two and three dimensions. *Physical Chemistry Chemical Physics*, **2018**, 20, 27059-27068	3.6	19
39	Solid□iquid and Solid□olid Phase Diagrams of Self-Assembled Triblock Janus Nanoparticles from Solution. *Journal of Physical Chemistry C*, **2018**, 122, 9235-9244	3.8	18
38	Investigation of interphase effects in silica-polystyrene nanocomposites based on a hybrid molecular-dynamics-finite-element simulation framework. *Physical Review E*, **2016**, 93, 052505	2.4	18

37	Distribution of the Number of Polymer Chains Grafted on Nanoparticles Fabricated by Grafting-to and Grafting-from Procedures. *Macromolecules*, **2018**, 51, 3758-3766	5.5	17
36	Do Transport Properties of Entangled Linear Polymers Scale with Excess Entropy?. *Macromolecules*, **2013**, 46, 8710-8723	5.5	16
35	Self-Assembly Mechanisms of Triblock Janus Particles. *Journal of Chemical Theory and Computation*, **2019**, 15, 1345-1354	6.4	16
34	Effect of grafted chains on the heat transfer between carbon nanotubes in a polyamide-6.6 matrix: A molecular dynamics study. *Polymer*, **2017**, 129, 228-234	3.9	13
33	A molecular dynamics study of viscosity in ionic liquids directed by quantitative structure-property relationships. *ChemPhysChem*, **2012**, 13, 1791-801	3.2	13
32	Influence of Polymer Bidispersity on the Effective Particle–Particle Interactions in Polymer Nanocomposites. *Macromolecules*, **2019**, 52, 8826-8839	5.5	12
31	Molecular dynamics method to locally resolve Poisson's ratio: Mechanical description of the solid-soft-matter interphase. *Physical Review E*, **2012**, 86, 036704	2.4	12
30	A steady-state non-equilibrium molecular dynamics approach for the study of evaporation processes. *Journal of Chemical Physics*, **2013**, 139, 134701	3.9	12
29	Fast relaxation of coarse-grained models of polymer interphases by hybrid particle-field molecular dynamics: Polystyrene-silica nanocomposites as an example. *European Physical Journal: Special Topics*, **2016**, 225, 1817-1841	2.3	11
28	Predicting the Mobility Increase of Coarse-Grained Polymer Models from Excess Entropy Differences. *Journal of Chemical Theory and Computation*, **2020**, 16, 1431-1447	6.4	10
27	Mechanisms of Nucleation and Solid-Solid-Phase Transitions in Triblock Janus Assemblies. *Journal of Chemical Theory and Computation*, **2021**, 17, 1742-1754	6.4	10
26	Adaptive-numerical-bias metadynamics. *Journal of Computational Chemistry*, **2017**, 38, 2721-2729	3.5	9
25	Excess entropy scaling for the segmental and global dynamics of polyethylene melts. *Physical Chemistry Chemical Physics*, **2014**, 16, 24301-11	3.6	9
24	A reverse nonequilibrium molecular dynamics method for calculating the mutual diffusion coefficient for binary fluids. *Chemical Engineering Science*, **2015**, 130, 1-7	4.4	9
23	Thermal Energy Transport across the Interface between Phase Change Material n-Heneicosane in Solid and Liquid Phases and Few-Layer Graphene. *Journal of Physical Chemistry C*, **2019**, 123, 29192-29202	3.8	8
22	A comparison of sulfur mustard and heptane penetrating a dipalmitoylphosphatidylcholine bilayer membrane. *Journal of Hazardous Materials*, **2009**, 168, 13-24	12.8	8
21	Coarse-Grained Molecular Simulation Model for Gecko Feet Keratin. *Journal of Physical Chemistry B*, **2018**, 122, 2203-2212	3.4	7
20	Polymer Chain Collapse upon Rapid Solvent Exchange: Slip-Spring Dissipative Particle Dynamics Simulations with an Explicit-Solvent Model. *Journal of Physical Chemistry C*, **2017**, 121, 27664-27673	3.8	7

