

Doros N Theodorou

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4676225/publications.pdf>

Version: 2024-02-01

239
papers

14,765
citations

18482

62
h-index

23533

111
g-index

272
all docs

272
docs citations

272
times ranked

6960
citing authors

#	ARTICLE	IF	CITATIONS
1	A coarse-grained model for capturing the helical behavior of isotactic polypropylene. <i>Soft Matter</i> , 2022, , .	2.7	1
2	Mixing Thermodynamics and Flory-Huggins Interaction Parameter of Polyethylene Oxide/Polyethylene Oligomeric Blends from Kirkwood-Buff Theory and Molecular Simulations. <i>Macromolecules</i> , 2022, 55, 4852-4862.	4.8	12
3	Molecular simulations of dopamine in a lipid bilayer. <i>AIP Conference Proceedings</i> , 2021, , .	0.4	2
4	Coarse-grained simulations of bidisperse polymer melts. <i>AIP Conference Proceedings</i> , 2021, , .	0.4	0
5	Molecular Dynamics Simulations of Polyethylene Bilayers. <i>Journal of Physics: Conference Series</i> , 2021, 1730, 012039.	0.4	0
6	Structure and thermodynamics of grafted silica/polystyrene dilute nanocomposites investigated through self-consistent field theory. <i>Soft Matter</i> , 2021, 17, 4077-4097.	2.7	10
7	Mesoscopic simulations of star polyethylene melts at equilibrium and under steady shear flow. <i>AIP Conference Proceedings</i> , 2021, , .	0.4	0
8	Molecular dynamics simulations of stretch-induced crystallization in layered polyethylene. <i>Polymer Crystallization</i> , 2021, 4, e10172.	0.8	1
9	Potential of Mean Force between Bare or Grafted Silica/Polystyrene Surfaces from Self-Consistent Field Theory. <i>Polymers</i> , 2021, 13, 1197.	4.5	9
10	RuSseL: A Self-Consistent Field Theory Code for Inhomogeneous Polymer Interphases. <i>Computation</i> , 2021, 9, 57.	2.0	2
11	Effect of Surface Nanopatterning on Slip: The Case of Couette Flow of Long-Chain Polyethylene Melt Flowing Past Gold Surfaces. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6681-6696.	2.6	1
12	In silico study of levodopa in hydrated lipid bilayers at the atomistic level. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 107, 107972.	2.4	4
13	A three-dimensional finite element methodology for addressing heterogeneous polymer systems with simulations based on self-consistent field theory. <i>AIP Conference Proceedings</i> , 2021, , .	0.4	2
14	Multiscale Simulations of Polyzwitterions in Aqueous Bulk Solutions and Brush Array Configurations. <i>Soft Matter</i> , 2021, , .	2.7	8
15	Thermodynamic analysis of oligomeric blends by applying the Kirkwood-Buff theory of solutions. <i>Journal of Physics: Conference Series</i> , 2021, 2090, 012079.	0.4	1
16	Free energy calculations by molecular simulations of deformed polymer glasses. <i>Computer Physics Communications</i> , 2020, 249, 107008.	7.5	8
17	Atomistic simulations of long-chain polyethylene melts flowing past gold surfaces: structure and wall-slip. <i>Molecular Physics</i> , 2020, 118, e1706775.	1.7	8
18	Promising Route for the Development of a Computational Framework for Self-Assembly and Phase Behavior Prediction of Ionic Surfactants Using MARTINI. <i>Journal of Physical Chemistry B</i> , 2020, 124, 556-567.	2.6	26

