

# 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

21215

62  
h-index

26792

111  
g-index

272  
all docs

272  
docs citations

272  
times ranked

7983  
citing authors

#	ARTICLE	IF	CITATIONS
1	Detailed molecular structure of a vinyl polymer glass. <i>Macromolecules</i> , 1985, 18, 1467-1478.	2.2	830
2	Atomistic modeling of mechanical properties of polymeric glasses. <i>Macromolecules</i> , 1986, 19, 139-154.	2.2	512
3	Shape of unperturbed linear polymers: polypropylene. <i>Macromolecules</i> , 1985, 18, 1206-1214.	2.2	401
4	Prediction of adsorption of aromatic hydrocarbons in silicalite from grand canonical Monte Carlo simulations with biased insertions. <i>The Journal of Physical Chemistry</i> , 1993, 97, 13742-13752.	2.9	366
5	Molecular dynamics simulation of a glassy polymer surface. <i>Macromolecules</i> , 1991, 24, 6283-6294.	2.2	331
6	Transport diffusivity of methane in silicalite from equilibrium and nonequilibrium simulations. <i>The Journal of Physical Chemistry</i> , 1993, 97, 4173-4181.	2.9	310
7	Topological Analysis of Linear Polymer Melts: A Statistical Approach. <i>Macromolecules</i> , 2006, 39, 4592-4604.	2.2	272
8	A concerted rotation algorithm for atomistic Monte Carlo simulation of polymer melts and glasses. <i>Molecular Physics</i> , 1993, 78, 961-996.	0.8	270
9	Molecular dynamics study of methane and xenon in silicalite. <i>The Journal of Physical Chemistry</i> , 1990, 94, 8232-8240.	2.9	258
10	Quasi-elastic neutron scattering and molecular dynamics simulation as complementary techniques for studying diffusion in zeolites. <i>Microporous and Mesoporous Materials</i> , 2007, 102, 21-50.	2.2	249
11	Molecular dynamics studies of butane and hexane in silicalite. <i>The Journal of Physical Chemistry</i> , 1992, 96, 1051-1060.	2.9	244
12	Variable Connectivity Method for the Atomistic Monte Carlo Simulation of Polydisperse Polymer Melts. <i>Macromolecules</i> , 1995, 28, 7224-7234.	2.2	244
13	Interface of Grafted and Ungrafted Silica Nanoparticles with a Polystyrene Matrix: Atomistic Molecular Dynamics Simulations. <i>Macromolecules</i> , 2011, 44, 2316-2327.	2.2	239
14	End-Bridging Monte Carlo: A Fast Algorithm for Atomistic Simulation of Condensed Phases of Long Polymer Chains. <i>Macromolecules</i> , 1999, 32, 5072-5096.	2.2	237
15	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.	2.9	218
16	Prediction of low occupancy sorption of alkanes in silicalite. <i>The Journal of Physical Chemistry</i> , 1990, 94, 1508-1516.	2.9	210
17	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.	2.2	198
18	Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts: Structure, Thermodynamic Properties, Chain Conformation, and Entanglements. <i>Macromolecules</i> , 2007, 40, 3876-3885.	2.2	190

