Vlasis G Mavrantzas

List of Publications by Citations

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	End-Bridging Monte Carlo: A Fast Algorithm for Atomistic Simulation of Condensed Phases of Long Polymer Chains. *Macromolecules*, **1999**, 32, 5072-5096	5.5	216
106	A novel Monte Carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture. *Physical Review Letters*, **2002**, 88, 105503	7.4	200
105	Detailed Atomistic Simulation of a Polymer Melt/Solid Interface: Structure, Density, and Conformation of a Thin Film of Polyethylene Melt Adsorbed on Graphite. *Macromolecules*, **2005**, 38, 5780-5795	5.5	166
104	Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts. *Macromolecules*, **1998**, 31, 7934-7943	5.5	159
103	Molecular Dynamics Simulation of a Polymer Melt/Solid Interface: Local Dynamics and Chain Mobility in a Thin Film of Polyethylene Melt Adsorbed on Graphite. *Macromolecules*, **2005**, 38, 5796-5809	5.5	152
102	Primitive Path Identification and Entanglement Statistics in Polymer Melts: Results from Direct Topological Analysis on Atomistic Polyethylene Models. *Macromolecules*, **2006**, 39, 4207-4216	5.5	137
101	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. *Macromolecules*, **2010**, 43, 6886-6902	5.5	128
100	Atomistic Simulation of Polymer Melt Elasticity: Calculation of the Free Energy of an Oriented Polymer Melt. *Macromolecules*, **1998**, 31, 6310-6332	5.5	125
99	Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm. *Journal of Chemical Physics*, **2002**, 117, 5465-5479	3.9	117
98	Detailed Atomistic Molecular Dynamics Simulation of cis-1,4-Poly(butadiene). *Macromolecules*, **2005**, 38, 1478-1492	5.5	104
97	Detailed Atomistic Simulation of the Segmental Dynamics and Barrier Properties of Amorphous Poly(ethylene terephthalate) and Poly(ethylene isophthalate). *Macromolecules*, **2004**, 37, 2978-2995	5.5	95
96	Melt Structure and Dynamics of Unentangled Polyethylene Rings: Rouse Theory, Atomistic Molecular Dynamics Simulation, and Comparison with the Linear Analogues. *Macromolecules*, **2010**, 43, 10692-10713	5.5	94
95	Quantifying chain reptation in entangled polymer melts: topological and dynamical mapping of atomistic simulation results onto the tube model. *Journal of Chemical Physics*, **2010**, 132, 124904	3.9	87
94	On the compatibility between various macroscopic formalisms for the concentration and flow of dilute polymer solutions. *Journal of Rheology*, **1994**, 38, 1235-1250	4.1	77
93	Determination of the Mechanical Properties of a Poly(methyl methacrylate) Nanocomposite with Functionalized Graphene Sheets through Detailed Atomistic Simulations. *Macromolecules*, **2014**, 47, 8072-8088	5.5	71
92	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. *Macromolecules*, **2013**, 46, 2450-2467	5.5	71
91	Analysis of Slow Modes in Ring Polymers: Threading of Rings Controls Long-Time Relaxation. *ACS Macro Letters*, **2016**, 5, 755-760	6.6	61

90	Structure and dynamics of polymer rings by neutron scattering: breakdown of the Rouse model. *Soft Matter*, **2011**, 7, 11169	3.6	55
89	Atomistic Monte Carlo Simulations of Polymer Melt Elasticity: Their Nonequilibrium Thermodynamics GENERIC Formulation in a Generalized Canonical Ensemble. *Macromolecules*, **2002**, 35, 960-975	5.5	53
88	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. *Macromolecules*, **2005**, 38, 8583-8596	5.5	52
87	Directed Bridging Methods for Fast Atomistic Monte Carlo Simulations of Bulk Polymers. *Macromolecules*, **2001**, 34, 8554-8568	5.5	51
86	Threading of Ring Poly(ethylene oxide) Molecules by Linear Chains in the Melt.. *ACS Macro Letters*, **2014**, 3, 763-766	6.6	50
85	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. *Macromolecules*, **2005**, 38, 7134-7149	5.5	47
84	Atomistic Simulation of Alkanethiol Self-Assembled Monolayers on Different Metal Surfaces via a Quantum, First-Principles Parametrization of the Sulfur–Metal Interaction. *Journal of Physical Chemistry C*, **2007**, 111, 6380-6391	3.8	46
83	Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities. *Chemical Engineering Science*, **2001**, 56, 2789-2801	4.4	42
82	Modeling of the rheology and flow-induced concentration changes in polymer solutions. *Physical Review Letters*, **1992**, 69, 273-276	7.4	42
81	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. *Journal of Chemical Physics*, **2003**, 118, 2451	3.9	41
80	Atomistic Molecular Dynamics Simulation of Stress Relaxation upon Cessation of Steady-State Uniaxial Elongational Flow. *Macromolecules*, **2000**, 33, 8062-8076	5.5	41
79	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. *Soft Matter*, **2011**, 7, 380-395	3.6	38
78	Detailed atomistic Monte Carlo simulation of grafted polymer melts. I. Thermodynamic and conformational properties. *Journal of Chemical Physics*, **2002**, 116, 11028-11038	3.9	38
77	A generalized differential constitutive equation for polymer melts based on principles of nonequilibrium thermodynamics. *Journal of Rheology*, **2009**, 53, 309-337	4.1	37
76	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. *Macromolecules*, **2017**, 50, 2565-2584	5.5	36
75	Atomistic molecular dynamics simulation of the temperature and pressure dependences of local and terminal relaxations in cis-1,4-polybutadiene. *Journal of Chemical Physics*, **2006**, 124, 084906	3.9	33
74	End-Bridging Monte Carlo Simulation of Bulk and Grafted Amorphous Polyethylene Above and Below the Glass Transition. *Macromolecules*, **2008**, 41, 987-996	5.5	31
73	Stress gradient-induced migration effects in the Taylor–Couette flow of a dilute polymer solution. *Journal of Non-Newtonian Fluid Mechanics*, **2002**, 102, 409-445	2.7	30

