Florian MÃ¼ller-Plathe

List of Publications by Year
in descending order

99 papers	7,961 citations	87843 38 h-index	48277 88 g-index
100 all docs	100 docs citations	100 times ranked	5667 citing authors

#	Article	IF	Citations
1	A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity. Journal of Chemical Physics, 1997, 106, 6082-6085.	1.2	1,262
2	Deriving effective mesoscale potentials from atomistic simulations. Journal of Computational Chemistry, 2003, 24, 1624-1636.	1.5	1,067
3	Coarse-Graining in Polymer Simulation: From the Atomistic to the Mesoscopic Scale and Back. ChemPhysChem, 2002, 3, 754-769.	1.0	764
4	Reversing the perturbation in nonequilibrium molecular dynamics: An easy way to calculate the shear viscosity of fluids. Physical Review E, 1999, 59, 4894-4898.	0.8	342
5	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, 15825-15833.	6.6	283
6	Mapping Atomistic Simulations to Mesoscopic Models:Â A Systematic Coarse-Graining Procedure for Vinyl Polymer Chains. Journal of Physical Chemistry B, 2005, 109, 18609-18619.	1.2	241
7	Temperature-Transferable Coarse-Grained Potentials for Ethylbenzene, Polystyrene, and Their Mixtures. Macromolecules, 2008, 41, 9919-9929.	2.2	210
8	Mapping Atomistic to Coarse-Grained Polymer Models Using Automatic Simplex Optimization To Fit Structural Properties. Macromolecules, 2001, 34, 2335-2345.	2.2	198
9	Transferability of coarse-grained force fields: The polymer case. Journal of Chemical Physics, 2008, 128, 064904.	1.2	192
10	Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts:Â Structure, Thermodynamic Properties, Chain Conformation, and Entanglements. Macromolecules, 2007, 40, 3876-3885.	2.2	190
11	YASP: A molecular simulation package. Computer Physics Communications, 1993, 78, 77-94.	3.0	174
12	Force field parametrization by weak coupling. Re-engineering SPC water. Chemical Physics Letters, 1995, 232, 429-436.	1.2	173
13	Interphase Structure in Silicaâ€“Polystyrene Nanocomposites: A Coarse-Grained Molecular Dynamics Study. Macromolecules, 2012, 45, 572-584.	2.2	163
14	Thermal Conductivities of Molecular Liquids by Reverse Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry B, 2005, 109, 15060-15067.	1.2	155
15	The thermal conductivity and thermal rectification of carbon nanotubes studied using reverse non-equilibrium molecular dynamics simulations. Nanotechnology, 2009, 20, 115704.	1.3	144
16	Interface and Interphase Dynamics of Polystyrene Chains near Grafted and Ungrafted Silica Nanoparticles. Macromolecules, 2012, 45, 171-179.	2.2	133
17	Molecular Dynamics Simulation of a Silica Nanoparticle in Oligomeric Poly(methyl methacrylate): A Model System for Studying the Interphase Thickness in a Polymerâ€“Nanocomposite via Different Properties. Macromolecules, 2013, 46, 8680-8692.	2.2	108
18	How Good Are Coarseâ€Grained Polymer Models? A Comparison for Atactic Polystyrene. ChemPhysChem, 2012, 13, 3428-3439.	1.0	100

