

Vlasis G Mavrantzas

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

107
papers

3,663
citations

33
h-index

57
g-index

114
ext. papers

3,998
ext. citations

4.5
avg, IF

5.61
L-index

#	Paper	IF	Citations
107	Individual Contributions of Adsorbed and Free Chains to Microscopic Dynamics of Unentangled poly(ethylene Glycol)/Silica Nanocomposite Melts and the Important Role of End Groups: Theory and Simulation. <i>Macromolecules</i> , 2021 , 54, 4470-4487	5.5	5
106	Using Monte Carlo to Simulate Complex Polymer Systems: Recent Progress and Outlook. <i>Frontiers in Physics</i> , 2021 , 9,	3.9	2
105	Molecular simulation of the morphology and viscosity of aqueous micellar solutions of sodium lauryl ether sulfate (SLEnS). <i>JPhys Materials</i> , 2021 , 4, 044001	4.2	0
104	Field-theoretic simulations beyond χ interactions: Overcoming the inverse potential problem in auxiliary field models. <i>Journal of Chemical Physics</i> , 2021 , 155, 024106	3.9	2
103	Conformation and Diffusivity of Ring and Linear Polyethylene Oxide in Aqueous Solution: Molecular Topology Dependent Concentration Effects and Comparison with Experimental Data. <i>Macromolecular Theory and Simulations</i> , 2020 , 29, 2000016	1.5	5
102	Effect of pH and Molecular Length on the Structure and Dynamics of Linear and Short-Chain Branched Poly(ethylene imine) in Dilute Solution: Scaling Laws from Detailed Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 6154-6169	3.4	4
101	Structure and Conformation of a Crystalline P3HT Film Adsorbed on an Alkanethiol Self-Assembled Monolayer Deposited on Gold. <i>Macromolecular Theory and Simulations</i> , 2020 , 29, 2000010	1.5	3
100	Simple, Accurate and User-Friendly Differential Constitutive Model for the Rheology of Entangled Polymer Melts and Solutions from Nonequilibrium Thermodynamics. <i>Materials</i> , 2020 , 13,	3.5	6
99	Conformational and Dynamic Properties of Short DNA Minicircles in Aqueous Solution from Atomistic Molecular Dynamics Simulations. <i>Macromolecules</i> , 2020 , 53, 5903-5918	5.5	2
98	Size and Diffusivity of Polymer Rings in Linear Polymer Matrices: The Key Role of Threading Events. <i>Macromolecules</i> , 2020 , 53, 803-820	5.5	13
97	Quantitative Prediction of the Structure and Viscosity of Aqueous Micellar Solutions of Ionic Surfactants: A Combined Approach Based on Coarse-Grained MARTINI Simulations Followed by Reverse-Mapped All-Atom Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2212-2220	6.4	8
96	Effect of Polymer Concentration on the Structure and Dynamics of Short Poly(ϵ -dimethylaminoethyl methacrylate) in Aqueous Solution: A Combined Experimental and Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 240-252	3.4	10
95	Two-species models for the rheology of associative polymer solutions: Derivation from nonequilibrium thermodynamics. <i>Journal of Rheology</i> , 2020 , 64, 1003-1016	4.1	8
94	Molecular Dynamics Simulation of the Diffusion Dynamics of Linear DNA Fragments in Dilute Solution with the Parmbsc1 Force Field and Comparison with Experimental Data and Theoretical Models. <i>Macromolecules</i> , 2020 , 53, 6135-6150	5.5	
93	Geometric Analysis of Clusters of Free Volume Accessible to Small Penetrants and Their Connectivity in Polymer Nanocomposites Containing Carbon Nanotubes. <i>Macromolecules</i> , 2020 , 53, 9563-9583 ¹	5.5	1
92	Phase Boundary and Salt Partitioning in Coacervate Complexes Formed between Poly(acrylic acid) and Poly(N,N-dimethylaminoethyl methacrylate) from Detailed Atomistic Simulations Combined with Free Energy Perturbation and Thermodynamic Integration Calculations. <i>Macromolecules</i> , 2020 , 53, 7618-7634	5.5	4
91	Molecular Dynamics Simulation of Amorphous Poly(3-hexylthiophene). <i>Macromolecules</i> , 2020 , 53, 7810-7824	5.5	3