#	ARTICLE	IF	CITATIONS
19	Kinetic concepts and local failure in the interfacial shear strength of epoxy-graphene nanocomposites. <i>Physical Review E</i> , 2020, 102, 030501.	2.1	7
20	Molecular Simulations and Mechanistic Analysis of the Effect of CO ₂ Sorption on Thermodynamics, Structure, and Local Dynamics of Molten Atactic Polystyrene. <i>Macromolecules</i> , 2020, 53, 3669-3689.	4.8	17
21	Molecular Dynamics Test of the Stress-Thermal Rule in Polyethylene and Polystyrene Entangled Melts. <i>Macromolecules</i> , 2020, 53, 789-802.	4.8	5
22	Self-Consistent Field Theory Coupled with Square Gradient Theory of Free Surfaces of Molten Polymers and Compared to Atomistic Simulations and Experiment. <i>Macromolecules</i> , 2019, 52, 5337-5356.	4.8	14
23	Molecular Modeling Investigations of Sorption and Diffusion of Small Molecules in Glassy Polymers. <i>Membranes</i> , 2019, 9, 98.	3.0	54
24	Multiscale Simulations of Graphite-Capped Polyethylene Melts: Brownian Dynamics/Kinetic Monte Carlo Compared to Atomistic Calculations and Experiment. <i>Macromolecules</i> , 2019, 52, 7503-7523.	4.8	17
25	Molecular dynamics simulations of EPON-862/DETDA epoxy networks: structure, topology, elastic constants, and local dynamics. <i>Soft Matter</i> , 2019, 15, 721-733.	2.7	41
26	Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2019, 9, e1414.	14.6	6
27	SimNano: A Trust Region Strategy for Large-Scale Molecular Systems Energy Minimization Based on Exact Second-Order Derivative Information. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 190-205.	5.4	2
28	Thermodynamic Analysis of <i>n</i> -Hexane-Ethanol Binary Mixtures Using the Kirkwood-Buff Theory. <i>Journal of Physical Chemistry B</i> , 2019, 123, 247-257.	2.6	9
29	Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites. <i>Archives of Computational Methods in Engineering</i> , 2018, 25, 591-645.	10.2	45
30	Thermodynamic analysis of Lennard-Jones binary mixtures using Kirkwood-Buff theory. <i>Fluid Phase Equilibria</i> , 2018, 470, 25-37.	2.5	19
31	Mesoscopic Simulations of Free Surfaces of Molten Polyethylene: Brownian Dynamics/Kinetic Monte Carlo Coupled with Square Gradient Theory and Compared to Atomistic Calculations and Experiment. <i>Macromolecules</i> , 2018, 51, 9798-9815.	4.8	20
32	Slip Spring-Based Mesoscopic Simulations of Polymer Networks: Methodology and the Corresponding Computational Code. <i>Polymers</i> , 2018, 10, 1156.	4.5	21
33	Tacticity Effect on the Conformational Properties of Polypropylene and Poly(ethylene-propylene) Copolymers. <i>Macromolecules</i> , 2018, 51, 6878-6891.	4.8	17
34	Computational Studies of Nanographene Systems: Extended Discotics, Covalently Linked Supermolecules, and Functionalized Supramolecular Assemblies. <i>Journal of Physical Chemistry C</i> , 2018, 122, 18715-18731.	3.1	7
35	Exploring the interactions of irbesartan and irbesartan-2-hydroxypropyl- β -cyclodextrin complex with model membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 1089-1098.	2.6	26
36	Slip-Spring Model for the Linear and Nonlinear Viscoelastic Properties of Molten Polyethylene Derived from Atomistic Simulations. <i>Macromolecules</i> , 2017, 50, 4524-4541.	4.8	48

#	ARTICLE	IF	CITATIONS
37	General Methodology for Estimating the Stiffness of Polymer Chains from Their Chemical Constitution: A Single Unperturbed Chain Monte Carlo Algorithm. <i>Macromolecules</i> , 2017, 50, 4575-4587.	4.8	20
38	Equation of State Based Slip Spring Model for Entangled Polymer Dynamics. <i>Macromolecules</i> , 2017, 50, 3004-3029.	4.8	45
39	Molecular Simulations of Free and Graphite Capped Polyethylene Films: Estimation of the Interfacial Free Energies. <i>Macromolecules</i> , 2017, 50, 8827-8844.	4.8	46
40	Mesoscopic Simulations of Crosslinked Polymer Networks. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012063.	0.4	9
41	Atomistic and Coarse-grained Simulations of Hexabenzocoronene Crystals. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012019.	0.4	1
42	Molecular Dynamics Study of Polyethylene under Extreme Confinement. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012012.	0.4	21
43	Molecular modeling and simulation of atactic polystyrene/amorphous silica nanocomposites. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012021.	0.4	2
44	Multiscale simulations of PS/SiO ₂ nanocomposites: from melt to glassy state. <i>Soft Matter</i> , 2016, 12, 7585-7605.	2.7	23
45	Diffusion of Aromatics in Silicalite-1: Experimental and Theoretical Evidence of Entropic Barriers. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21410-21426.	3.1	20
46	Melting Point and Solid-Liquid Coexistence Properties of ± 1 Isotactic Polypropylene as Functions of Its Molar Mass: A Molecular Dynamics Study. <i>Macromolecules</i> , 2016, 49, 4663-4673.	4.8	17
47	Molecular Modeling and Simulation of Polymer Nanocomposites at Multiple Length Scales. <i>IEEE Nanotechnology Magazine</i> , 2016, 15, 416-422.	2.0	12
48	Application of bi-Helmholtz nonlocal elasticity and molecular simulations to the dynamical response of carbon nanotubes. <i>AIP Conference Proceedings</i> , 2015, , .	0.4	20
49	Multiscale simulations of hexa-peri-hexabenzocoronene and hexa-n-dodecyl-hexa-peri-hexabenzocoronene. <i>AIP Conference Proceedings</i> , 2015, , .	0.4	1
50	Molecular modeling and simulation of polymer nanocomposites at multiple length scales. , 2015, , .		0
51	Structural and dynamical properties of nanographene molecular wires: A Molecular Dynamics study. , 2015, , .		0
52	Molecular dynamics simulations of alkyl substituted nanographene crystals. <i>Molecular Physics</i> , 2015, 113, 2776-2790.	1.7	10
53	Monte Carlo simulations of structure and entanglements in polymer melts. <i>Molecular Simulation</i> , 2015, 41, 993-995.	2.0	2
54	Local Segmental Dynamics and Stresses in Polystyrene-C ₆₀ Mixtures. <i>Macromolecules</i> , 2014, 47, 387-404.	4.8	85