#	Article	IF	Citations
19	Recovering the reptation dynamics of polymer melts in dissipative particle dynamics simulations via slip-springs. Journal of Chemical Physics, 2013, 138, 104907.	1.2	76
20	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.	1.5	69
21	IBIsCO: A molecular dynamics simulation package for coarseâ€grained simulation. Journal of Computational Chemistry, 2011, 32, 1475-1487.	1.5	68
22	Molecular Dynamics Simulation of Sorption of Gases in Polystyrene. Macromolecules, 2007, 40, 6413-6421.	2.2	66
23	Mechanical behavior and interphase structure in a silicaâ€“polystyrene nanocomposite under uniaxial deformation. Nanotechnology, 2012, 23, 305702.	1.3	65
24	Molecular dynamics simulation in the grand canonical ensemble. Journal of Computational Chemistry, 2007, 28, 1763-1773.	1.5	64
25	Pinning of the Contact Line during Evaporation on Heterogeneous Surfaces: Slowdown or Temporary Immobilization? Insights from a Nanoscale Study. Langmuir, 2015, 31, 7544-7552.	1.6	63
26	Nonequilibrium Molecular Dynamics Calculation of the Thermal Conductivity of Amorphous Polyamide-6,6. Journal of Physical Chemistry B, 2007, 111, 11516-11523.	1.2	57
27	Temperature dependence of coarse-grained potentials for liquid hexane. Physical Chemistry Chemical Physics, 2011, 13, 2894-2902.	1.3	57
28	Parallelizing a Molecular Dynamics Algorithm on a Multiprocessor Workstation Using OpenMP. Journal of Chemical Information and Modeling, 2005, 45, 1943-1952.	2.5	56
29	Thermal Transport at Solidâ€“Liquid Interfaces: High Pressure Facilitates Heat Flow through Nonlocal Liquid Structuring. Journal of Physical Chemistry Letters, 2017, 8, 1946-1951.	2.1	55
30	A kinetic chain growth algorithm in coarse-grained simulations. Journal of Computational Chemistry, 2016, 37, 2634-2646.	1.5	51
31	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, 1336-1346.	1.2	51
32	Influence of Contact-Line Curvature on the Evaporation of Nanodroplets from Solid Substrates. Physical Review Letters, 2014, 113, 046101.	2.9	49
33	Effective control of the transport coefficients of a coarse-grained liquid and polymer models using the dissipative particle dynamics and Loweâ€“Andersen equations of motion. Physical Chemistry Chemical Physics, 2009, 11, 1962.	1.3	46
34	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, 8129-8133.	1.2	45
35	Cyclohexaneâ^'Benzene Mixtures:Â Thermodynamics and Structure from Atomistic Simulations. Journal of Physical Chemistry B, 2004, 108, 7415-7423.	1.2	44
36	Reactive Molecular Dynamics with Material-Specific Coarse-Grained Potentials: Growth of Polystyrene Chains from Styrene Monomers. Journal of Physical Chemistry B, 2010, 114, 13656-13666.	1.2	42

#	Article	IF	Citations
37	Molecular Dynamics Calculations of the Thermal Conductivity of Molecular Liquids, Polymers, and Carbon Nanotubes. Soft Materials, 2012, 10, 42-80.	0.8	41
38	Molecular structure and multi-body potential of mean force in silica-polystyrene nanocomposites. Nanoscale, 2018, 10, 21656-21670.	2.8	40
39	Sorption and diffusion of carbon dioxide and nitrogen in poly(methyl methacrylate). Journal of Chemical Physics, 2013, 139, 124902.	1.2	38
40	Local bond order parameters for accurate determination of crystal structures in two and three dimensions. Physical Chemistry Chemical Physics, 2018, 20, 27059-27068.	1.3	35
41	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, 14596-14603.	1.2	33
42	Thermal conductivity of carbon nanotubeâ€"polyamide-6,6 nanocomposites: Reverse non-equilibrium molecular dynamics simulations. Journal of Chemical Physics, 2011, 135, 184905.	1.2	33
43	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.	2.3	33
44	A Multichain Slip-Spring Dissipative Particle Dynamics Simulation Method for Entangled Polymer Solutions. Macromolecules, 2016, 49, 9186-9191.	2.2	32
45	Mechanisms of Nucleation and Solidâ€"Solid-Phase Transitions in Triblock Janus Assemblies. Journal of Chemical Theory and Computation, 2021, 17, 1742-1754.	2.3	32
46	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.	2.3	28
47	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.	2.3	28
48	Solidâ€"Liquid and Solidâ€"Solid Phase Diagrams of Self-Assembled Triblock Janus Nanoparticles from Solution. Journal of Physical Chemistry C, 2018, 122, 9235-9244.	1.5	27
49	Predicting the Mobility Increase of Coarse-Grained Polymer Models from Excess Entropy Differences. Journal of Chemical Theory and Computation, 2020, 16, 1431-1447.	2.3	27
50	Nonperiodic stochastic boundary conditions for molecular dynamics simulations of materials embedded into a continuum mechanics domain. Journal of Chemical Physics, 2011, 134, 154108.	1.2	26
51	Reptation and constraint release dynamics in bidisperse polymer melts. Journal of Chemical Physics, 2014, 141, 194904.	1.2	26
52	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.	1.5	26
53	Distribution of the Number of Polymer Chains Grafted on Nanoparticles Fabricated by Grafting-to and Grafting-from Procedures. Macromolecules, 2018, 51, 3758-3766.	2.2	25
54	Self-Assembly Mechanisms of Triblock Janus Particles. Journal of Chemical Theory and Computation, 2019, 15, 1345-1354.	2.3	25