90	Dynamic Heterogeneity in Ring-Linear Polymer Blends. <i>Polymers</i> , 2020 , 12,	4.5	11
89	3-Arm star pyrene-functional PMMAs for efficient exfoliation of graphite in chloroform: fabrication of graphene-reinforced fibrous veils. <i>Nanoscale</i> , 2019 , 11, 915-931	7.7	13
88	The impact of molecular simulations in gas-phase manufacture of nanomaterials. <i>Current Opinion in Chemical Engineering</i> , 2019 , 23, 174-183	5.4	6
87	Ultrafast rotational motions of supported nanoclusters probed by electron diffraction. <i>Nanoscale Horizons</i> , 2019 , 4, 1164-1173	10.8	6
86	Insights into the morphology of multicomponent organic and inorganic aerosols from molecular dynamics simulations. <i>Atmospheric Chemistry and Physics</i> , 2019 , 19, 5571-5587	6.8	10
85	Effect of pH and Molecular Length on the Structure and Dynamics of Short Poly(acrylic acid) in Dilute Solution: Detailed Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 4204-4219	13.4	23
84	Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019 , 9, e1414	7.9	2
83	High Polymer Mass Densities at the Mouths of Carbon Nanotubes (CNTs) Control the Diffusion of Small Molecules through CNT-Based Polymer Nanocomposite Membranes. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 6892-6900	3.4	1
82	Shear Rheology of Unentangled and Marginally Entangled Ring Polymer Melts from Large-Scale Nonequilibrium Molecular Dynamics Simulations. <i>Polymers</i> , 2019 , 11,	4.5	13
81	Molecular dynamics simulation of π -substituted oligo-thiophenes: dependence of their high-temperature liquid-crystalline phase behaviour on molecular length. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 9984-9995	7.1	2
80	Mobility and settling rate of agglomerates of polydisperse nanoparticles. <i>Journal of Chemical Physics</i> , 2018 , 148, 064703	3.9	5
79	Pressure- and Temperature-Induced Monoclinic-to-Orthorhombic Phase Transition in Silicalite-1. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 6217-6229	3.8	4
78	A constitutive rheological model for agglomerating blood derived from nonequilibrium thermodynamics. <i>Physics of Fluids</i> , 2018 , 30, 030710	4.4	22
77	Scaling Laws for the Conformation and Viscosity of Ring Polymers in the Crossover Region around Me from Detailed Molecular Dynamics Simulations. <i>ACS Macro Letters</i> , 2018 , 7, 916-920	6.6	23
76	Molecular simulation of the high temperature phase behaviour of π -substituted sexithiophene. <i>Soft Matter</i> , 2018 , 14, 8253-8266	3.6	5
75	Understanding the rheological behavior of polymer nanocomposites: Non-equilibrium thermodynamics modeling coupled with detailed atomistic non-equilibrium molecular dynamics simulations. <i>Materials Today: Proceedings</i> , 2018 , 5, 27589-27598	1.4	
74	Monte Carlo Algorithm Based on Internal Bridging Moves for the Atomistic Simulation of Thiophene Oligomers and Polymers. <i>Macromolecules</i> , 2018 , 51, 8406-8423	5.5	5
73	Molecular Dynamics Study of an Atactic Poly(methyl methacrylate)-Carbon Nanotube Nanocomposite. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 9007-9021	3.4	14