#	ARTICLE	IF	CITATIONS
19	Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts. <i>Macromolecules</i> , 1998, 31, 7934-7943.	2.2	182
20	Prediction of Permeation Properties of CO <sub>2</sub> and N <sub>2</sub> through Silicalite via Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2001, 105, 777-788.	1.2	182
21	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
22	Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature Range. <i>Journal of Physical Chemistry B</i> , 1998, 102, 1029-1035.	1.2	159
23	Sorption Thermodynamics, Siting, and Conformation of Long n-Alkanes in Silicalite As Predicted by Configurational-Bias Monte Carlo Integration. <i>The Journal of Physical Chemistry</i> , 1995, 99, 2057-2079.	2.9	148
24	Diffusion and reaction in blocked and high occupancy zeolite catalysts. <i>Journal of Catalysis</i> , 1983, 83, 205-224.	3.1	139
25	Geometric analysis of diffusion pathways in glassy and melt atactic polypropylene. <i>Macromolecules</i> , 1993, 26, 5461-5472.	2.2	139
26	Atomistic simulation of a glassy polymer/graphite interface. <i>Macromolecules</i> , 1991, 24, 4295-4309.	2.2	138
27	Atomistic Simulation of Polymer Melt Elasticity: Calculation of the Free Energy of an Oriented Polymer Melt. <i>Macromolecules</i> , 1998, 31, 6310-6332.	2.2	136
28	Dynamics of Long n-Alkanes in Silicalite: A Hierarchical Simulation Approach. <i>The Journal of Physical Chemistry</i> , 1996, 100, 7155-7173.	2.9	132
29	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.	1.2	130
30	Atomistic simulation of a glassy polymer surface. <i>Macromolecules</i> , 1990, 23, 4430-4445.	2.2	127
31	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.	0.8	124
32	Interfacial structure and dynamics of macromolecular liquids: a Monte Carlo simulation approach. <i>Macromolecules</i> , 1989, 22, 3143-3152.	2.2	121
33	Detailed Atomistic Molecular Dynamics Simulation of cis-1,4-Poly(butadiene). <i>Macromolecules</i> , 2005, 38, 1478-1492.	2.2	118
34	Molecular Simulation of Phase Equilibria for Water~Methane and Water~Ethane Mixtures. <i>Journal of Physical Chemistry B</i> , 1998, 102, 8865-8873.	1.2	115
35	Local structure and the mechanism of response to elastic deformation in a glassy polymer. <i>Macromolecules</i> , 1986, 19, 379-387.	2.2	111
36	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.	2.2	109

#	ARTICLE	IF	CITATIONS
37	Transport Diffusivity of N <sub>2</sub> and CO <sub>2</sub> in Silicalite: A Coherent Quasielastic Neutron Scattering Measurements and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 12748-12756.	1.2	104
38	The effects of local structural relaxation on aluminum siting within H-ZSM-5. <i>Catalysis Letters</i> , 1991, 11, 209-217.	1.4	103
39	Progress and Outlook in Monte Carlo Simulations. <i>Industrial &amp; Engineering Chemistry Research</i> , 2010, 49, 3047-3058.	1.8	102
40	Structure of Polymer Layers Grafted to Nanoparticles in Silica-Polystyrene Nanocomposites. <i>Macromolecules</i> , 2013, 46, 4670-4683.	2.2	95
41	Investigation of the dynamics of benzene in silicalite using Transition-State Theory. <i>The Journal of Physical Chemistry</i> , 1994, 98, 11948-11961.	2.9	93
42	Variable-density model of polymer melt surfaces: structure and surface tension. <i>Macromolecules</i> , 1989, 22, 4578-4589.	2.2	90
43	A hierarchical atomistic/lattice simulation approach for the prediction of adsorption thermodynamics of benzene in silicalite. <i>The Journal of Physical Chemistry</i> , 1994, 98, 5111-5119.	2.9	87
44	Molecular Modeling of Methane Diffusion in Glassy Atactic Polypropylene via Multidimensional Transition State Theory. <i>Macromolecules</i> , 1998, 31, 7068-7090.	2.2	86
45	Monte Carlo Simulation of Short Chain Branched Polyolefins in the Molten State. <i>Macromolecules</i> , 2007, 40, 9640-9650.	2.2	86
46	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.	1.2	85
47	Chain and local dynamics of polyisoprene as probed by experiments and computer simulations. <i>Journal of Chemical Physics</i> , 2003, 119, 6883-6894.	1.2	85
48	Local Segmental Dynamics and Stresses in Polystyrene-C <sub>60</sub> Mixtures. <i>Macromolecules</i> , 2014, 47, 387-404.	2.2	85
49	Geometrical considerations in model systems with periodic boundaries. <i>Journal of Chemical Physics</i> , 1985, 82, 955-966.	1.2	83
50	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.	2.2	83
51	Structure and thermodynamics of bulk homopolymer solid interfaces: a site lattice model approach. <i>Macromolecules</i> , 1988, 21, 1400-1410.	2.2	77
52	Dynamics of n-Butane-Methane Mixtures in Silicalite, Using Quasielastic Neutron Scattering and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2000, 104, 5541-5552.	1.2	77
53	A chain of states method for investigating infrequent event processes occurring in multistate, multidimensional systems. <i>Journal of Chemical Physics</i> , 1993, 98, 3196-3212.	1.2	75
54	Lattice models for bulk polymers at interfaces. <i>Macromolecules</i> , 1988, 21, 1391-1400.	2.2	74