#	ARTICLE	IF	CITATIONS
55	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.	4.8	83
56	Dimensionality reduction of free energy profiles of benzene in silicalite-1: calculation of diffusion coefficients using transition state theory. <i>Molecular Simulation</i> , 2014, 40, 80-100.	2.0	19
57	Self-Consistent-Field Study of Adsorption and Desorption Kinetics of Polyethylene Melts on Graphite and Comparison with Atomistic Simulations. <i>Macromolecules</i> , 2014, 47, 6964-6981.	4.8	17
58	Atomistic simulations of cavitation in a model polyethylene network. <i>Polymer Science - Series C</i> , 2013, 55, 212-218.	1.7	10
59	Structure of Polymer Layers Grafted to Nanoparticles in Silicaâ€“Polystyrene Nanocomposites. <i>Macromolecules</i> , 2013, 46, 4670-4683.	4.8	95
60	Structure and entanglements in short chain branched polyolefin melts. <i>AIP Conference Proceedings</i> , 2013, , .	0.4	2
61	Tracking a glassy polymer on its energy landscape in the course of elastic deformation. <i>Molecular Physics</i> , 2013, 111, 3430-3441.	1.7	21
62	Temporal disconnectivity of the energy landscape in glassy systems. <i>Journal of Chemical Physics</i> , 2013, 138, 12A545.	3.0	6
63	On solving the master equation in spatially periodic systems. <i>Journal of Chemical Physics</i> , 2012, 137, 034112.	3.0	12
64	Microscopic Description of Entanglements in Polyethylene Networks and Melts: Strong, Weak, Pairwise, and Collective Attributes. <i>Macromolecules</i> , 2012, 45, 9475-9492.	4.8	45
65	Monte Carlo Simulation of Short Chain Branched Polyolefins: Structure and Properties. <i>Macromolecules</i> , 2012, 45, 8453-8466.	4.8	25
66	Diffusional Effects in Zeolite Catalysts. , 2012, , 807-837.		1
67	Systematic Coarse Graining of 4-Cyano-4â€²-pentylbiphenyl. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 546-556.	3.7	35
68	Interface of Grafted and Ungrafted Silica Nanoparticles with a Polystyrene Matrix: Atomistic Molecular Dynamics Simulations. <i>Macromolecules</i> , 2011, 44, 2316-2327.	4.8	239
69	Monte Carlo simulations of a coarse grained model for an athermal all-polystyrene nanocomposite system. <i>European Polymer Journal</i> , 2011, 47, 699-712.	5.4	64
70	Lumping analysis for the prediction of long-time dynamics: From monomolecular reaction systems to inherent structure dynamics of glassy materials. <i>Journal of Chemical Physics</i> , 2011, 135, 204507.	3.0	16
71	A Study of the Entanglement in Systems with Periodic Boundary Conditions. <i>Progress of Theoretical Physics Supplement</i> , 2011, 191, 172-181.	0.1	27
72	Temperature Accelerated Dynamics in Glass-Forming Materials. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7844-7853.	2.6	8

#	ARTICLE	IF	CITATIONS
73	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. <i>Journal of Supercritical Fluids</i> , 2010, 55, 503-509.	3.2	7
74	Diffusion via space discretization method to study the concentration dependence of self-diffusivity under confinement. <i>Journal of Chemical Physics</i> , 2010, 132, 134108.	3.0	6
75	Crystallization and Melting Simulations of Oligomeric $\hat{\pm}1$ Isotactic Polypropylene. <i>Macromolecules</i> , 2010, 43, 5455-5469.	4.8	35
76	Prediction of Infinite Dilution Benzene Solubility in Linear Polyethylene Melts via the Direct Particle Deletion Method. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6233-6246.	2.6	17
77	Efficient Parallel Decomposition of Dynamical Sampling in Glass-Forming Materials Based on an $\hat{\epsilon}$ On the Fly $\hat{\epsilon}$ Definition of Metabasins. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1307-1322.	5.3	12
78	Progress and Outlook in Monte Carlo Simulations. <i>Industrial & Engineering Chemistry Research</i> , 2010, 49, 3047-3058.	3.7	102
79	Simulation studies of methane, carbon dioxide, hydrogen and deuterium in ITQ-1 and NaX zeolites. <i>Molecular Simulation</i> , 2009, 35, 79-89.	2.0	18
80	Molecular Dynamics of Carbon Dioxide, Methane and Their Mixtures in a Zeolite Possessing Two Independent Pore Networks as Revealed by Computer Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 13761-13767.	2.6	18
81	Benefit of Microscopic Diffusion Measurement for the Characterization of Nanoporous Materials. <i>Chemical Engineering and Technology</i> , 2009, 32, 1494-1511.	1.5	28
82	Diffusion in micropores. <i>Microporous and Mesoporous Materials</i> , 2009, 125, 1-2.	4.4	0
83	Onset of Entanglements Revisited. Dynamical Analysis. <i>Macromolecules</i> , 2009, 42, 7485-7494.	4.8	66
84	Onset of Entanglements Revisited. Topological Analysis. <i>Macromolecules</i> , 2009, 42, 7474-7484.	4.8	53
85	Probing subglass relaxation in polymers via a geometric representation of probabilities, observables, and relaxation modes for discrete stochastic systems. <i>Journal of Chemical Physics</i> , 2009, 130, 044905.	3.0	19
86	Prediction of Sorption of CO ₂ in Glassy Atactic Polystyrene at Elevated Pressures Through a New Computational Scheme. <i>Macromolecules</i> , 2009, 42, 1759-1769.	4.8	50
87	Combined Atomistic Simulation and Quasielastic Neutron Scattering Study of the Low-Temperature Dynamics of Hydrogen and Deuterium Confined in NaX Zeolite. <i>Journal of Physical Chemistry B</i> , 2008, 112, 11708-11715.	2.6	23
88	Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data. <i>Macromolecules</i> , 2008, 41, 2959-2962.	4.8	46
89	On the Role of Inherent Structures in Glass-forming Materials: II. Reconstruction of the Mean Square Displacement by Rigorous Lifting of the Inherent Structure Dynamics. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10628-10637.	2.6	9
90	On the Role of Inherent Structures in Glass-Forming Materials: I. The Vitrification Process. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10619-10627.	2.6	22