72	Microscopic Structure, Conformation, and Dynamics of Ring and Linear Poly(ethylene oxide) Melts from Detailed Atomistic Molecular Dynamics Simulations: Dependence on Chain Length and Direct Comparison with Experimental Data. <i>Macromolecules</i> , 2017 , 50, 2565-2584	5.5	36
71	Molecular dynamics simulation of the local concentration and structure in multicomponent aerosol nanoparticles under atmospheric conditions. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16681-16692 ^{3,6}	3.6	11
70	Detailed Molecular Dynamics Simulation of the Structure and Self-Diffusion of Linear and Cyclic n-Alkanes in Melt and Blends. <i>Macromolecular Theory and Simulations</i> , 2017 , 26, 1600049	1.5	9
69	Analysis of Slow Modes in Ring Polymers: Threading of Rings Controls Long-Time Relaxation. <i>ACS Macro Letters</i> , 2016 , 5, 755-760	6.6	61
68	Molecular Modeling Combined with Advanced Chemistry for the Rational Design of Efficient Graphene Dispersing Agents. <i>ACS Macro Letters</i> , 2016 , 5, 24-29	6.6	18
67	Microscopic Dynamics and Topology of Polymer Rings Immersed in a Host Matrix of Longer Linear Polymers: Results from a Detailed Molecular Dynamics Simulation Study and Comparison with Experimental Data. <i>Polymers</i> , 2016 , 8,	4.5	22
66	Flow-Induced Orientation and Stretching of Entangled Polymers in the Framework of Nonequilibrium Thermodynamics. <i>Macromolecules</i> , 2016 , 49, 3161-3173	5.5	20
65	Atomistic Monte Carlo and molecular dynamics simulation of the bulk phase self-assembly of semifluorinated alkanes. <i>Chemical Engineering Science</i> , 2015 , 121, 32-50	4.4	9
64	Determination of the effective diffusivity of water in a poly (methyl methacrylate) membrane containing carbon nanotubes using kinetic Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2015 , 143, 164903	3.9	3
63	Molecular Structure and Work of Adhesion of Poly(n-butyl acrylate) and Poly(n-butyl acrylate-co-acrylic acid) on Quartz, Ferric Oxide, and Ferrite from Detailed Molecular Dynamics Simulations. <i>Macromolecules</i> , 2015 , 48, 8262-8284	5.5	15
62	Accurate prediction of the linear viscoelastic properties of highly entangled mono and bidisperse polymer melts. <i>Journal of Chemical Physics</i> , 2014 , 140, 214903	3.9	15
61	Determination of the Mechanical Properties of a Poly(methyl methacrylate) Nanocomposite with Functionalized Graphene Sheets through Detailed Atomistic Simulations. <i>Macromolecules</i> , 2014 , 47, 8072-8088 ⁷¹	5.5	8088 ⁷¹
60	Threading of Ring Poly(ethylene oxide) Molecules by Linear Chains in the Melt.. <i>ACS Macro Letters</i> , 2014 , 3, 763-766	6.6	50
59	Stress-gradient induced migration of polymers in corrugated channels. <i>Journal of Rheology</i> , 2014 , 58, 911-947	4.1	23
58	Dynamic, conformational and topological properties of ring-linear poly(ethylene oxide) blends from molecular dynamics simulations. <i>Reactive and Functional Polymers</i> , 2014 , 80, 61-70	4.6	23
57	Continuum Model for the Phase Behavior, Microstructure, and Rheology of Unentangled Polymer Nanocomposite Melts. <i>Macromolecules</i> , 2014 , 47, 4493-4513	5.5	23
56	Quantitative predictions of the linear viscoelastic properties of entangled polyethylene and polybutadiene melts via modified versions of modern tube models on the basis of atomistic simulation data. <i>Journal of Non-Newtonian Fluid Mechanics</i> , 2013 , 200, 111-130	2.7	14
55	All-Atom Molecular Dynamics Simulation of Temperature Effects on the Structural, Thermodynamic, and Packing Properties of the Pure Amorphous and Pure Crystalline Phases of Regioregular P3HT. <i>Macromolecules</i> , 2013 , 46, 2450-2467	5.5	71