#	ARTICLE	IF	CITATIONS
55	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.	3.2	74
56	Transition-State Theory Model for the Diffusion Coefficients of Small Penetrants in Glassy Polymers. <i>Macromolecules</i> , 1997, 30, 7296-7306.	2.2	69
57	Molecular Dynamics Simulation of n-Butane-Methane Mixtures in Silicalite. <i>Journal of Physical Chemistry B</i> , 1999, 103, 3380-3390.	1.2	66
58	Onset of Entanglements Revisited. <i>Dynamical Analysis. Macromolecules</i> , 2009, 42, 7485-7494.	2.2	66
59	On the calculation of the chemical potential using the particle deletion scheme. <i>Molecular Physics</i> , 1999, 96, 905-913.	0.8	64
60	Monte Carlo simulations of a coarse grained model for an athermal all-polystyrene nanocomposite system. <i>European Polymer Journal</i> , 2011, 47, 699-712.	2.6	64
61	Electronic Structure Calculations of Ammonia Adsorption in H-ZSM-5 Zeolites. <i>The Journal of Physical Chemistry</i> , 1995, 99, 1505-1515.	2.9	63
62	Coarse Grained End Bridging Monte Carlo Simulations of Poly(ethylene terephthalate) Melt. <i>Macromolecules</i> , 2007, 40, 710-722.	2.2	63
63	Hierarchical modelling of polymeric materials. <i>Chemical Engineering Science</i> , 2007, 62, 5697-5714.	1.9	62
64	Molecular Simulations of Methane Adsorption in Silicalite. <i>Molecular Simulation</i> , 1991, 8, 73-92.	0.9	61
65	Stress tensor in model polymer systems with periodic boundaries. <i>Die Makromolekulare Chemie Theory and Simulations</i> , 1993, 2, 191-238.	1.0	61
66	Coarse-Grained Molecular Simulation of Penetrant Diffusion in a Glassy Polymer Using Reverse and Kinetic Monte Carlo. <i>Macromolecules</i> , 2001, 34, 8541-8553.	2.2	61
67	Connectivity-Altering Monte Carlo Simulations of the End Group Effects on Volumetric Properties for Poly(ethylene oxide). <i>Macromolecules</i> , 2004, 37, 7026-7033.	2.2	60
68	Static atomistic modelling of the structure and ring dynamics of bulk amorphous polystyrene. <i>Macromolecular Theory and Simulations</i> , 1994, 3, 19-43.	0.6	57
69	Phase Equilibria of Mixtures Containing Chain Molecules Predicted through a Novel Simulation Scheme. <i>Physical Review Letters</i> , 1998, 80, 4466-4469.	2.9	57
70	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.	1.2	56
71	From atomistic simulations to slip-link models of entangled polymer melts: Hierarchical strategies for the prediction of rheological properties. <i>Current Opinion in Solid State and Materials Science</i> , 2006, 10, 61-72.	5.6	56
72	Molecular Dynamics of Atactic Polypropylene Melts. <i>Macromolecules</i> , 1998, 31, 7944-7952.	2.2	55