#	ARTICLE	IF	CITATIONS
91	A second-order Markov process for modeling diffusive motion through spatial discretization. Journal of Chemical Physics, 2008, 128, 024504.	3.0	6
92	Dynamical integration of a Markovian web: A first passage time approach. Journal of Chemical Physics, 2007, 127, 084903.	3.0	42
93	Formation of rodlike structures of water between oppositely charged ions in decane and polyethylene. Journal of Chemical Physics, 2007, 127, 191101.	3.0	2
94	Mesoscopic simulations of the diffusivity of ethane in beds of NaX zeolite crystals: Comparison with pulsed field gradient NMR measurements. Journal of Chemical Physics, 2007, 126, 094702.	3.0	28
95	Monte Carlo simulations of equilibrium solubilities and structure of water in n-alkanes and polyethylene. Journal of Chemical Physics, 2007, 126, 224902.	3.0	25
96	Coarse Grained End Bridging Monte Carlo Simulations of Poly(ethylene terephthalate) Melt. Macromolecules, 2007, 40, 710-722.	4.8	63
97	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.	4.8	190
98	Monte Carlo Simulation of Short Chain Branched Polyolefins in the Molten State. Macromolecules, 2007, 40, 9640-9650.	4.8	86
99	Segmental and Chain Dynamics of Isotactic Polypropylene Melts. Macromolecules, 2007, 40, 2235-2245.	4.8	40
100	Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends. Macromolecules, 2007, 40, 2904-2914.	4.8	8
101	Hierarchical modelling of polymeric materials. Chemical Engineering Science, 2007, 62, 5697-5714.	3.8	62
102	Quasi-elastic neutron scattering and molecular dynamics simulation as complementary techniques for studying diffusion in zeolites. Microporous and Mesoporous Materials, 2007, 102, 21-50.	4.4	249
103	Sorption Thermodynamics of CO ₂ , CH ₄ , and Their Mixtures in the ITQ-1 Zeolite as Revealed by Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 22742-22753.	2.6	39
104	Diffusion of Longn-Alkanes in Silicalite. A Comparison between Neutron Scattering Experiments and Hierarchical Simulation Results. Journal of Physical Chemistry B, 2006, 110, 1964-1967.	2.6	51
105	Topological Analysis of Linear Polymer Melts: A Statistical Approach. Macromolecules, 2006, 39, 4592-4604.	4.8	272
106	From atomistic simulations to slip-link models of entangled polymer melts: Hierarchical strategies for the prediction of rheological properties. Current Opinion in Solid State and Materials Science, 2006, 10, 61-72.	11.5	56
107	Principles of Molecular Simulation of Gas Transport in Polymers. , 2006, , 49-94.		34
108	Accelerating molecular simulations by reversible mapping between local minima. Journal of Chemical Physics, 2006, 125, 084107.	3.0	15

#	ARTICLE	IF	CITATIONS
109	A reversible minimum-to-minimum mapping method for the calculation of free-energy differences. <i>Journal of Chemical Physics</i> , 2006, 124, 034109.	3.0	23
110	Equilibration and Coarse-Graining Methods for Polymers. , 2006, , 419-448.		4
111	Pulsed-field gradient nuclear magnetic resonance study of transport properties of fluid catalytic cracking catalysts. <i>Magnetic Resonance Imaging</i> , 2005, 23, 233-237.	1.8	14
112	Molecular simulation of structure, thermodynamic and transport properties of polymeric membrane materials for hydrocarbon separation. <i>Fluid Phase Equilibria</i> , 2005, 228-229, 15-20.	2.5	16
113	Hierarchical modeling of amorphous polymers. <i>Computer Physics Communications</i> , 2005, 169, 82-88.	7.5	22
114	Structure and Volumetric Properties of Linear and Triarm Star Polyethylenes from Atomistic Monte Carlo Simulation Using New Internal Rearrangement Moves. <i>Macromolecules</i> , 2005, 38, 386-397.	4.8	38
115	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.	4.8	48
116	Microscopic Origins for the Favorable Solvation of Carbonate Ether Copolymers in CO ₂ . <i>Journal of the American Chemical Society</i> , 2005, 127, 12338-12342.	13.7	28
117	Detailed Atomistic Molecular Dynamics Simulation of cis-1,4-Poly(butadiene). <i>Macromolecules</i> , 2005, 38, 1478-1492.	4.8	118
118	Coarse graining using pretabulated potentials: Liquid benzene. <i>Journal of Chemical Physics</i> , 2005, 122, 244111.	3.0	23
119	Diffusion in Fluid Catalytic Cracking Catalysts on Various Displacement Scales and Its Role in Catalytic Performance. <i>Chemistry of Materials</i> , 2005, 17, 2466-2474.	6.7	74
120	Multiscale Modeling of Polymers. , 2005, , 2757-2761.		2
121	Multiscale Modeling of Polymers. , 2005, , 2757-2761.		0
122	Connectivity-Altering Monte Carlo Simulations of the End Group Effects on Volumetric Properties for Poly(ethylene oxide). <i>Macromolecules</i> , 2004, 37, 7026-7033.	4.8	60
123	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.	4.8	109
124	Experimental and Self-Consistent-Field Theoretical Study of Styrene Block Copolymer Self-Adhesive Materials. <i>Macromolecules</i> , 2004, 37, 5093-5109.	4.8	37
125	Molecular Dynamics Simulation of Structure and Thermodynamic Properties of Poly(dimethylsilamethylene) and Hydrocarbon Solubility Therein: Toward the Development of Novel Membrane Materials for Hydrocarbon Separation. <i>Macromolecules</i> , 2004, 37, 1102-1112.	4.8	46
126	Transport Diffusivity of N ₂ and CO ₂ in Silicalite: A Coherent Quasielastic Neutron Scattering Measurements and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12748-12756.	2.6	104