#	Article	IF	Citations
55	Polymeric Flower-Like Microparticles from Self-Assembled Cellulose Stearoyl Esters. ACS Macro Letters, 2015, 4, 214-219.	2.3	24
56	Do Transport Properties of Entangled Linear Polymers Scale with Excess Entropy?. Macromolecules, 2013, 46, 8710-8723.	2.2	22
57	How Alcoholic Disinfectants Affect Coronavirus Model Membranes: Membrane Fluidity, Permeability, and Disintegration. Journal of Physical Chemistry B, 2020, 124, 10374-10385.	1.2	22
58	Molecular Mobility in Cyclic Hydrocarbons:Â A Simulation Study. Journal of Physical Chemistry B, 1999, 103, 9731-9737.	1.2	21
59	Water permeability of poly(ethylene terephthalate): A grand canonical ensemble molecular dynamics simulation study. Journal of Chemical Physics, 2009, 131, 234904.	1.2	21
60	Investigation of interphase effects in silica-polystyrene nanocomposites based on a hybrid molecular-dynamicsâ€“finite-element simulation framework. Physical Review E, 2016, 93, 052505.	0.8	21
61	Influence of Polymer Bidispersity on the Effective Particleâ€“Particle Interactions in Polymer Nanocomposites. Macromolecules, 2019, 52, 8826-8839.	2.2	20
62	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.	2.3	20
63	Sequence-Engineering Polyethyleneâ€“Polypropylene Copolymers with High Thermal Conductivity Using a Molecular-Dynamics-Based Genetic Algorithm. Journal of Chemical Theory and Computation, 2021, 17, 3772-3782.	2.3	18
64	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.	1.2	17
65	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.	1.8	16
66	Self-Assembly of Model Triblock Janus Colloidal Particles in Two Dimensions. Journal of Chemical Theory and Computation, 2022, 18, 1870-1882.	2.3	16
67	A Molecular Dynamics Study of Viscosity in Ionic Liquids Directed by Quantitative Structureâ€“Property Relationships. ChemPhysChem, 2012, 13, 1791-1801.	1.0	14
68	Molecular dynamics method to locally resolve Poisson's ratio: Mechanical description of the solid--soft-matter interphase. Physical Review E, 2012, 86, 036704.	0.8	13
69	A steady-state non-equilibrium molecular dynamics approach for the study of evaporation processes. Journal of Chemical Physics, 2013, 139, 134701.	1.2	13
70	Excess entropy scaling for the segmental and global dynamics of polyethylene melts. Physical Chemistry Chemical Physics, 2014, 16, 24301-24311.	1.3	13
71	Adaptiveâ€numericalâ€bias metadynamics. Journal of Computational Chemistry, 2017, 38, 2721-2729.	1.5	13
72	Simulation of Elastomers by Slip-Spring Dissipative Particle Dynamics. Macromolecules, 2021, 54, 5155-5166.	2.2	12

