Doros N Theodorou

List of Publications by Year
in descending order

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239	14,765	18482	23533
papers	citations	62 h-index	111 g-index

272	272	272	6960
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Detailed molecular structure of a vinyl polymer glass. Macromolecules, 1985, 18, 1467-1478.	4.8	830
2	Atomistic modeling of mechanical properties of polymeric glasses. Macromolecules, 1986, 19, 139-154.	4.8	512
3	Shape of unperturbed linear polymers: polypropylene. Macromolecules, 1985, 18, 1206-1214.	4.8	401
4	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
5	Molecular dynamics simulation of a glassy polymer surface. Macromolecules, 1991, 24, 6283-6294.	4.8	331
6	Transport diffusivity of methane in silicalite from equilibrium and nonequilibrium simulations. The Journal of Physical Chemistry, 1993, 97, 4173-4181.	2.9	310
7	Topological Analysis of Linear Polymer Melts:Â A Statistical Approach. Macromolecules, 2006, 39, 4592-4604.	4.8	272
8	A concerted rotation algorithm for atomistic Monte Carlo simulation of polymer melts and glasses. Molecular Physics, 1993, 78, 961-996.	1.7	270
9	Molecular dynamics study of methane and xenon in silicalite. The Journal of Physical Chemistry, 1990, 94, 8232-8240.	2.9	258
10	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
11	Molecular dynamics studies of butane and hexane in silicalite. The Journal of Physical Chemistry, 1992, 96, 1051-1060.	2.9	244
12	Variable Connectivity Method for the Atomistic Monte Carlo Simulation of Polydisperse Polymer Melts. Macromolecules, 1995, 28, 7224-7234.	4.8	244
13	Interface of Grafted and Ungrafted Silica Nanoparticles with a Polystyrene Matrix: Atomistic Molecular Dynamics Simulations. Macromolecules, 2011, 44, 2316-2327.	4.8	239
14	End-Bridging Monte Carlo:Â A Fast Algorithm for Atomistic Simulation of Condensed Phases of Long Polymer Chains. Macromolecules, 1999, 32, 5072-5096.	4.8	237
15	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.	7.8	218
16	Prediction of low occupancy sorption of alkanes in silicalite. The Journal of Physical Chemistry, 1990, 94, 1508-1516.	2.9	210
17	Crossover from the Rouse to the Entangled Polymer Melt Regime:Â Signals from Long, Detailed Atomistic Molecular Dynamics Simulations, Supported by Rheological Experiments. Macromolecules, 2003, 36, 1376-1387.	4.8	198
18	Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts:Â Structure, Thermodynamic Properties, Chain Conformation, and Entanglements. Macromolecules, 2007, 40, 3876-3885.	4.8	190

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19	Atomistic Molecular Dynamics Simulation of Polydisperse Linear Polyethylene Melts. Macromolecules, 1998, 31, 7934-7943.	4.8	182
20	Prediction of Permeation Properties of CO2 and N2 through Silicalite via Molecular Simulations. Journal of Physical Chemistry B, 2001, 105, 777-788.	2.6	182
21	Transition-state studies of xenon and sulfur hexafluoride diffusion in silicalite. The Journal of Physical Chemistry, 1991, 95, 8866-8878.	2.9	180
22	Engineering a Molecular Model for Water Phase Equilibrium over a Wide Temperature Range. Journal of Physical Chemistry B, 1998, 102, 1029-1035.	2.6	159
23	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
24	Diffusion and reaction in blocked and high occupancy zeolite catalysts. Journal of Catalysis, 1983, 83, 205-224.	6.2	139
25	Geometric analysis of diffusion pathways in glassy and melt atactic polypropylene. Macromolecules, 1993, 26, 5461-5472.	4.8	139
26	Atomistic simulation of a glassy polymer/graphite interface. Macromolecules, 1991, 24, 4295-4309.	4.8	138
27	Atomistic Simulation of Polymer Melt Elasticity:Â Calculation of the Free Energy of an Oriented Polymer Melt. Macromolecules, 1998, 31, 6310-6332.	4.8	136
28	Dynamics of Longn-Alkanes in Silicalite:Â A Hierarchical Simulation Approach. The Journal of Physical Chemistry, 1996, 100, 7155-7173.	2.9	132
29	Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm. Journal of Chemical Physics, 2002, 117, 5465-5479.	3.0	130
30	Atomistic simulation of a glassy polymer surface. Macromolecules, 1990, 23, 4430-4445.	4.8	127
31	Analytical treatment of the volume and surface area of molecules formed by an arbitrary collection of unequal spheres intersected by planes. Molecular Physics, 1991, 72, 1313-1345.	1.7	124
32	Interfacial structure and dynamics of macromolecular liquids: a Monte Carlo simulation approach. Macromolecules, 1989, 22, 3143-3152.	4.8	121
33	Detailed Atomistic Molecular Dynamics Simulation ofcis-1,4-Poly(butadiene). Macromolecules, 2005, 38, 1478-1492.	4.8	118
34	Molecular Simulation of Phase Equilibria for Waterâ^'Methane and Waterâ^'Ethane Mixtures. Journal of Physical Chemistry B, 1998, 102, 8865-8873.	2.6	115
35	Local structure and the mechanism of response to elastic deformation in a glassy polymer. Macromolecules, 1986, 19, 379-387.	4.8	111
36	Detailed Atomistic Simulation of the Segmental Dynamics and Barrier Properties of Amorphous Poly(ethylene terephthalate) and Poly(ethylene isophthalate). Macromolecules, 2004, 37, 2978-2995.	4.8	109