#	ARTICLE	IF	CITATIONS
127	Understanding and predicting structure-property relations in polymeric materials through molecular simulations. <i>Molecular Physics</i> , 2004, 102, 147-166.	1.7	52
128	On the separation between torsion-vibration and conformational relaxation processes in the incoherent intermediate scattering function of polyethylene. <i>Chemical Physics</i> , 2003, 292, 371-382.	1.9	14
129	Chain and local dynamics of polyisoprene as probed by experiments and computer simulations. <i>Journal of Chemical Physics</i> , 2003, 119, 6883-6894.	3.0	85
130	Crossover from the Rouse to the Entangled Polymer Melt Regime: Signals from Long, Detailed Atomistic Molecular Dynamics Simulations, Supported by Rheological Experiments. <i>Macromolecules</i> , 2003, 36, 1376-1387.	4.8	198
131	Atomistic Monte Carlo Simulation of Polybutadiene Isomers: cis-1,4-Polybutadiene and 1,2-Polybutadiene. <i>Macromolecules</i> , 2003, 36, 6925-6938.	4.8	50
132	Microscopic calculation of the static electric susceptibility of polyethylene. <i>Journal of Chemical Physics</i> , 2003, 119, 11458-11466.	3.0	8
133	Polymers at Surfaces and Interfaces. , 2003, , 329-419.		11
134	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.	7.8	218
135	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.	3.0	130
136	Atomistic molecular dynamics simulation of diffusion in binary liquid n-alkane mixtures. <i>Journal of Chemical Physics</i> , 2002, 116, 7656-7665.	3.0	49
137	Detailed molecular dynamics simulation of the self-diffusion of n-alkane and cis-1,4 polyisoprene oligomer melts. <i>Journal of Chemical Physics</i> , 2002, 116, 436.	3.0	85
138	Variable-Connectivity Monte Carlo Algorithms for the Atomistic Simulation of Long-Chain Polymer Systems. <i>Lecture Notes in Physics</i> , 2002, , 67-127.	0.7	14
139	Atomic structure of a high polymer melt. <i>Europhysics Letters</i> , 2002, 57, 506-511.	2.0	42
140	Mushrooms and Brushes in Thin Films of Diblock Copolymer/Homopolymer Mixtures. <i>Macromolecules</i> , 2002, 35, 1116-1132.	4.8	24
141	Entanglement Network of the Polypropylene/Polyamide Interface. 3. Deformation to Fracture. <i>Macromolecules</i> , 2002, 35, 508-521.	4.8	32
142	Parallel tempering method for reconstructing isotropic and anisotropic porous media. <i>Journal of Chemical Physics</i> , 2002, 117, 5876-5884.	3.0	24
143	Segmental Dynamics of Atactic Polypropylene As Revealed by Molecular Simulations and Quasielastic Neutron Scattering. <i>Macromolecules</i> , 2002, 35, 7110-7124.	4.8	35
144	Linking the atomistic scale and the mesoscale: molecular orbital and solid state packing calculations on poly(p-phenylene). <i>Polymer</i> , 2002, 43, 185-193.	3.8	9