54	Detailed atomistic simulation of the nano-sorption and nano-diffusivity of water, tyrosol, vanillic acid, and p-coumaric acid in single wall carbon nanotubes. <i>Journal of Chemical Physics</i> , 2013 , 139, 16471-16480	3.9	8
53	Effects of tube persistence length on dynamics of mildly entangled polymers. <i>Journal of Rheology</i> , 2012 , 56, 707-723	4.1	19
52	Projection of atomistic simulation data for the dynamics of entangled polymers onto the tube theory: calculation of the segment survival probability function and comparison with modern tube models. <i>Soft Matter</i> , 2011 , 7, 380-395	3.6	38
51	Toward an Improved Description of Constraint Release and Contour Length Fluctuations in Tube Models for Entangled Polymer Melts Guided by Atomistic Simulations. <i>Macromolecular Theory and Simulations</i> , 2011 , 20, 752-768	1.5	21
50	Structure and dynamics of polymer rings by neutron scattering: breakdown of the Rouse model. <i>Soft Matter</i> , 2011 , 7, 11169	3.6	55
49	On Maxwell's Relations of Thermodynamics for Polymeric Liquids away from Equilibrium. <i>Macromolecules</i> , 2011 , 44, 640-646	5.5	7
48	Flow Effects on Melt Structure and Entanglement Network of Linear Polymers: Results from a Nonequilibrium Molecular Dynamics Simulation Study of a Polyethylene Melt in Steady Shear. <i>Macromolecules</i> , 2010 , 43, 6886-6902	5.5	128
47	Melt Structure and Dynamics of Unentangled Polyethylene Rings: Rouse Theory, Atomistic Molecular Dynamics Simulation, and Comparison with the Linear Analogues. <i>Macromolecules</i> , 2010 , 43, 10692-10713	5.5	94
46	Advanced Monte Carlo Algorithm for the Atomistic Simulation of Short- and Long-Chain Branched Polymers: Implementation for Model H-Shaped, A3AA3 Multiarm (Pom-Pom), and Short-Chain Branched Polyethylene Melts. <i>Macromolecules</i> , 2010 , 43, 986-1002	5.5	28
45	Understanding Dynamics in Binary Mixtures of Entangled cis-1,4-Polybutadiene Melts at the Level of Primitive Path Segments by Mapping Atomistic Simulation Data onto the Tube Model. <i>Macromolecules</i> , 2010 , 43, 8239-8250	5.5	28
44	Quantifying chain reptation in entangled polymer melts: topological and dynamical mapping of atomistic simulation results onto the tube model. <i>Journal of Chemical Physics</i> , 2010 , 132, 124904	3.9	87
43	From atomistic trajectories to primitive paths to tube models: linking atomistic simulations with the reptation theory of polymer dynamics. <i>Soft Matter</i> , 2010 , 6, 4603	3.6	12
42	Multiscale Modeling and Coarse Graining of Polymer Dynamics: Simulations Guided by Statistical Beyond-Equilibrium Thermodynamics 2010 , 343-383		4
41	A generalized differential constitutive equation for polymer melts based on principles of nonequilibrium thermodynamics. <i>Journal of Rheology</i> , 2009 , 53, 309-337	4.1	37
40	End-Bridging Monte Carlo Simulation of Bulk and Grafted Amorphous Polyethylene Above and Below the Glass Transition. <i>Macromolecules</i> , 2008 , 41, 987-996	5.5	31
39	An efficient Monte Carlo algorithm for the fast equilibration and atomistic simulation of alkanethiol self-assembled monolayers on a Au(111) substrate. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 1198-211	3.4	19
38	Atomistic Simulation of the Sorption of Small Gas Molecules in Polyisobutylene. <i>Macromolecules</i> , 2008 , 41, 6228-6238	5.5	16
37	Molecular dynamics simulation of temperature and pressure effects on the intermediate length scale dynamics and zero shear rate viscosity of cis-1,4-polybutadiene: Rouse mode analysis and dynamic structure factor spectra. <i>Journal of Non-Newtonian Fluid Mechanics</i> , 2008 , 152, 184-194	2.7	14