72	A hierarchical model for surface effects on chain conformation and rheology of polymer solutions. I. General formulation. *Journal of Chemical Physics*, **1999**, 110, 616-627	3.9	29
71	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. *Macromolecules*, **2010**, 43, 986-1002	5.5	28
70	Understanding Dynamics in Binary Mixtures of Entangledcis-1,4-Polybutadiene Melts at the Level of Primitive Path Segments by Mapping Atomistic Simulation Data onto the Tube Model. *Macromolecules*, **2010**, 43, 8239-8250	5.5	28
69	Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors. *Computer Physics Communications*, **2002**, 144, 1-22	4.2	28
68	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. *Macromolecular Theory and Simulations*, **2000**, 9, 500-515	1.5	26
67	A hierarchical model for surface effects on chain conformation and rheology of polymer solutions. II. Application to a neutral surface. *Journal of Chemical Physics*, **1999**, 110, 628-638	3.9	24
66	Effect of pH and Molecular Length on the Structure and Dynamics of Short Poly(acrylic acid) in Dilute Solution: Detailed Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2019**, 123, 4204-4219	3.4	23
65	Scaling Laws for the Conformation and Viscosity of Ring Polymers in the Crossover Region around Me from Detailed Molecular Dynamics Simulations. *ACS Macro Letters*, **2018**, 7, 916-920	6.6	23
64	Stress-gradient induced migration of polymers in corrugated channels. *Journal of Rheology*, **2014**, 58, 911-947	4.1	23
63	Dynamic, conformational and topological properties of ring□inear poly(ethylene oxide) blends from molecular dynamics simulations. *Reactive and Functional Polymers*, **2014**, 80, 61-70	4.6	23
62	Continuum Model for the Phase Behavior, Microstructure, and Rheology of Unentangled Polymer Nanocomposite Melts. *Macromolecules*, **2014**, 47, 4493-4513	5.5	23
61	A constitutive rheological model for agglomerating blood derived from nonequilibrium thermodynamics. *Physics of Fluids*, **2018**, 30, 030710	4.4	22
60	Numerical simulation of bubble growth in Newtonian and viscoelastic filaments undergoing stretching. *Journal of Non-Newtonian Fluid Mechanics*, **2004**, 122, 177-200	2.7	22
59	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. *Polymers*, **2016**, 8,	4.5	22
58	Toward an Improved Description of Constraint Release and Contour Length Fluctuations in Tube Models for Entangled Polymer Melts Guided by Atomistic Simulations. *Macromolecular Theory and Simulations*, **2011**, 20, 752-768	1.5	21
57	Temperature and Pressure Effects on Local Structure and Chain Packing in cis-1,4-Polybutadiene from Detailed Molecular Dynamics Simulations. *Macromolecular Theory and Simulations*, **2006**, 15, 381-393	1.5	20
56	Detailed atomistic molecular-dynamics simulation of the orthorhombic phase of crystalline polyethylene and alkane crystals. *Journal of Chemical Physics*, **2001**, 115, 3937-3950	3.9	20
55	Flow-Induced Orientation and Stretching of Entangled Polymers in the Framework of Nonequilibrium Thermodynamics. *Macromolecules*, **2016**, 49, 3161-3173	5.5	20