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37	Transport Diffusivity of N2and CO2in Silicalite:Â Coherent Quasielastic Neutron Scattering Measurements and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 12748-12756.	2.6	104
38	The effects of local structural relaxation on aluminum siting within H-ZSM-5. Catalysis Letters, 1991, 11, 209-217.	2.6	103
39	Progress and Outlook in Monte Carlo Simulations. Industrial & Engineering Chemistry Research, 2010, 49, 3047-3058.	3.7	102
40	Structure of Polymer Layers Grafted to Nanoparticles in Silicaâ€“Polystyrene Nanocomposites. Macromolecules, 2013, 46, 4670-4683.	4.8	95
41	Investigation of the dynamics of benzene in silicalite using Transition-State Theory. The Journal of Physical Chemistry, 1994, 98, 11948-11961.	2.9	93
42	Variable-density model of polymer melt surfaces: structure and surface tension. Macromolecules, 1989, 22, 4578-4589.	4.8	90
43	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
44	Molecular Modeling of Methane Diffusion in Glassy Atactic Polypropylene via Multidimensional Transition State Theory. Macromolecules, 1998, 31, 7068-7090.	4.8	86
45	Monte Carlo Simulation of Short Chain Branched Polyolefins in the Molten State. Macromolecules, 2007, 40, 9640-9650.	4.8	86
46	Detailed molecular dynamics simulation of the self-diffusion of n-alkane and cis-1,4 polyisoprene oligomer melts. Journal of Chemical Physics, 2002, 116, 436.	3.0	85
47	Chain and local dynamics of polyisoprene as probed by experiments and computer simulations. Journal of Chemical Physics, 2003, 119, 6883-6894.	3.0	85
48	Local Segmental Dynamics and Stresses in Polystyreneâ€“C₆₀ Mixtures. Macromolecules, 2014, 47, 387-404.	4.8	85
49	Geometrical considerations in model systems with periodic boundaries. Journal of Chemical Physics, 1985, 82, 955-966.	3.0	83
50	Determination of the Mechanical Properties of a Poly(methyl methacrylate) Nanocomposite with Functionalized Graphene Sheets through Detailed Atomistic Simulations. Macromolecules, 2014, 47, 8072-8088.	4.8	83
51	Structure and thermodynamics of bulk homopolymer solid interfaces: a site lattice model approach. Macromolecules, 1988, 21, 1400-1410.	4.8	77
52	Dynamics ofn-Butaneâ€™Methane Mixtures in Silicalite, Using Quasielastic Neutron Scattering and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2000, 104, 5541-5552.	2.6	77
53	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
54	Lattice models for bulk polymers at interfaces. Macromolecules, 1988, 21, 1391-1400.	4.8	74