#	ARTICLE	IF	CITATIONS
145	Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors. <i>Computer Physics Communications</i> , 2002, 144, 1-22.	7.5	32
146	Local Structure and Dynamics of trans-Polyisoprene Oligomers. <i>Macromolecules</i> , 2001, 34, 1436-1448.	4.8	45
147	Calculation of refractive indices and third-harmonic generation susceptibilities of liquid benzene and water: Comparison of continuum and discrete local-field theories. <i>Journal of Chemical Physics</i> , 2001, 114, 876.	3.0	29
148	Atomistic Monte Carlo simulation of cis-1,4 polyisoprene melts. I. Single temperature end-bridging Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2001, 115, 11339-11351.	3.0	56
149	Prediction of Permeation Properties of CO ₂ and N ₂ through Silicalite via Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2001, 105, 777-788.	2.6	182
150	Coarse-Grained Molecular Simulation of Penetrant Diffusion in a Glassy Polymer Using Reverse and Kinetic Monte Carlo. <i>Macromolecules</i> , 2001, 34, 8541-8553.	4.8	61
151	Henry's Constant Analysis for Water and Nonpolar Solvents from Experimental Data, Macroscopic Models, and Molecular Simulation. <i>Journal of Physical Chemistry B</i> , 2001, 105, 7792-7798.	2.6	36
152	Directed Bridging Methods for Fast Atomistic Monte Carlo Simulations of Bulk Polymers. <i>Macromolecules</i> , 2001, 34, 8554-8568.	4.8	53
153	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.	3.8	42
154	A new Monte Carlo simulation approach for the prediction of sorption equilibria of oligomers in polymer melts: Solubility of long alkanes in linear polyethylene. <i>Journal of Chemical Physics</i> , 2001, 115, 2860-2875.	3.0	32
155	Calculation of the chemical potential of chain molecules using the staged particle deletion scheme. <i>Journal of Chemical Physics</i> , 2001, 115, 8231-8237.	3.0	41
156	Atomistic Monte Carlo simulation of cis-1,4 polyisoprene melts. II. Parallel tempering end-bridging Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2001, 115, 11352-11361.	3.0	48
157	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.	1.4	26
158	Atomistic simulation of the birefringence of uniaxially stretched polyethylene melts. <i>Computational and Theoretical Polymer Science</i> , 2000, 10, 1-13.	1.1	35
159	Component segmental mobilities in an athermal polymer blend: Quasielastic incoherent neutron scattering versus simulation. <i>Journal of Chemical Physics</i> , 2000, 112, 8687-8694.	3.0	50
160	Molecular Simulation of Phase Equilibria for Water ⁿ -Butane and Water ⁿ -Hexane Mixtures. <i>Journal of Physical Chemistry B</i> , 2000, 104, 4958-4963.	2.6	47
161	Dynamics of n-Butane ⁿ Methane Mixtures in Silicalite, Using Quasielastic Neutron Scattering and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2000, 104, 5541-5552.	2.6	77
162	Entanglement Network of the Polypropylene/Polyamide Interface. 2. Network Generation. <i>Macromolecules</i> , 2000, 33, 1397-1410.	4.8	22

#	ARTICLE	IF	CITATIONS
163	Atomistic Molecular Dynamics Simulation of Stress Relaxation upon Cessation of Steady-State Uniaxial Elongational Flow. <i>Macromolecules</i> , 2000, 33, 8062-8076.	4.8	49
164	Entanglement Network of the Polypropylene/Polyamide Interface. 1. Self-Consistent Field Model. <i>Macromolecules</i> , 2000, 33, 1385-1396.	4.8	28
165	Dynamics of alkane mixtures in silicalite pores. <i>European Physical Journal Special Topics</i> , 2000, 10, Pr7-143-Pr7-146.	0.2	1
166	Molecular simulation of static hyper-Rayleigh scattering: A calculation of the depolarization ratio and the local fields for liquid nitrobenzene. <i>Journal of Chemical Physics</i> , 1999, 111, 9711-9719.	3.0	32
167	On the calculation of the chemical potential using the particle deletion scheme. <i>Molecular Physics</i> , 1999, 96, 905-913.	1.7	64
168	Computer simulation of the linear and nonlinear optical properties of liquid benzene: Its local fields, refractive index, and second nonlinear susceptibility. <i>Journal of Chemical Physics</i> , 1999, 110, 6463-6474.	3.0	33
169	Effect of Tacticity on the Molecular Dynamics of Polypropylene Melts. <i>Macromolecules</i> , 1999, 32, 8635-8644.	4.8	40
170	Molecular Dynamics Simulation of n-Butane~Methane Mixtures in Silicalite. <i>Journal of Physical Chemistry B</i> , 1999, 103, 3380-3390.	2.6	66
171	Molecular Simulation of $\hat{\pm}$ -Olefins Using a New United-Atom Potential Model: Vapor~Liquid Equilibria of Pure Compounds and Mixtures. <i>Journal of the American Chemical Society</i> , 1999, 121, 3407-3413.	13.7	29
172	Van Hove Function for Diffusion in Zeolites. <i>Journal of Physical Chemistry B</i> , 1999, 103, 4721-4729.	2.6	19
173	End-Bridging Monte Carlo: A Fast Algorithm for Atomistic Simulation of Condensed Phases of Long Polymer Chains. <i>Macromolecules</i> , 1999, 32, 5072-5096.	4.8	237
174	On the calculation of the chemical potential using the particle deletion scheme. <i>Molecular Physics</i> , 1999, 96, 905-913.	1.7	3
175	Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts. <i>Macromolecules</i> , 1998, 31, 7934-7943.	4.8	182
176	Calculation of macroscopic first- and third-order optical susceptibilities for the benzene crystal. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 384-390.	1.4	26
177	Hierarchical simulation approach to structure and dynamics of polymers. <i>Current Opinion in Solid State and Materials Science</i> , 1998, 3, 544-551.	11.5	40
178	Monte Carlo Simulations of a Single Polyelectrolyte in Solution: Activity Coefficients of the Simple Ions and Application to Viscosity Measurements. <i>Macromolecules</i> , 1998, 31, 7921-7933.	4.8	15
179	Molecular Simulation of the Puren-Hexadecane Vapor~Liquid Equilibria at Elevated Temperature. <i>Macromolecules</i> , 1998, 31, 1430-1431.	4.8	10
180	Molecular Modeling of Methane Diffusion in Glassy Atactic Polypropylene via Multidimensional Transition State Theory. <i>Macromolecules</i> , 1998, 31, 7068-7090.	4.8	86