54	Effects of tube persistence length on dynamics of mildly entangled polymers. *Journal of Rheology*, **2012**, 56, 707-723	4.1	19
53	An efficient Monte Carlo algorithm for the fast equilibration and atomistic simulation of alkanethiol self-assembled monolayers on a Au(111) substrate. *Journal of Physical Chemistry B*, **2008**, 112, 1198-211	3.4	19
52	Molecular Modeling Combined with Advanced Chemistry for the Rational Design of Efficient Graphene Dispersing Agents. *ACS Macro Letters*, **2016**, 5, 24-29	6.6	18
51	Atomistic Simulation of the Sorption of Small Gas Molecules in Polyisobutylene. *Macromolecules*, **2008**, 41, 6228-6238	5.5	16
50	Numerical simulation of multiple bubbles growing in a Newtonian liquid filament undergoing stretching. *Physics of Fluids*, **2006**, 18, 042106	4.4	16
49	Accurate prediction of the linear viscoelastic properties of highly entangled mono and bidisperse polymer melts. *Journal of Chemical Physics*, **2014**, 140, 214903	3.9	15
48	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. *Macromolecules*, **2015**, 48, 8262-8284	5.5	15
47	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. *Macromolecules*, **2003**, 36, 6674-6682	5.5	15
46	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. *Journal of Non-Newtonian Fluid Mechanics*, **2013**, 200, 111-130	2.7	14
45	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. *Journal of Non-Newtonian Fluid Mechanics*, **2008**, 152, 184-194	2.7	14
44	Molecular Dynamics Study of an Atactic Poly(methyl methacrylate)-Carbon Nanotube Nanocomposite. *Journal of Physical Chemistry B*, **2018**, 122, 9007-9021	3.4	14
43	3-Arm star pyrene-functional PMMAs for efficient exfoliation of graphite in chloroform: fabrication of graphene-reinforced fibrous veils. *Nanoscale*, **2019**, 11, 915-931	7.7	13
42	Size and Diffusivity of Polymer Rings in Linear Polymer Matrices: The Key Role of Threading Events. *Macromolecules*, **2020**, 53, 803-820	5.5	13
41	Shear Rheology of Unentangled and Marginally Entangled Ring Polymer Melts from Large-Scale Nonequilibrium Molecular Dynamics Simulations. *Polymers*, **2019**, 11,	4.5	13
40	From atomistic trajectories to primitive paths to tube models: linking atomistic simulations with the reptation theory of polymer dynamics. *Soft Matter*, **2010**, 6, 4603	3.6	12
39	Molecular dynamics simulation of the local concentration and structure in multicomponent aerosol nanoparticles under atmospheric conditions. *Physical Chemistry Chemical Physics*, **2017**, 19, 16681-16692	3.6	11
38	Dynamic Heterogeneity in Ring-Linear Polymer Blends. *Polymers*, **2020**, 12,	4.5	11
37	Insights into the morphology of multicomponent organic and inorganic aerosols from molecular dynamics simulations. *Atmospheric Chemistry and Physics*, **2019**, 19, 5571-5587	6.8	10

36	Modeling of the Rheology and Flow-Induced Concentration Changes in Polymer Solutions. *Physical Review Letters*, **1993**, 70, 2659-2659	7.4	10
35	Effect of Polymer Concentration on the Structure and Dynamics of Short Poly(,-dimethylaminoethyl methacrylate) in Aqueous Solution: A Combined Experimental and Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2020**, 124, 240-252	3.4	10
34	Atomistic Monte Carlo and molecular dynamics simulation of the bulk phase self-assembly of semifluorinated alkanes. *Chemical Engineering Science*, **2015**, 121, 32-50	4.4	9
33	Detailed Molecular Dynamics Simulation of the Structure and Self-Diffusion of Linear and Cyclic n-Alkanes in Melt and Blends. *Macromolecular Theory and Simulations*, **2017**, 26, 1600049	1.5	9
32	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. *Journal of Chemical Theory and Computation*, **2020**, 16, 3363-3372	6.4	8
31	Detailed atomistic simulation of the nano-sorption and nano-diffusivity of water, tyrosol, vanillic acid, and p-coumaric acid in single wall carbon nanotubes. *Journal of Chemical Physics*, **2013**, 139, 164711	3.9	8
30	Two-species models for the rheology of associative polymer solutions: Derivation from nonequilibrium thermodynamics. *Journal of Rheology*, **2020**, 64, 1003-1016	4.1	8
29	On Maxwell Relations of Thermodynamics for Polymeric Liquids away from Equilibrium. *Macromolecules*, **2011**, 44, 640-646	5.5	7
28	The impact of molecular simulations in gas-phase manufacture of nanomaterials. *Current Opinion in Chemical Engineering*, **2019**, 23, 174-183	5.4	6
27	Ultrafast rotational motions of supported nanoclusters probed by electron diffraction. *Nanoscale Horizons*, **2019**, 4, 1164-1173	10.8	6
26	Simple, Accurate and User-Friendly Differential Constitutive Model for the Rheology of Entangled Polymer Melts and Solutions from Nonequilibrium Thermodynamics. *Materials*, **2020**, 13,	3.5	6
25	Conformation and Diffusivity of Ring and Linear Polyethylene Oxide in Aqueous Solution: Molecular Topology Dependent Concentration Effects and Comparison with Experimental Data. *Macromolecular Theory and Simulations*, **2020**, 29, 2000016	1.5	5
24	Mobility and settling rate of agglomerates of polydisperse nanoparticles. *Journal of Chemical Physics*, **2018**, 148, 064703	3.9	5
23	Molecular simulation of the high temperature phase behaviour of unsubstituted sexithiophene. *Soft Matter*, **2018**, 14, 8253-8266	3.6	5
22	Continuum formulation of the Scheutjens-Fleer lattice statistical theory for homopolymer adsorption from solution. *Journal of Chemical Physics*, **2005**, 123, 174901	3.9	5
21	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. *Macromolecules*, **2021**, 54, 4470-4487	5.5	5
20	Monte Carlo Algorithm Based on Internal Bridging Moves for the Atomistic Simulation of Thiophene Oligomers and Polymers. *Macromolecules*, **2018**, 51, 8406-8423	5.5	5
19	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. *Journal of Physical Chemistry B*, **2020**, 124, 6154-6169	3.4	4