#	ARTICLE	IF	CITATIONS
73	Molecular Modeling Investigations of Sorption and Diffusion of Small Molecules in Glassy Polymers. Membranes, 2019, 9, 98.	1.4	54
74	Variable-density model of polymer melt/solid interfaces: structure, adhesion tension, and surface forces. Macromolecules, 1989, 22, 4589-4597.	2.2	53
75	Directed Bridging Methods for Fast Atomistic Monte Carlo Simulations of Bulk Polymers. Macromolecules, 2001, 34, 8554-8568.	2.2	53
76	Onset of Entanglements Revisited. Topological Analysis. Macromolecules, 2009, 42, 7474-7484.	2.2	53
77	Understanding and predicting structure-property relations in polymeric materials through molecular simulations. Molecular Physics, 2004, 102, 147-166.	0.8	52
78	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.	1.2	51
79	Component segmental mobilities in an athermal polymer blend: Quasielastic incoherent neutron scattering versus simulation. Journal of Chemical Physics, 2000, 112, 8687-8694.	1.2	50
80	Atomistic Monte Carlo Simulation of Polybutadiene Isomers: cis-1,4-Polybutadiene and 1,2-Polybutadiene. Macromolecules, 2003, 36, 6925-6938.	2.2	50
81	Prediction of Sorption of CO <sub>2</sub> in Glassy Atactic Polystyrene at Elevated Pressures Through a New Computational Scheme. Macromolecules, 2009, 42, 1759-1769.	2.2	50
82	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
83	Atomistic Molecular Dynamics Simulation of Stress Relaxation upon Cessation of Steady-State Uniaxial Elongational Flow. Macromolecules, 2000, 33, 8062-8076.	2.2	49
84	Atomistic molecular dynamics simulation of diffusion in binary liquid n-alkane mixtures. Journal of Chemical Physics, 2002, 116, 7656-7665.	1.2	49
85	Atomistic Monte Carlo simulation of cis-1,4 polyisoprene melts. II. Parallel tempering end-bridging Monte Carlo simulations. Journal of Chemical Physics, 2001, 115, 11352-11361.	1.2	48
86	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. Macromolecules, 2005, 38, 7134-7149.	2.2	48
87	Slip-Spring Model for the Linear and Nonlinear Viscoelastic Properties of Molten Polyethylene Derived from Atomistic Simulations. Macromolecules, 2017, 50, 4524-4541.	2.2	48
88	Thermodynamics of Chain Fluids from Atomistic Simulation: A Test of the Chain Increment Method for Chemical Potential. Macromolecules, 1997, 30, 4744-4755.	2.2	47
89	Molecular Simulation of Phase Equilibria for Water~n-Butane and Water~n-Hexane Mixtures. Journal of Physical Chemistry B, 2000, 104, 4958-4963.	1.2	47
90	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. Macromolecules, 2004, 37, 1102-1112.	2.2	46

#	ARTICLE	IF	CITATIONS
91	Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data. <i>Macromolecules</i> , 2008, 41, 2959-2962.	2.2	46
92	Molecular Simulations of Free and Graphite Capped Polyethylene Films: Estimation of the Interfacial Free Energies. <i>Macromolecules</i> , 2017, 50, 8827-8844.	2.2	46
93	Local Structure and Dynamics of trans-Polyisoprene Oligomers. <i>Macromolecules</i> , 2001, 34, 1436-1448.	2.2	45
94	Microscopic Description of Entanglements in Polyethylene Networks and Melts: Strong, Weak, Pairwise, and Collective Attributes. <i>Macromolecules</i> , 2012, 45, 9475-9492.	2.2	45
95	Equation of State Based Slip Spring Model for Entangled Polymer Dynamics. <i>Macromolecules</i> , 2017, 50, 3004-3029.	2.2	45
96	Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites. <i>Archives of Computational Methods in Engineering</i> , 2018, 25, 591-645.	6.0	45
97	Structural and electronic features of a Brønsted acid site in H-ZSM-5. <i>The Journal of Physical Chemistry</i> , 1993, 97, 6679-6685.	2.9	43
98	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.	1.9	42
99	Atomic structure of a high polymer melt. <i>Europhysics Letters</i> , 2002, 57, 506-511.	0.7	42
100	Dynamical integration of a Markovian web: A first passage time approach. <i>Journal of Chemical Physics</i> , 2007, 127, 084903.	1.2	42
101	Calculation of the chemical potential of chain molecules using the staged particle deletion scheme. <i>Journal of Chemical Physics</i> , 2001, 115, 8231-8237.	1.2	41
102	Molecular dynamics simulations of EPON-862/DETDA epoxy networks: structure, topology, elastic constants, and local dynamics. <i>Soft Matter</i> , 2019, 15, 721-733.	1.2	41
103	Hierarchical simulation approach to structure and dynamics of polymers. <i>Current Opinion in Solid State and Materials Science</i> , 1998, 3, 544-551.	5.6	40
104	Effect of Tacticity on the Molecular Dynamics of Polypropylene Melts. <i>Macromolecules</i> , 1999, 32, 8635-8644.	2.2	40
105	Segmental and Chain Dynamics of Isotactic Polypropylene Melts. <i>Macromolecules</i> , 2007, 40, 2235-2245.	2.2	40
106	Sorption Thermodynamics of CO <sub>2</sub> , CH <sub>4</sub> , and Their Mixtures in the ITQ-1 Zeolite as Revealed by Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 22742-22753.	1.2	39
107	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.	2.2	38
108	Experimental and Self-Consistent-Field Theoretical Study of Styrene Block Copolymer Self-Adhesive Materials. <i>Macromolecules</i> , 2004, 37, 5093-5109.	2.2	37