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55	Diffusion in Fluid Catalytic Cracking Catalysts on Various Displacement Scales and Its Role in Catalytic Performance. Chemistry of Materials, 2005, 17, 2466-2474.	6.7	74
56	Transition-State Theory Model for the Diffusion Coefficients of Small Penetrants in Glassy Polymers. Macromolecules, 1997, 30, 7296-7306.	4.8	69
57	Molecular Dynamics Simulation ofn-Butaneâ^'Methane Mixtures in Silicalite. Journal of Physical Chemistry B, 1999, 103, 3380-3390.	2.6	66
58	Onset of Entanglements Revisited. Dynamical Analysis. Macromolecules, 2009, 42, 7485-7494.	4.8	66
59	On the calculation of the chemical potential using the particle deletion scheme. Molecular Physics, 1999, 96, 905-913.	1.7	64
60	Monte Carlo simulations of a coarse grained model for an athermal all-polystyrene nanocomposite system. European Polymer Journal, 2011, 47, 699-712.	5.4	64
61	Electronic Structure Calculations of Ammonia Adsorption in H-ZSM-5 Zeolites. The Journal of Physical Chemistry, 1995, 99, 1505-1515.	2.9	63
62	Coarse Grained End Bridging Monte Carlo Simulations of Poly(ethylene terephthalate) Melt. Macromolecules, 2007, 40, 710-722.	4.8	63
63	Hierarchical modelling of polymeric materials. Chemical Engineering Science, 2007, 62, 5697-5714.	3.8	62
64	Molecular Simulations of Methane Adsorption in Silicalite. Molecular Simulation, 1991, 8, 73-92.	2.0	61
65	Stress tensor in model polymer systems with periodic boundaries. Die Makromolekulare Chemie Theory and Simulations, 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. Macromolecules, 2001, 34, 8541-8553.	4.8	61
67	Connectivity-Altering Monte Carlo Simulations of the End Group Effects on Volumetric Properties for Poly(ethylene oxide). Macromolecules, 2004, 37, 7026-7033.	4.8	60
68	Static atomistic modelling of the structure and ring dynamics of bulk amorphous polystyrene. Macromolecular Theory and Simulations, 1994, 3, 19-43.	1.4	57
69	Phase Equilibria of Mixtures Containing Chain Molecules Predicted through a Novel Simulation Scheme. Physical Review Letters, 1998, 80, 4466-4469.	7.8	57
70	Atomistic Monte Carlo simulation of cis-1,4 polyisoprene melts. I. Single temperature end-bridging Monte Carlo simulations. Journal of Chemical Physics, 2001, 115, 11339-11351.	3.0	56
71	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
72	Molecular Dynamics of Atactic Polypropylene Melts. Macromolecules, 1998, 31, 7944-7952.	4.8	55

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73	Molecular Modeling Investigations of Sorption and Diffusion of Small Molecules in Glassy Polymers. Membranes, 2019, 9, 98.	3.0	54
74	Variable-density model of polymer melt/solid interfaces: structure, adhesion tension, and surface forces. Macromolecules, 1989, 22, 4589-4597.	4.8	53
75	Directed Bridging Methods for Fast Atomistic Monte Carlo Simulations of Bulk Polymers. Macromolecules, 2001, 34, 8554-8568.	4.8	53
76	Onset of Entanglements Revisited. Topological Analysis. Macromolecules, 2009, 42, 7474-7484.	4.8	53
77	Understanding and predicting structureâ€“property relations in polymeric materials through molecular simulations. Molecular Physics, 2004, 102, 147-166.	1.7	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.	2.6	51
79	Component segmental mobilities in an athermal polymer blend: Quasielastic incoherent neutron scattering versus simulation. Journal of Chemical Physics, 2000, 112, 8687-8694.	3.0	50
80	Atomistic Monte Carlo Simulation of Polybutadiene Isomers:Âcis-1,4-Polybutadiene and 1,2-Polybutadiene. Macromolecules, 2003, 36, 6925-6938.	4.8	50
81	Prediction of Sorption of CO₂ in Glassy Atactic Polystyrene at Elevated Pressures Through a New Computational Scheme. Macromolecules, 2009, 42, 1759-1769.	4.8	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.	4.8	49
84	Atomistic molecular dynamics simulation of diffusion in binary liquid n-alkane mixtures. Journal of Chemical Physics, 2002, 116, 7656-7665.	3.0	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.	3.0	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.	4.8	48
87	Slip-Spring Model for the Linear and Nonlinear Viscoelastic Properties of Molten Polyethylene Derived from Atomistic Simulations. Macromolecules, 2017, 50, 4524-4541.	4.8	48
88	Thermodynamics of Chain Fluids from Atomistic Simulation:â€‰ A Test of the Chain Increment Method for Chemical Potential. Macromolecules, 1997, 30, 4744-4755.	4.8	47
89	Molecular Simulation of Phase Equilibria for Waterâ^'n-Butane and Waterâ^'n-Hexane Mixtures. Journal of Physical Chemistry B, 2000, 104, 4958-4963.	2.6	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.	4.8	46

