Doros N Theodorou

List of Publications by Year in descending order

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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	A coarse-grained model for capturing the helical behavior of isotactic polypropylene. Soft Matter, 2022, , .	1.2	1
2	Mixing Thermodynamics and Floryâ€“Huggins Interaction Parameter of Polyethylene Oxide/Polyethylene Oligomeric Blends from Kirkwoodâ€“Buff Theory and Molecular Simulations. Macromolecules, 2022, 55, 4852-4862.	2.2	12
3	Molecular simulations of dopamine in a lipid bilayer. AIP Conference Proceedings, 2021, , .	0.3	2
4	Coarse-grained simulations of bidisperse polymer melts. AIP Conference Proceedings, 2021, , .	0.3	0
5	Molecular Dynamics Simulations of Polyethylene Bilayers. Journal of Physics: Conference Series, 2021, 1730, 012039.	0.3	0
6	Structure and thermodynamics of grafted silica/polystyrene dilute nanocomposites investigated through self-consistent field theory. Soft Matter, 2021, 17, 4077-4097.	1.2	10
7	Mesoscopic simulations of star polyethylene melts at equilibrium and under steady shear flow. AIP Conference Proceedings, 2021, , .	0.3	0
8	Molecular dynamics simulations of stretchâ€induced crystallization in layered polyethylene. Polymer Crystallization, 2021, 4, e10172.	0.5	1
9	Potential of Mean Force between Bare or Grafted Silica/Polystyrene Surfaces from Self-Consistent Field Theory. Polymers, 2021, 13, 1197.	2.0	9
10	RuSseL: A Self-Consistent Field Theory Code for Inhomogeneous Polymer Interphases. Computation, 2021, 9, 57.	1.0	2
11	Effect of Surface Nanopatterning on Slip: The Case of Couette Flow of Long-Chain Polyethylene Melt Flowing Past Gold Surfaces. Journal of Physical Chemistry B, 2021, 125, 6681-6696.	1.2	1
12	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
13	A three-dimensional finite element methodology for addressing heterogeneous polymer systems with simulations based on self-consistent field theory. AIP Conference Proceedings, 2021, , .	0.3	2
14	Multiscale Simulations of Polyzwitterions in Aqueous Bulk Solutions and Brush Array Configurations. Soft Matter, 2021, , .	1.2	8
15	Thermodynamic analysis of oligomeric blends by applying the Kirkwood-Buff theory of solutions. Journal of Physics: Conference Series, 2021, 2090, 012079.	0.3	1
16	Free energy calculations by molecular simulations of deformed polymer glasses. Computer Physics Communications, 2020, 249, 107008.	3.0	8
17	Atomistic simulations of long-chain polyethylene melts flowing past gold surfaces: structure and wall-slip. Molecular Physics, 2020, 118, e1706775.	0.8	8
18	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.	1.2	26

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19	Kinetic concepts and local failure in the interfacial shear strength of epoxy-graphene nanocomposites. Physical Review E, 2020, 102, 030501.	0.8	7
20	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.	2.2	17
21	Molecular Dynamics Test of the Stress-Thermal Rule in Polyethylene and Polystyrene Entangled Melts. Macromolecules, 2020, 53, 789-802.	2.2	5
22	Self-Consistent Field Theory Coupled with Square Gradient Theory of Free Surfaces of Molten Polymers and Compared to Atomistic Simulations and Experiment. Macromolecules, 2019, 52, 5337-5356.	2.2	14
23	Molecular Modeling Investigations of Sorption and Diffusion of Small Molecules in Glassy Polymers. Membranes, 2019, 9, 98.	1.4	54
24	Multiscale Simulations of Graphite-Capped Polyethylene Melts: Brownian Dynamics/Kinetic Monte Carlo Compared to Atomistic Calculations and Experiment. Macromolecules, 2019, 52, 7503-7523.	2.2	17
25	Molecular dynamics simulations of EPON-862/DETDA epoxy networks: structure, topology, elastic constants, and local dynamics. Soft Matter, 2019, 15, 721-733.	1.2	41
26	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
27	SimNano: A Trust Region Strategy for Large-Scale Molecular Systems Energy Minimization Based on Exact Second-Order Derivative Information. Journal of Chemical Information and Modeling, 2019, 59, 190-205.	2.5	2
28	Thermodynamic Analysis of n-Hexaneâ€“Ethanol Binary Mixtures Using the Kirkwoodâ€“Buff Theory. Journal of Physical Chemistry B, 2019, 123, 247-257.	1.2	9
29	Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites. Archives of Computational Methods in Engineering, 2018, 25, 591-645.	6.0	45
30	Thermodynamic analysis of Lennard-Jones binary mixtures using Kirkwood-Buff theory. Fluid Phase Equilibria, 2018, 470, 25-37.	1.4	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. Macromolecules, 2018, 51, 9798-9815.	2.2	20
32	Slip Spring-Based Mesoscopic Simulations of Polymer Networks: Methodology and the Corresponding Computational Code. Polymers, 2018, 10, 1156.	2.0	21
33	Tacticity Effect on the Conformational Properties of Polypropylene and Poly(ethyleneâ€“propylene) Copolymers. Macromolecules, 2018, 51, 6878-6891.	2.2	17
34	Computational Studies of Nanographene Systems: Extended Discotics, Covalently Linked â€œSupermolecules,â€• and Functionalized Supramolecular Assemblies. Journal of Physical Chemistry C, 2018, 122, 18715-18731.	1.5	7
35	Exploring the interactions of irbesartan and irbesartanâ€“2-hydroxypropyl-Î²-cyclodextrin complex with model membranes. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1089-1098.	1.4	26
36	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