#	ARTICLE	IF	CITATIONS
109	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.	1.2	36
110	Coupling of Penetrant and Polymer Motions During Small-Molecule Diffusion In a Glassy Polymer. <i>Molecular Simulation</i> , 1997, 19, 329-361.	0.9	35
111	Atomistic simulation of the birefringence of uniaxially stretched polyethylene melts. <i>Computational and Theoretical Polymer Science</i> , 2000, 10, 1-13.	1.1	35
112	Segmental Dynamics of Atactic Polypropylene As Revealed by Molecular Simulations and Quasielastic Neutron Scattering. <i>Macromolecules</i> , 2002, 35, 7110-7124.	2.2	35
113	Crystallization and Melting Simulations of Oligomeric $\hat{\pm}1$ Isotactic Polypropylene. <i>Macromolecules</i> , 2010, 43, 5455-5469.	2.2	35
114	Systematic Coarse Graining of 4-Cyano-4- $\hat{\epsilon}^2$ -pentylbiphenyl. <i>Industrial &amp; Engineering Chemistry Research</i> , 2011, 50, 546-556.	1.8	35
115	Principles of Molecular Simulation of Gas Transport in Polymers. , 2006, , 49-94.		34
116	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.	1.2	33
117	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.	1.2	32
118	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.	1.2	32
119	Entanglement Network of the Polypropylene/Polyamide Interface. 3. Deformation to Fracture. <i>Macromolecules</i> , 2002, 35, 508-521.	2.2	32
120	Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors. <i>Computer Physics Communications</i> , 2002, 144, 1-22.	3.0	32
121	Microscopic structure and thermodynamic properties of bulk copolymers and surface-active polymers at interfaces. 1. Theory. <i>Macromolecules</i> , 1988, 21, 1411-1421.	2.2	31
122	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.	2.2	30
123	Self-consistent field model of the polymer/diblock copolymer/polymer interface. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1995, 91, 2381.	1.7	29
124	Elementary structural transitions in the amorphous Lennard-Jones solid using multidimensional transition-state theory. <i>Journal of Chemical Physics</i> , 1998, 109, 8573-8582.	1.2	29
125	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.	6.6	29
126	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.	1.2	29



#	ARTICLE	IF	CITATIONS
127	Analysis of Computed Trajectories of Penetrant Micromolecules in a Simulated Polymeric Material. <i>Macromolecules</i> , 1996, 29, 3615-3624.	2.2	28
128	Entanglement Network of the Polypropylene/Polyamide Interface. 1. Self-Consistent Field Model. <i>Macromolecules</i> , 2000, 33, 1385-1396.	2.2	28
129	Microscopic Origins for the Favorable Solvation of Carbonate Ether Copolymers in CO <sub>2</sub> . <i>Journal of the American Chemical Society</i> , 2005, 127, 12338-12342.	6.6	28
130	Mesoscopic simulations of the diffusivity of ethane in beds of NaX zeolite crystals: Comparison with pulsed field gradient NMR measurements. <i>Journal of Chemical Physics</i> , 2007, 126, 094702.	1.2	28
131	Benefit of Microscopic Diffusion Measurement for the Characterization of Nanoporous Materials. <i>Chemical Engineering and Technology</i> , 2009, 32, 1494-1511.	0.9	28
132	A Study of the Entanglement in Systems with Periodic Boundary Conditions. <i>Progress of Theoretical Physics Supplement</i> , 2011, 191, 172-181.	0.2	27
133	Calculation of macroscopic first- and third-order optical susceptibilities for the benzene crystal. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 384-390.	0.5	26
134	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.	0.6	26
135	Exploring the interactions of irbesartan and irbesartan- $\beta$ -2-hydroxypropyl- $\beta$ -cyclodextrin complex with model membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 1089-1098.	1.4	26
136	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.	1.2	26
137	Monte Carlo simulations of equilibrium solubilities and structure of water in n-alkanes and polyethylene. <i>Journal of Chemical Physics</i> , 2007, 126, 224902.	1.2	25
138	Monte Carlo Simulation of Short Chain Branched Polyolefins: Structure and Properties. <i>Macromolecules</i> , 2012, 45, 8453-8466.	2.2	25
139	Mushrooms and Brushes in Thin Films of Diblock Copolymer/Homopolymer Mixtures. <i>Macromolecules</i> , 2002, 35, 1116-1132.	2.2	24
140	Parallel tempering method for reconstructing isotropic and anisotropic porous media. <i>Journal of Chemical Physics</i> , 2002, 117, 5876-5884.	1.2	24
141	Coarse graining using pretabulated potentials: Liquid benzene. <i>Journal of Chemical Physics</i> , 2005, 122, 244111.	1.2	23
142	A reversible minimum-to-minimum mapping method for the calculation of free-energy differences. <i>Journal of Chemical Physics</i> , 2006, 124, 034109.	1.2	23
143	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.	1.2	23
144	Multiscale simulations of PS-SiO <sub>2</sub> nanocomposites: from melt to glassy state. <i>Soft Matter</i> , 2016, 12, 7585-7605.	1.2	23