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91	Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data. Macromolecules, 2008, 41, 2959-2962.	4.8	46
92	Molecular Simulations of Free and Graphite Capped Polyethylene Films: Estimation of the Interfacial Free Energies. Macromolecules, 2017, 50, 8827-8844.	4.8	46
93	Local Structure and Dynamics oftrans-Polyisoprene Oligomers. Macromolecules, 2001, 34, 1436-1448.	4.8	45
94	Microscopic Description of Entanglements in Polyethylene Networks and Melts: Strong, Weak, Pairwise, and Collective Attributes. Macromolecules, 2012, 45, 9475-9492.	4.8	45
95	Equation of State Based Slip Spring Model for Entangled Polymer Dynamics. Macromolecules, 2017, 50, 3004-3029.	4.8	45
96	Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites. Archives of Computational Methods in Engineering, 2018, 25, 591-645.	10.2	45
97	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
98	Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities. Chemical Engineering Science, 2001, 56, 2789-2801.	3.8	42
99	Atomic structure of a high polymer melt. Europhysics Letters, 2002, 57, 506-511.	2.0	42
100	Dynamical integration of a Markovian web: A first passage time approach. Journal of Chemical Physics, 2007, 127, 084903.	3.0	42
101	Calculation of the chemical potential of chain molecules using the staged particle deletion scheme. Journal of Chemical Physics, 2001, 115, 8231-8237.	3.0	41
102	Molecular dynamics simulations of EPON-862/DETDA epoxy networks: structure, topology, elastic constants, and local dynamics. Soft Matter, 2019, 15, 721-733.	2.7	41
103	Hierarchical simulation approach to structure and dynamics of polymers. Current Opinion in Solid State and Materials Science, 1998, 3, 544-551.	11.5	40
104	Effect of Tacticity on the Molecular Dynamics of Polypropylene Melts. Macromolecules, 1999, 32, 8635-8644.	4.8	40
105	Segmental and Chain Dynamics of Isotactic Polypropylene Melts. Macromolecules, 2007, 40, 2235-2245.	4.8	40
106	Sorption Thermodynamics of CO2, CH4, 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
107	Structure and Volumetric Properties of Linear and Triarm Star Polyethylenes from Atomistic Monte Carlo Simulation Using New Internal Rearrangement Moves. Macromolecules, 2005, 38, 386-397.	4.8	38
108	Experimental and Self-Consistent-Field Theoretical Study of Styrene Block Copolymer Self-Adhesive Materials. Macromolecules, 2004, 37, 5093-5109.	4.8	37

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109	Henry's Constant Analysis for Water and Nonpolar Solvents from Experimental Data, Macroscopic Models, and Molecular Simulation. Journal of Physical Chemistry B, 2001, 105, 7792-7798.	2.6	36
110	Coupling of Penetrant and Polymer Motions During Small-Molecule Diffusion In a Glassy Polymer. Molecular Simulation, 1997, 19, 329-361.	2.0	35
111	Atomistic simulation of the birefringence of uniaxially stretched polyethylene melts. Computational and Theoretical Polymer Science, 2000, 10, 1-13.	1.1	35
112	Segmental Dynamics of Atactic Polypropylene As Revealed by Molecular Simulations and Quasielastic Neutron Scattering. Macromolecules, 2002, 35, 7110-7124.	4.8	35
113	Crystallization and Melting Simulations of Oligomeric Î±1 Isotactic Polypropylene. Macromolecules, 2010, 43, 5455-5469.	4.8	35
114	Systematic Coarse Graining of 4-Cyano-4â€²-pentylbiphenyl. Industrial & Engineering Chemistry Research, 2011, 50, 546-556.	3.7	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. Journal of Chemical Physics, 1999, 110, 6463-6474.	3.0	33
117	Molecular simulation of static hyper-Rayleigh scattering: A calculation of the depolarization ratio and the local fields for liquid nitrobenzene. Journal of Chemical Physics, 1999, 111, 9711-9719.	3.0	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. Journal of Chemical Physics, 2001, 115, 2860-2875.	3.0	32
119	Entanglement Network of the Polypropylene/Polyamide Interface. 3. Deformation to Fracture. Macromolecules, 2002, 35, 508-521.	4.8	32
120	Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors. Computer Physics Communications, 2002, 144, 1-22.	7.5	32
121	Microscopic structure and thermodynamic properties of bulk copolymers and surface-active polymers at interfaces. 1. Theory. Macromolecules, 1988, 21, 1411-1421.	4.8	31
122	Microscopic structure and thermodynamic properties of bulk copolymers and surface-active polymers at interfaces. 2. Results for some representative chain architectures. Macromolecules, 1988, 21, 1422-1436.	4.8	30
123	Self-consistent field model of the polymer/diblock copolymer/polymer interface. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 2381.	1.7	29
124	Elementary structural transitions in the amorphous Lennard-Jones solid using multidimensional transition-state theory. Journal of Chemical Physics, 1998, 109, 8573-8582.	3.0	29
125	Molecular Simulation of Î±-Olefins Using a New United-Atom Potential Model:â€‰ Vaporâ€“Liquid Equilibria of Pure Compounds and Mixtures. Journal of the American Chemical Society, 1999, 121, 3407-3413.	13.7	29
126	Calculation of refractive indices and third-harmonic generation susceptibilities of liquid benzene and water: Comparison of continuum and discrete local-field theories. Journal of Chemical Physics, 2001, 114, 876.	3.0	29