36	Atomistic Simulation of Alkanethiol Self-Assembled Monolayers on Different Metal Surfaces via a Quantum, First-Principles Parametrization of the Sulfur-Metal Interaction. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 6380-6391	3.8	46
35	Temperature and Pressure Effects on Local Structure and Chain Packing in cis-1,4-Polybutadiene from Detailed Molecular Dynamics Simulations. <i>Macromolecular Theory and Simulations</i> , 2006 , 15, 381-393	3.5	20
34	Atomistic molecular dynamics simulation of the temperature and pressure dependences of local and terminal relaxations in cis-1,4-polybutadiene. <i>Journal of Chemical Physics</i> , 2006 , 124, 084906	3.9	33
33	Primitive Path Identification and Entanglement Statistics in Polymer Melts: Results from Direct Topological Analysis on Atomistic Polyethylene Models. <i>Macromolecules</i> , 2006 , 39, 4207-4216	5.5	137
32	Numerical simulation of multiple bubbles growing in a Newtonian liquid filament undergoing stretching. <i>Physics of Fluids</i> , 2006 , 18, 042106	4.4	16
31	Advanced Monte Carlo Methods for the atomistic simulation of polymers with a linear or a non-linear molecular architecture. <i>Computer Aided Chemical Engineering</i> , 2006 , 31-67	0.6	2
30	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. <i>Macromolecules</i> , 2005 , 38, 7134-7149	5.5	47
29	Hierarchical Modeling of the Dynamics of Polymers with a Nonlinear Molecular Architecture: Calculation of Branch Point Friction and Chain Reptation Time of H-Shaped Polyethylene Melts from Long Molecular Dynamics Simulations. <i>Macromolecules</i> , 2005 , 38, 8583-8596	5.5	52
28	Molecular Dynamics Simulation of a Polymer Melt/Solid Interface: Local Dynamics and Chain Mobility in a Thin Film of Polyethylene Melt Adsorbed on Graphite. <i>Macromolecules</i> , 2005 , 38, 5796-5809	5.5	152
27	Detailed Atomistic Simulation of a Polymer Melt/Solid Interface: Structure, Density, and Conformation of a Thin Film of Polyethylene Melt Adsorbed on Graphite. <i>Macromolecules</i> , 2005 , 38, 5780-5795	5.5	166
26	Detailed Atomistic Molecular Dynamics Simulation of cis-1,4-Poly(butadiene). <i>Macromolecules</i> , 2005 , 38, 1478-1492	5.5	104
25	Continuum formulation of the Scheutjens-Fleer lattice statistical theory for homopolymer adsorption from solution. <i>Journal of Chemical Physics</i> , 2005 , 123, 174901	3.9	5
24	Numerical simulation of bubble growth in Newtonian and viscoelastic filaments undergoing stretching. <i>Journal of Non-Newtonian Fluid Mechanics</i> , 2004 , 122, 177-200	2.7	22
23	Detailed Atomistic Simulation of the Segmental Dynamics and Barrier Properties of Amorphous Poly(ethylene terephthalate) and Poly(ethylene isophthalate). <i>Macromolecules</i> , 2004 , 37, 2978-2995	5.5	95
22	Variable Connectivity Methods for the Atomistic Monte Carlo Simulation of Inhomogeneous and/or Anisotropic Polymer Systems of Precisely Defined Chain Length Distribution: Tuning the Spectrum of Chain Relative Chemical Potentials. <i>Macromolecules</i> , 2003 , 36, 6674-6682	5.5	15
21	An advanced Monte Carlo method for the equilibration of model long-chain branched polymers with a well-defined molecular architecture: Detailed atomistic simulation of an H-shaped polyethylene melt. <i>Journal of Chemical Physics</i> , 2003 , 118, 2451	3.9	41
20	Stress gradient-induced migration effects in the Taylor-Couette flow of a dilute polymer solution. <i>Journal of Non-Newtonian Fluid Mechanics</i> , 2002 , 102, 409-445	2.7	30
19	Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors. <i>Computer Physics Communications</i> , 2002 , 144, 1-22	4.2	28