#	ARTICLE	IF	CITATIONS
145	Entanglement Network of the Polypropylene/Polyamide Interface. 2. Network Generation. <i>Macromolecules</i> , 2000, 33, 1397-1410.	2.2	22
146	Hierarchical modeling of amorphous polymers. <i>Computer Physics Communications</i> , 2005, 169, 82-88.	3.0	22
147	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.	1.2	22
148	Tracking a glassy polymer on its energy landscape in the course of elastic deformation. <i>Molecular Physics</i> , 2013, 111, 3430-3441.	0.8	21
149	Molecular Dynamics Study of Polyethylene under Extreme Confinement. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012012.	0.3	21
150	Slip Spring-Based Mesoscopic Simulations of Polymer Networks: Methodology and the Corresponding Computational Code. <i>Polymers</i> , 2018, 10, 1156.	2.0	21
151	Application of bi-Helmholtz nonlocal elasticity and molecular simulations to the dynamical response of carbon nanotubes. <i>AIP Conference Proceedings</i> , 2015, , .	0.3	20
152	Diffusion of Aromatics in Silicalite-1: Experimental and Theoretical Evidence of Entropic Barriers. <i>Journal of Physical Chemistry C</i> , 2016, 120, 21410-21426.	1.5	20
153	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.	2.2	20
154	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.	2.2	20
155	Van Hove Function for Diffusion in Zeolites. <i>Journal of Physical Chemistry B</i> , 1999, 103, 4721-4729.	1.2	19
156	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.	1.2	19
157	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.	0.9	19
158	Thermodynamic analysis of Lennard-Jones binary mixtures using Kirkwood-Buff theory. <i>Fluid Phase Equilibria</i> , 2018, 470, 25-37.	1.4	19
159	Simulation studies of methane, carbon dioxide, hydrogen and deuterium in ITQ-1 and NaX zeolites. <i>Molecular Simulation</i> , 2009, 35, 79-89.	0.9	18
160	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.	1.2	18
161	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.	1.2	17
162	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.	2.2	17

#	ARTICLE	IF	CITATIONS
163	Melting Point and Solid-Liquid Coexistence Properties of $\pm 1$ Isotactic Polypropylene as Functions of Its Molar Mass: A Molecular Dynamics Study. <i>Macromolecules</i> , 2016, 49, 4663-4673.	2.2	17
164	Tacticity Effect on the Conformational Properties of Polypropylene and Poly(ethylene-propylene) Copolymers. <i>Macromolecules</i> , 2018, 51, 6878-6891.	2.2	17
165	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.	2.2	17
166	Molecular Simulations and Mechanistic Analysis of the Effect of CO <sub>2</sub> Sorption on Thermodynamics, Structure, and Local Dynamics of Molten Atactic Polystyrene. <i>Macromolecules</i> , 2020, 53, 3669-3689.	2.2	17
167	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.	1.4	16
168	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.	1.2	16
169	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.	2.2	15
170	Accelerating molecular simulations by reversible mapping between local minima. <i>Journal of Chemical Physics</i> , 2006, 125, 084107.	1.2	15
171	Variable-Connectivity Monte Carlo Algorithms for the Atomistic Simulation of Long-Chain Polymer Systems. <i>Lecture Notes in Physics</i> , 2002, , 67-127.	0.3	14
172	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.	0.9	14
173	Pulsed-field gradient nuclear magnetic resonance study of transport properties of fluid catalytic cracking catalysts. <i>Magnetic Resonance Imaging</i> , 2005, 23, 233-237.	1.0	14
174	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.	2.2	14
175	Calculation of macroscopic first- and third-order optical susceptibilities for the benzene crystal. <i>Theoretical Chemistry Accounts</i> , 1998, 99, 384.	0.5	14
176	Efficient Parallel Decomposition of Dynamical Sampling in Glass-Forming Materials Based on an On the Fly-Definition of Metabasins. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1307-1322.	2.3	12
177	On solving the master equation in spatially periodic systems. <i>Journal of Chemical Physics</i> , 2012, 137, 034112.	1.2	12
178	Molecular Modeling and Simulation of Polymer Nanocomposites at Multiple Length Scales. <i>IEEE Nanotechnology Magazine</i> , 2016, 15, 416-422.	1.1	12
179	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.	2.2	12
180	Polymers at Surfaces and Interfaces. , 2003, , 329-419.		11