18	Pressure- and Temperature-Induced Monoclinic-to-Orthorhombic Phase Transition in Silicalite-1. *Journal of Physical Chemistry C*, **2018**, 122, 6217-6229	3.8	4
17	Multiscale Modeling and Coarse Graining of Polymer Dynamics: Simulations Guided by Statistical Beyond-Equilibrium Thermodynamics **2010**, 343-383		4
16	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. *Macromolecules*, **2020**, 53, 7618-7634	5.5	4
15	Structure and Conformation of a Crystalline P3HT Film Adsorbed on an Alkanethiol Self-Assembled Monolayer Deposited on Gold. *Macromolecular Theory and Simulations*, **2020**, 29, 2000010	1.5	3
14	Determination of the effective diffusivity of water in a poly (methyl methacrylate) membrane containing carbon nanotubes using kinetic Monte Carlo simulations. *Journal of Chemical Physics*, **2015**, 143, 164903	3.9	3
13	Molecular Dynamics Simulation of Amorphous Poly(3-hexylthiophene). *Macromolecules*, **2020**, 53, 7810-7824	5.5	3
12	Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1414	7.9	2
11	Conformational and Dynamic Properties of Short DNA Minicircles in Aqueous Solution from Atomistic Molecular Dynamics Simulations. *Macromolecules*, **2020**, 53, 5903-5918	5.5	2
10	Molecular dynamics simulation of α,ω-unsubstituted oligo-thiophenes: dependence of their high-temperature liquid-crystalline phase behaviour on molecular length. *Journal of Materials Chemistry C*, **2019**, 7, 9984-9995	7.1	2
9	Advanced Monte Carlo Methods for the atomistic simulation of polymers with a linear or a non-linear molecular architecture. *Computer Aided Chemical Engineering*, **2006**, 31-67	0.6	2
8	Using Monte Carlo to Simulate Complex Polymer Systems: Recent Progress and Outlook. *Frontiers in Physics*, **2021**, 9,	3.9	2
7	Field-theoretic simulations beyond π-interactions: Overcoming the inverse potential problem in auxiliary field models. *Journal of Chemical Physics*, **2021**, 155, 024106	3.9	2
6	High Polymer Mass Densities at the Mouths of Carbon Nanotubes (CNTs) Control the Diffusion of Small Molecules through CNT-Based Polymer Nanocomposite Membranes. *Journal of Physical Chemistry B*, **2019**, 123, 6892-6900	3.4	1
5	Geometric Analysis of Clusters of Free Volume Accessible to Small Penetrants and Their Connectivity in Polymer Nanocomposites Containing Carbon Nanotubes. *Macromolecules*, **2020**, 53, 9563-9583	5.5	1
4	Molecular simulation of the morphology and viscosity of aqueous micellar solutions of sodium lauryl ether sulfate (SLEnS). *JPhys Materials*, **2021**, 4, 044001	4.2	0
3	The 3rd International Conference of the Hellenic Society of Rheology (HSR). *Applied Rheology*, **2002**, 12, 35-36	1.2	
2	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. *Macromolecules*, **2020**, 53, 6135-6150	5.5	
1	Understanding the rheological behavior of polymer nanocomposites: Non-equilibrium thermodynamics modeling coupled with detailed atomistic non-equilibrium molecular dynamics simulations. *Materials Today: Proceedings*, **2018**, 5, 27589-27598	1.4	