#	ARTICLE	IF	CITATIONS
181	Molecular Dynamics of Atactic Polypropylene Melts. <i>Macromolecules</i> , 1998, 31, 7944-7952.	4.8	55
182	Molecular Simulation of Phase Equilibria for Water~Methane and Water~Ethane Mixtures. <i>Journal of Physical Chemistry B</i> , 1998, 102, 8865-8873.	2.6	115
183	Atomistic Simulation of Polymer Melt Elasticity:Â Calculation of the Free Energy of an Oriented Polymer Melt. <i>Macromolecules</i> , 1998, 31, 6310-6332.	4.8	136
184	Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature Range. <i>Journal of Physical Chemistry B</i> , 1998, 102, 1029-1035.	2.6	159
185	Transition-state theory investigations of small molecule diffusion in glassy polymers. , 1998, , .		0
186	Phase Equilibria of Mixtures Containing Chain Molecules Predicted through a Novel Simulation Scheme. <i>Physical Review Letters</i> , 1998, 80, 4466-4469.	7.8	57
187	Elementary structural transitions in the amorphous Lennard-Jones solid using multidimensional transition-state theory. <i>Journal of Chemical Physics</i> , 1998, 109, 8573-8582.	3.0	29
188	Calculation of macroscopic first- and third-order optical susceptibilities for the benzene crystal. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 384.	1.4	14
189	Surface tension and phase coexistence properties of the lattice fluid from a virtual site removal Monte Carlo strategy. <i>Journal of Chemical Physics</i> , 1997, 107, 5125-5140.	3.0	5
190	Simulation of hydrocarbon diffusion in zeolites. <i>Studies in Surface Science and Catalysis</i> , 1997, 105, 1851-1858.	1.5	5
191	Segment density of a block copolymer chain tethered at both ends. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 4355-4370.	1.7	2
192	Transition-State Theory Model for the Diffusion Coefficients of Small Penetrants in Glassy Polymers. <i>Macromolecules</i> , 1997, 30, 7296-7306.	4.8	69
193	Thermodynamics of Chain Fluids from Atomistic Simulation:â€ A Test of the Chain Increment Method for Chemical Potential. <i>Macromolecules</i> , 1997, 30, 4744-4755.	4.8	47
194	Coupling of Penetrant and Polymer Motions During Small-Molecule Diffusion In a Glassy Polymer. <i>Molecular Simulation</i> , 1997, 19, 329-361.	2.0	35
195	Analysis of Computed Trajectories of Penetrant Micromolecules in a Simulated Polymeric Material. <i>Macromolecules</i> , 1996, 29, 3615-3624.	4.8	28
196	Dynamics of Longn-Alkanes in Silicalite:Â A Hierarchical Simulation Approach. <i>The Journal of Physical Chemistry</i> , 1996, 100, 7155-7173.	2.9	132
197	Investigation of the dynamics of benzene in silicalite using transition-state theory. <i>Studies in Surface Science and Catalysis</i> , 1995, 98, 240-241.	1.5	5
198	Variable Connectivity Method for the Atomistic Monte Carlo Simulation of Polydisperse Polymer Melts. <i>Macromolecules</i> , 1995, 28, 7224-7234.	4.8	244

#	ARTICLE	IF	CITATIONS
199	Sorption Thermodynamics, Siting, and Conformation of Long n-Alkanes in Silicalite As Predicted by Configurational-Bias Monte Carlo Integration. The Journal of Physical Chemistry, 1995, 99, 2057-2079.	2.9	148
200	Self-consistent field model of the polymer/diblock copolymer/polymer interface. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 2381.	1.7	29
201	Electronic Structure Calculations of Ammonia Adsorption in H-ZSM-5 Zeolites. The Journal of Physical Chemistry, 1995, 99, 1505-1515.	2.9	63
202	Investigation of the dynamics of benzene in silicalite using Transition-State Theory. The Journal of Physical Chemistry, 1994, 98, 11948-11961.	2.9	93
203	Atomistic Monte Carlo simulation and continuum mean field theory of the structure and equation of state properties of alkane and polymer melts. , 1994, , 249-281.		49
204	Static atomistic modelling of the structure and ring dynamics of bulk amorphous polystyrene. Macromolecular Theory and Simulations, 1994, 3, 19-43.	1.4	57
205	A hierarchical atomistic/lattice simulation approach for the prediction of adsorption thermodynamics of benzene in silicalite. The Journal of Physical Chemistry, 1994, 98, 5111-5119.	2.9	87
206	Low-Occupancy Sorption Thermodynamics of Long Alkanes in Silicalite Via Molecular Simulation. Studies in Surface Science and Catalysis, 1994, 84, 2099-2105.	1.5	4
207	Stress tensor in model polymer systems with periodic boundaries. Die Makromolekulare Chemie Theory and Simulations, 1993, 2, 191-238.	1.0	61
208	Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulations with biased insertions. The Journal of Physical Chemistry, 1993, 97, 13742-13752.	2.9	366
209	Transport diffusivity of methane in silicalite from equilibrium and nonequilibrium simulations. The Journal of Physical Chemistry, 1993, 97, 4173-4181.	2.9	310
210	Geometric analysis of diffusion pathways in glassy and melt atactic polypropylene. Macromolecules, 1993, 26, 5461-5472.	4.8	139
211	A concerted rotation algorithm for atomistic Monte Carlo simulation of polymer melts and glasses. Molecular Physics, 1993, 78, 961-996.	1.7	270
212	Structural and electronic features of a Broensted acid site in H-ZSM-5. The Journal of Physical Chemistry, 1993, 97, 6679-6685.	2.9	43
213	A chain of states method for investigating infrequent event processes occurring in multistate, multidimensional systems. Journal of Chemical Physics, 1993, 98, 3196-3212.	3.0	75
214	Molecular dynamics studies of butane and hexane in silicalite. The Journal of Physical Chemistry, 1992, 96, 1051-1060.	2.9	244
215	Molecular Modeling of Polymer Surfaces and Polymer/Solid Interfaces. , 1992, , 139-162.		6
216	Molecular Simulations of Methane Adsorption in Silicalite. Molecular Simulation, 1991, 8, 73-92.	2.0	61