#	ARTICLE	IF	CITATIONS
181	Molecular Simulation of the Puren-Hexadecane Vapor~Liquid Equilibria at Elevated Temperature. <i>Macromolecules</i> , 1998, 31, 1430-1431.	2.2	10
182	Atomistic simulations of cavitation in a model polyethylene network. <i>Polymer Science - Series C</i> , 2013, 55, 212-218.	0.8	10
183	Molecular dynamics simulations of alkyl substituted nanographene crystals. <i>Molecular Physics</i> , 2015, 113, 2776-2790.	0.8	10
184	Structure and thermodynamics of grafted silica/polystyrene dilute nanocomposites investigated through self-consistent field theory. <i>Soft Matter</i> , 2021, 17, 4077-4097.	1.2	10
185	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.	1.8	9
186	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.	1.2	9
187	Mesoscopic Simulations of Crosslinked Polymer Networks. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012063.	0.3	9
188	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.	1.2	9
189	Potential of Mean Force between Bare or Grafted Silica/Polystyrene Surfaces from Self-Consistent Field Theory. <i>Polymers</i> , 2021, 13, 1197.	2.0	9
190	Microscopic calculation of the static electric susceptibility of polyethylene. <i>Journal of Chemical Physics</i> , 2003, 119, 11458-11466.	1.2	8
191	Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends. <i>Macromolecules</i> , 2007, 40, 2904-2914.	2.2	8
192	Temperature Accelerated Dynamics in Glass-Forming Materials. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7844-7853.	1.2	8
193	Free energy calculations by molecular simulations of deformed polymer glasses. <i>Computer Physics Communications</i> , 2020, 249, 107008.	3.0	8
194	Atomistic simulations of long-chain polyethylene melts flowing past gold surfaces: structure and wall-slip. <i>Molecular Physics</i> , 2020, 118, e1706775.	0.8	8
195	Multiscale Simulations of Polyzwitterions in Aqueous Bulk Solutions and Brush Array Configurations. <i>Soft Matter</i> , 2021, , .	1.2	8
196	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. <i>Journal of Supercritical Fluids</i> , 2010, 55, 503-509.	1.6	7
197	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.	1.5	7
198	Kinetic concepts and local failure in the interfacial shear strength of epoxy-graphene nanocomposites. <i>Physical Review E</i> , 2020, 102, 030501.	0.8	7