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127	Analysis of Computed Trajectories of Penetrant Micromolecules in a Simulated Polymeric Material. Macromolecules, 1996, 29, 3615-3624.	4.8	28
128	Entanglement Network of the Polypropylene/Polyamide Interface. 1. Self-Consistent Field Model. Macromolecules, 2000, 33, 1385-1396.	4.8	28
129	Microscopic Origins for the Favorable Solvation of Carbonate Ether Copolymers in CO2. Journal of the American Chemical Society, 2005, 127, 12338-12342.	13.7	28
130	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
131	Benefit of Microscopic Diffusion Measurement for the Characterization of Nanoporous Materials. Chemical Engineering and Technology, 2009, 32, 1494-1511.	1.5	28
132	A Study of the Entanglement in Systems with Periodic Boundary Conditions. Progress of Theoretical Physics Supplement, 2011, 191, 172-181.	0.1	27
133	Calculation of macroscopic first- and third-order optical susceptibilities for the benzene crystal. Theoretical Chemistry Accounts, 1998, 99, 384-390.	1.4	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. Macromolecular Theory and Simulations, 2000, 9, 500-515.	1.4	26
135	Exploring the interactions of irbesartan and irbesartanâ€“2-hydroxypropyl-Î²-cyclodextrin complex with model membranes. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1089-1098.	2.6	26
136	Promising Route for the Development of a Computational Framework for Self-Assembly and Phase Behavior Prediction of Ionic Surfactants Using MARTINI. Journal of Physical Chemistry B, 2020, 124, 556-567.	2.6	26
137	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
138	Monte Carlo Simulation of Short Chain Branched Polyolefins: Structure and Properties. Macromolecules, 2012, 45, 8453-8466.	4.8	25
139	Mushrooms and Brushes in Thin Films of Diblock Copolymer/Homopolymer Mixtures. Macromolecules, 2002, 35, 1116-1132.	4.8	24
140	Parallel tempering method for reconstructing isotropic and anisotropic porous media. Journal of Chemical Physics, 2002, 117, 5876-5884.	3.0	24
141	Coarse graining using pretabulated potentials: Liquid benzene. Journal of Chemical Physics, 2005, 122, 244111.	3.0	23
142	A reversible minimum-to-minimum mapping method for the calculation of free-energy differences. Journal of Chemical Physics, 2006, 124, 034109.	3.0	23
143	Combined Atomistic Simulation and Quasielastic Neutron Scattering Study of the Low-Temperature Dynamics of Hydrogen and Deuterium Confined in NaX Zeolite. Journal of Physical Chemistry B, 2008, 112, 11708-11715.	2.6	23
144	Multiscale simulations of PSâ€“SiO2nanocomposites: from melt to glassy state. Soft Matter, 2016, 12, 7585-7605.	2.7	23