#	ARTICLE	IF	CITATIONS
217	Analytical treatment of the volume and surface area of molecules formed by an arbitrary collection of unequal spheres intersected by planes. <i>Molecular Physics</i> , 1991, 72, 1313-1345.	1.7	124
218	Atomistic simulation of a glassy polymer/graphite interface. <i>Macromolecules</i> , 1991, 24, 4295-4309.	4.8	138
219	Molecular dynamics simulation of a glassy polymer surface. <i>Macromolecules</i> , 1991, 24, 6283-6294.	4.8	331
220	Molecular dynamics study of methane and xenon in silicalite [Erratum to document cited in CA113(20):183284q]. <i>The Journal of Physical Chemistry</i> , 1991, 95, 1014-1014.	2.9	4
221	Transition-state studies of xenon and sulfur hexafluoride diffusion in silicalite. <i>The Journal of Physical Chemistry</i> , 1991, 95, 8866-8878.	2.9	180
222	The effects of local structural relaxation on aluminum siting within H-ZSM-5. <i>Catalysis Letters</i> , 1991, 11, 209-217.	2.6	103
223	Prediction of low occupancy sorption of alkanes in silicalite. <i>The Journal of Physical Chemistry</i> , 1990, 94, 1508-1516.	2.9	210
224	Molecular dynamics study of methane and xenon in silicalite. <i>The Journal of Physical Chemistry</i> , 1990, 94, 8232-8240.	2.9	258
225	Atomistic simulation of a glassy polymer surface. <i>Macromolecules</i> , 1990, 23, 4430-4445.	4.8	127
226	Variable-density model of polymer melt/solid interfaces: structure, adhesion tension, and surface forces. <i>Macromolecules</i> , 1989, 22, 4589-4597.	4.8	53
227	Variable-density model of polymer melt surfaces: structure and surface tension. <i>Macromolecules</i> , 1989, 22, 4578-4589.	4.8	90
228	Interfacial structure and dynamics of macromolecular liquids: a Monte Carlo simulation approach. <i>Macromolecules</i> , 1989, 22, 3143-3152.	4.8	121
229	Microscopic structure and thermodynamic properties of bulk copolymers and surface-active polymers at interfaces. 2. Results for some representative chain architectures. <i>Macromolecules</i> , 1988, 21, 1422-1436.	4.8	30
230	Structure and thermodynamics of bulk homopolymer solid interfaces: a site lattice model approach. <i>Macromolecules</i> , 1988, 21, 1400-1410.	4.8	77
231	Lattice models for bulk polymers at interfaces. <i>Macromolecules</i> , 1988, 21, 1391-1400.	4.8	74
232	Microscopic structure and thermodynamic properties of bulk copolymers and surface-active polymers at interfaces. 1. Theory. <i>Macromolecules</i> , 1988, 21, 1411-1421.	4.8	31
233	Detailed Modeling of Structure and Deformation of Glassy Polymers. <i>Materials Research Society Symposia Proceedings</i> , 1986, 79, 387.	0.1	0
234	Local structure and the mechanism of response to elastic deformation in a glassy polymer. <i>Macromolecules</i> , 1986, 19, 379-387.	4.8	111

#	ARTICLE	IF	CITATIONS
235	Atomistic modeling of mechanical properties of polymeric glasses. <i>Macromolecules</i> , 1986, 19, 139-154.	4.8	512
236	Geometrical considerations in model systems with periodic boundaries. <i>Journal of Chemical Physics</i> , 1985, 82, 955-966.	3.0	83
237	Detailed molecular structure of a vinyl polymer glass. <i>Macromolecules</i> , 1985, 18, 1467-1478.	4.8	830
238	Shape of unperturbed linear polymers: polypropylene. <i>Macromolecules</i> , 1985, 18, 1206-1214.	4.8	401
239	Diffusion and reaction in blocked and high occupancy zeolite catalysts. <i>Journal of Catalysis</i> , 1983, 83, 205-224.	6.2	139