#	ARTICLE	IF	CITATIONS
199	A second-order Markov process for modeling diffusive motion through spatial discretization. Journal of Chemical Physics, 2008, 128, 024504.	1.2	6
200	Diffusion via space discretization method to study the concentration dependence of self-diffusivity under confinement. Journal of Chemical Physics, 2010, 132, 134108.	1.2	6
201	Temporal disconnectivity of the energy landscape in glassy systems. Journal of Chemical Physics, 2013, 138, 12A545.	1.2	6
202	Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1414.	6.2	6
203	Molecular Modeling of Polymer Surfaces and Polymer/Solid Interfaces. , 1992, , 139-162.		6
204	Investigation of the dynamics of benzene in silicalite using transition-state theory. Studies in Surface Science and Catalysis, 1995, 98, 240-241.	1.5	5
205	Surface tension and phase coexistence properties of the lattice fluid from a virtual site removal Monte Carlo strategy. Journal of Chemical Physics, 1997, 107, 5125-5140.	1.2	5
206	Simulation of hydrocarbon diffusion in zeolites. Studies in Surface Science and Catalysis, 1997, 105, 1851-1858.	1.5	5
207	Molecular Dynamics Test of the Stress-Thermal Rule in Polyethylene and Polystyrene Entangled Melts. Macromolecules, 2020, 53, 789-802.	2.2	5
208	Molecular dynamics study of methane and xenon in silicalite [Erratum to document cited in CA113(20):183284q]. The Journal of Physical Chemistry, 1991, 95, 1014-1014.	2.9	4
209	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
210	Equilibration and Coarse-Graining Methods for Polymers. , 2006, , 419-448.		4
211	In silico study of levodopa in hydrated lipid bilayers at the atomistic level. Journal of Molecular Graphics and Modelling, 2021, 107, 107972.	1.3	4
212	On the calculation of the chemical potential using the particle deletion scheme. , 0, .		3
213	Segment density of a block copolymer chain tethered at both ends. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 4355-4370.	1.7	2
214	Multiscale Modeling of Polymers. , 2005, , 2757-2761.		2
215	Formation of rodlike structures of water between oppositely charged ions in decane and polyethylene. Journal of Chemical Physics, 2007, 127, 191101.	1.2	2
216	Structure and entanglements in short chain branched polyolefin melts. AIP Conference Proceedings, 2013, , .	0.3	2

#	ARTICLE	IF	CITATIONS
217	Monte Carlo simulations of structure and entanglements in polymer melts. <i>Molecular Simulation</i> , 2015, 41, 993-995.	0.9	2
218	Molecular modeling and simulation of atactic polystyrene/amorphous silica nanocomposites. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012021.	0.3	2
219	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.	2.5	2
220	Molecular simulations of dopamine in a lipid bilayer. <i>AIP Conference Proceedings</i> , 2021, , .	0.3	2
221	RuSseL: A Self-Consistent Field Theory Code for Inhomogeneous Polymer Interphases. <i>Computation</i> , 2021, 9, 57.	1.0	2
222	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, , .	0.3	2
223	Diffusional Effects in Zeolite Catalysts. , 2012, , 807-837.		1
224	Multiscale simulations of hexa-peri-hexabenzocoronene and hexa-n-dodecyl-hexa-peri-hexabenzocoronene. <i>AIP Conference Proceedings</i> , 2015, , .	0.3	1
225	Atomistic and Coarse-grained Simulations of Hexabenzocoronene Crystals. <i>Journal of Physics: Conference Series</i> , 2016, 738, 012019.	0.3	1
226	Molecular dynamics simulations of stretch-induced crystallization in layered polyethylene. <i>Polymer Crystallization</i> , 2021, 4, e10172.	0.5	1
227	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.	1.2	1
228	Dynamics of alkane mixtures in silicalite pores. <i>European Physical Journal Special Topics</i> , 2000, 10, Pr7-143-Pr7-146.	0.2	1
229	Thermodynamic analysis of oligomeric blends by applying the Kirkwood-Buff theory of solutions. <i>Journal of Physics: Conference Series</i> , 2021, 2090, 012079.	0.3	1
230	A coarse-grained model for capturing the helical behavior of isotactic polypropylene. <i>Soft Matter</i> , 2022, , .	1.2	1
231	Detailed Modeling of Structure and Deformation of Glassy Polymers. <i>Materials Research Society Symposia Proceedings</i> , 1986, 79, 387.	0.1	0
232	Transition-state theory investigations of small molecule diffusion in glassy polymers. , 1998, , .		0
233	Diffusion in micropores. <i>Microporous and Mesoporous Materials</i> , 2009, 125, 1-2.	2.2	0
234	Molecular modeling and simulation of polymer nanocomposites at multiple length scales. , 2015, , .		0

#	ARTICLE	IF	CITATIONS
235	Structural and dynamical properties of nanographene molecular wires: A Molecular Dynamics study. , 2015, , .		0
236	Coarse-grained simulations of bidisperse polymer melts. AIP Conference Proceedings, 2021, , .	0.3	0
237	Molecular Dynamics Simulations of Polyethylene Bilayers. Journal of Physics: Conference Series, 2021, 1730, 012039.	0.3	0
238	Mesoscopic simulations of star polyethylene melts at equilibrium and under steady shear flow. AIP Conference Proceedings, 2021, , .	0.3	0
239	Multiscale Modeling of Polymers. , 2005, , 2757-2761.		0