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145	Entanglement Network of the Polypropylene/Polyamide Interface. 2. Network Generation. Macromolecules, 2000, 33, 1397-1410.	4.8	22
146	Hierarchical modeling of amorphous polymers. Computer Physics Communications, 2005, 169, 82-88.	7.5	22
147	On the Role of Inherent Structures in Glass-Forming Materials: I. The Vitrification Process. Journal of Physical Chemistry B, 2008, 112, 10619-10627.	2.6	22
148	Tracking a glassy polymer on its energy landscape in the course of elastic deformation. Molecular Physics, 2013, 111, 3430-3441.	1.7	21
149	Molecular Dynamics Study of Polyethylene under Extreme Confinement. Journal of Physics: Conference Series, 2016, 738, 012012.	0.4	21
150	Slip Spring-Based Mesoscopic Simulations of Polymer Networks: Methodology and the Corresponding Computational Code. Polymers, 2018, 10, 1156.	4.5	21
151	Application of bi-Helmholtz nonlocal elasticity and molecular simulations to the dynamical response of carbon nanotubes. AIP Conference Proceedings, 2015, , .	0.4	20
152	Diffusion of Aromatics in Silicalite-1: Experimental and Theoretical Evidence of Entropic Barriers. Journal of Physical Chemistry C, 2016, 120, 21410-21426.	3.1	20
153	General Methodology for Estimating the Stiffness of Polymer Chains from Their Chemical Constitution: A Single Unperturbed Chain Monte Carlo Algorithm. Macromolecules, 2017, 50, 4575-4587.	4.8	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. Macromolecules, 2018, 51, 9798-9815.	4.8	20
155	Van Hove Function for Diffusion in Zeolites. Journal of Physical Chemistry B, 1999, 103, 4721-4729.	2.6	19
156	Probing subglass relaxation in polymers via a geometric representation of probabilities, observables, and relaxation modes for discrete stochastic systems. Journal of Chemical Physics, 2009, 130, 044905.	3.0	19
157	Dimensionality reduction of free energy profiles of benzene in silicalite-1: calculation of diffusion coefficients using transition state theory. Molecular Simulation, 2014, 40, 80-100.	2.0	19
158	Thermodynamic analysis of Lennard-Jones binary mixtures using Kirkwood-Buff theory. Fluid Phase Equilibria, 2018, 470, 25-37.	2.5	19
159	Simulation studies of methane, carbon dioxide, hydrogen and deuterium in ITQ-1 and NaX zeolites. Molecular Simulation, 2009, 35, 79-89.	2.0	18
160	Molecular Dynamics of Carbon Dioxide, Methane and Their Mixtures in a Zeolite Possessing Two Independent Pore Networks as Revealed by Computer Simulations. Journal of Physical Chemistry B, 2009, 113, 13761-13767.	2.6	18
161	Prediction of Infinite Dilution Benzene Solubility in Linear Polyethylene Melts via the Direct Particle Deletion Method. Journal of Physical Chemistry B, 2010, 114, 6233-6246.	2.6	17
162	Self-Consistent-Field Study of Adsorption and Desorption Kinetics of Polyethylene Melts on Graphite and Comparison with Atomistic Simulations. Macromolecules, 2014, 47, 6964-6981.	4.8	17

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163	Melting Point and Solidâ€“Liquid Coexistence Properties of Î±1 Isotactic Polypropylene as Functions of Its Molar Mass: A Molecular Dynamics Study. Macromolecules, 2016, 49, 4663-4673.	4.8	17
164	Tacticity Effect on the Conformational Properties of Polypropylene and Poly(ethyleneâ€“propylene) Copolymers. Macromolecules, 2018, 51, 6878-6891.	4.8	17
165	Multiscale Simulations of Graphite-Capped Polyethylene Melts: Brownian Dynamics/Kinetic Monte Carlo Compared to Atomistic Calculations and Experiment. Macromolecules, 2019, 52, 7503-7523.	4.8	17
166	Molecular Simulations and Mechanistic Analysis of the Effect of CO₂ Sorption on Thermodynamics, Structure, and Local Dynamics of Molten Atactic Polystyrene. Macromolecules, 2020, 53, 3669-3689.	4.8	17
167	Molecular simulation of structure, thermodynamic and transport properties of polymeric membrane materials for hydrocarbon separation. Fluid Phase Equilibria, 2005, 228-229, 15-20.	2.5	16
168	Lumping analysis for the prediction of long-time dynamics: From monomolecular reaction systems to inherent structure dynamics of glassy materials. Journal of Chemical Physics, 2011, 135, 204507.	3.0	16
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