18	A novel Monte Carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture. <i>Physical Review Letters</i> , 2002 , 88, 105503	7.4	200
17	Detailed atomistic Monte Carlo simulation of grafted polymer melts. I. Thermodynamic and conformational properties. <i>Journal of Chemical Physics</i> , 2002 , 116, 11028-11038	3.9	38
16	Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm. <i>Journal of Chemical Physics</i> , 2002 , 117, 5465-5479	3.9	117
15	Atomistic Monte Carlo Simulations of Polymer Melt Elasticity: Their Nonequilibrium Thermodynamics GENERIC Formulation in a Generalized Canonical Ensemble. <i>Macromolecules</i> , 2002 , 35, 960-975	5.5	53
14	The 3rd International Conference of the Hellenic Society of Rheology (HSR). <i>Applied Rheology</i> , 2002 , 12, 35-36	1.2	
13	Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities. <i>Chemical Engineering Science</i> , 2001 , 56, 2789-2801	4.4	42
12	Detailed atomistic molecular-dynamics simulation of the orthorhombic phase of crystalline polyethylene and alkane crystals. <i>Journal of Chemical Physics</i> , 2001 , 115, 3937-3950	3.9	20
11	Directed Bridging Methods for Fast Atomistic Monte Carlo Simulations of Bulk Polymers. <i>Macromolecules</i> , 2001 , 34, 8554-8568	5.5	51
10	Atomistic Monte Carlo simulation of steady-state uniaxial elongational flow of long-chain polyethylene melts: dependence of the melt degree of orientation on stress, molecular length and elongational strain rate. <i>Macromolecular Theory and Simulations</i> , 2000 , 9, 500-515	1.5	26
9	Atomistic Molecular Dynamics Simulation of Stress Relaxation upon Cessation of Steady-State Uniaxial Elongational Flow. <i>Macromolecules</i> , 2000 , 33, 8062-8076	5.5	41
8	A hierarchical model for surface effects on chain conformation and rheology of polymer solutions. II. Application to a neutral surface. <i>Journal of Chemical Physics</i> , 1999 , 110, 628-638	3.9	24
7	A hierarchical model for surface effects on chain conformation and rheology of polymer solutions. I. General formulation. <i>Journal of Chemical Physics</i> , 1999 , 110, 616-627	3.9	29
6	End-Bridging Monte Carlo: A Fast Algorithm for Atomistic Simulation of Condensed Phases of Long Polymer Chains. <i>Macromolecules</i> , 1999 , 32, 5072-5096	5.5	216
5	Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts. <i>Macromolecules</i> , 1998 , 31, 7934-7943	5.5	159
4	Atomistic Simulation of Polymer Melt Elasticity: Calculation of the Free Energy of an Oriented Polymer Melt. <i>Macromolecules</i> , 1998 , 31, 6310-6332	5.5	125
3	On the compatibility between various macroscopic formalisms for the concentration and flow of dilute polymer solutions. <i>Journal of Rheology</i> , 1994 , 38, 1235-1250	4.1	77
2	Modeling of the Rheology and Flow-Induced Concentration Changes in Polymer Solutions. <i>Physical Review Letters</i> , 1993 , 70, 2659-2659	7.4	10
1	Modeling of the rheology and flow-induced concentration changes in polymer solutions. <i>Physical Review Letters</i> , 1992 , 69, 273-276	7.4	42