#	Article	IF	Citations
73	A comparison of sulfur mustard and heptane penetrating a dipalmitoylphosphatidylcholine bilayer membrane. Journal of Hazardous Materials, 2009, 168, 13-24.	6.5	11
74	Coarse-Grained Molecular Simulation Model for Gecko Feet Keratin. Journal of Physical Chemistry B, 2018, 122, 2203-2212.	1.2	11
75	Thermal Energy Transport across the Interface between Phase Change Materialn-Heneicosane in Solid and Liquid Phases and Few-Layer Graphene. Journal of Physical Chemistry C, 2019, 123, 29192-29202.	1.5	11
76	Atomistic hybrid <scp>particleâ€field</scp> molecular dynamics combined with <scp>slipâ€springs</scp>: Restoring entangled dynamics to simulations of polymer melts. Journal of Computational Chemistry, 2021, 42, 6-18.	1.5	11
77	A reverse nonequilibrium molecular dynamics method for calculating the mutual diffusion coefficient for binary fluids. Chemical Engineering Science, 2015, 130, 1-7.	1.9	10
78	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.	1.5	9
79	Gecko adhesion: a molecular-simulation perspective on the effect of humidity. Soft Matter, 2022, 18, 1247-1263.	1.2	9
80	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.	1.2	8
81	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.	1.0	8
82	Rebound Suppression of a Droplet Impacting on a Supersolvophobic Surface by a Small Amount of Polymer Additives. ACS Macro Letters, 2021, 10, 192-196.	2.3	8
83	Robustness of a new molecular dynamicsâ€“finite element coupling approach for soft matter systems analyzed by uncertainty quantification. Journal of Chemical Physics, 2015, 142, 104105.	1.2	7
84	Different Stages of Polymer-Chain Collapse Following Solvent Quenchingâ€“Scaling Relations from Dissipative Particle Dynamics Simulations. Macromolecules, 2020, 53, 8889-8900.	2.2	7
85	Suppressing the rebound of impacting droplets from solvophobic surfaces by polymer additives: polymer adsorption and molecular mechanisms. Soft Matter, 2021, 17, 6952-6963.	1.2	7
86	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, 18, 2375-2387.	2.3	7
87	Knotting behaviour of polymer chains in the melt state for soft-core models with and without slip-springs. Journal of Physics Condensed Matter, 2021, 33, 244001.	0.7	6
88	Compatibilization Efficiency of Additives in Homopolymer Blends: A Dissipative Particle Dynamics Study. Macromolecules, 2021, 54, 9551-9564.	2.2	5
89	Effect of Polymer on the Contact Line Friction of a Capillary Bridge. Macromolecules, 2022, 55, 2649-2658.	2.2	5
90	How Ethanolic Disinfectants Disintegrate Coronavirus Model Membranes: A Dissipative Particle Dynamics Simulation Study. Journal of Chemical Theory and Computation, 2022, 18, 2597-2615.	2.3	5

#	Article	IF	Citations
91	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.	1.2	4
92	Roughness Volumes: An Improved RoughMob Concept for Predicting the Increase of Molecular Mobility upon Coarse-Graining. Journal of Physical Chemistry B, 2022, 126, 3737-3747.	1.2	4
93	Contact Line Friction and Dynamic Contact Angles of a Capillary Bridge between Superhydrophobic Nanostructured Surfaces. Journal of Chemical Physics, 0, , .	1.2	3
94	Extending reverse nonequilibrium molecular dynamics to the calculation of mutual diffusion coefficients in molecular fluid mixtures. Molecular Simulation, 2016, 42, 1379-1384.	0.9	2
95	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.	2.3	2
96	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.	1.5	2
97	Slip-Spring Hybrid Particle-Field Molecular Dynamics for Coarse-Graining Branched Polymer Melts: Polystyrene Melts as an Example. Journal of Chemical Theory and Computation, 2022, 18, 3814-3828.	2.3	2
98	Mobility of Polymer Melts in a Regular Array of Carbon Nanotubes. Journal of Chemical Theory and Computation, 2022, 18, 3285-3295.	2.3	1
99	Conductance Switching in Liquid Crystal-Inspired Self-Assembled Monolayer Junctions. ACS Applied Materials & Interfaces, 2022, 14, 31044-31053.	4.0	1