19	Application of Reverse Nonequilibrium Molecular Dynamics to the Calculation of the Mutual Diffusion Coefficient of Alkane Mixtures. *Journal of Physical Chemistry B*, **2018**, 122, 9210-9217	3.4	7
18	How Alcoholic Disinfectants Affect Coronavirus Model Membranes: Membrane Fluidity, Permeability, and Disintegration. *Journal of Physical Chemistry B*, **2020**, 124, 10374-10385	3.4	6
17	Robustness of a new molecular dynamics-finite element coupling approach for soft matter systems analyzed by uncertainty quantification. *Journal of Chemical Physics*, **2015**, 142, 104105	3.9	5
16	The Influence of Entanglements on the Dynamics of Flash Nanoprecipitation: A Slip-Spring Dissipative-Particle-Dynamics Investigation. *Journal of Chemical & Engineering Data*, **2020**, 65, 1264-1272	2.8	5
15	Atomistic hybrid particle-field molecular dynamics combined with slip-springs: Restoring entangled dynamics to simulations of polymer melts. *Journal of Computational Chemistry*, **2021**, 42, 6-18	3.5	5
14	Combination of Hybrid Particle-Field Molecular Dynamics and Slip-Springs for the Efficient Simulation of Coarse-Grained Polymer Models: Static and Dynamic Properties of Polystyrene Melts. *Journal of Chemical Theory and Computation*, **2021**, 17, 474-487	6.4	5
13	Gecko adhesion: a molecular-simulation perspective on the effect of humidity.. *Soft Matter*, **2022**,	3.6	4
12	Different Stages of Polymer-Chain Collapse Following Solvent Quenching: Scaling Relations from Dissipative Particle Dynamics Simulations. *Macromolecules*, **2020**, 53, 8889-8900	5.5	4
11	Rebound Suppression of a Droplet Impacting on a Supersolvophobic Surface by a Small Amount of Polymer Additives.. *ACS Macro Letters*, **2021**, 10, 192-196	6.6	4
10	Simulation of Elastomers by Slip-Spring Dissipative Particle Dynamics. *Macromolecules*, **2021**, 54, 5155-5166	5.5	3
9	Sequence-Engineering Polyethylene-Polypropylene Copolymers with High Thermal Conductivity Using a Molecular-Dynamics-Based Genetic Algorithm. *Journal of Chemical Theory and Computation*, **2021**, 17, 3772-3782	6.4	3
8	Extending reverse nonequilibrium molecular dynamics to the calculation of mutual diffusion coefficients in molecular fluid mixtures. *Molecular Simulation*, **2016**, 42, 1379-1384	2	2
7	Suppressing the rebound of impacting droplets from solvophobic surfaces by polymer additives: polymer adsorption and molecular mechanisms. *Soft Matter*, **2021**, 17, 6952-6963	3.6	2
6	Addressing Surface Effects at the Particle-Continuum Interface in a Molecular Dynamics and Finite Elements Coupled Multiscale Simulation Technique.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
5	Compatibilization Efficiency of Additives in Homopolymer Blends: A Dissipative Particle Dynamics Study. *Macromolecules*, **2021**, 54, 9551-9564	5.5	1
4	Uncertainty Quantification Guided Parameter Selection in a Fully Coupled Molecular Dynamics-Finite Element Model of the Mechanical Behavior of Polymers. *Journal of Chemical Theory and Computation*, **2021**, 17, 3760-3771	6.4	1
3	Effect of Defects on the Interfacial Thermal Conductance between n-Heneicosane in Solid and Liquid Phases and a Graphene Monolayer. *Journal of Physical Chemistry C*, **2021**, 125, 14149-14162	3.8	1
2	The role of the envelope protein in the stability of a coronavirus model membrane against an ethanolic disinfectant. *Journal of Chemical Physics*, **2021**, 154, 245101	3.9	1

List of Publications

1 Keine Angst vor der Entropie. *Chemie in Unserer Zeit*, **2020**, 54, 250-253 0.2