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37	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.	2.2	20
38	Equation of State Based Slip Spring Model for Entangled Polymer Dynamics. Macromolecules, 2017, 50, 3004-3029.	2.2	45
39	Molecular Simulations of Free and Graphite Capped Polyethylene Films: Estimation of the Interfacial Free Energies. Macromolecules, 2017, 50, 8827-8844.	2.2	46
40	Mesoscopic Simulations of Crosslinked Polymer Networks. Journal of Physics: Conference Series, 2016, 738, 012063.	0.3	9
41	Atomistic and Coarse-grained Simulations of Hexabenzocoronene Crystals. Journal of Physics: Conference Series, 2016, 738, 012019.	0.3	1
42	Molecular Dynamics Study of Polyethylene under Extreme Confinement. Journal of Physics: Conference Series, 2016, 738, 012012.	0.3	21
43	Molecular modeling and simulation of atactic polystyrene/amorphous silica nanocomposites. Journal of Physics: Conference Series, 2016, 738, 012021.	0.3	2
44	Multiscale simulations of PSâ€“SiO2nanocomposites: from melt to glassy state. Soft Matter, 2016, 12, 7585-7605.	1.2	23
45	Diffusion of Aromatics in Silicalite-1: Experimental and Theoretical Evidence of Entropic Barriers. Journal of Physical Chemistry C, 2016, 120, 21410-21426.	1.5	20
46	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.	2.2	17
47	Molecular Modeling and Simulation of Polymer Nanocomposites at Multiple Length Scales. IEEE Nanotechnology Magazine, 2016, 15, 416-422.	1.1	12
48	Application of bi-Helmholtz nonlocal elasticity and molecular simulations to the dynamical response of carbon nanotubes. AIP Conference Proceedings, 2015, , .	0.3	20
49	Multiscale simulations of hexa-peri-hexabenzocoronene and hexa-n-dodecyl-hexa-peri-hexabenzocoronene. AIP Conference Proceedings, 2015, , .	0.3	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. Molecular Physics, 2015, 113, 2776-2790.	0.8	10
53	Monte Carlo simulations of structure and entanglements in polymer melts. Molecular Simulation, 2015, 41, 993-995.	0.9	2
54	Local Segmental Dynamics and Stresses in Polystyreneâ€“C₆₀ Mixtures. Macromolecules, 2014, 47, 387-404.	2.2	85

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55	Determination of the Mechanical Properties of a Poly(methyl methacrylate) Nanocomposite with Functionalized Graphene Sheets through Detailed Atomistic Simulations. Macromolecules, 2014, 47, 8072-8088.	2.2	83
56	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.	0.9	19
57	Self-Consistent-Field Study of Adsorption and Desorption Kinetics of Polyethylene Melts on Graphite and Comparison with Atomistic Simulations. Macromolecules, 2014, 47, 6964-6981.	2.2	17
58	Atomistic simulations of cavitation in a model polyethylene network. Polymer Science - Series C, 2013, 55, 212-218.	0.8	10
59	Structure of Polymer Layers Grafted to Nanoparticles in Silicaâ€“Polystyrene Nanocomposites. Macromolecules, 2013, 46, 4670-4683.	2.2	95
60	Structure and entanglements in short chain branched polyolefin melts. AIP Conference Proceedings, 2013, , .	0.3	2
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62	Temporal disconnectivity of the energy landscape in glassy systems. Journal of Chemical Physics, 2013, 138, 12A545.	1.2	6
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64	Microscopic Description of Entanglements in Polyethylene Networks and Melts: Strong, Weak, Pairwise, and Collective Attributes. Macromolecules, 2012, 45, 9475-9492.	2.2	45
65	Monte Carlo Simulation of Short Chain Branched Polyolefins: Structure and Properties. Macromolecules, 2012, 45, 8453-8466.	2.2	25
66	Diffusional Effects in Zeolite Catalysts. , 2012, , 807-837.		1
67	Systematic Coarse Graining of 4-Cyano-4â€²-pentylbiphenyl. Industrial & Engineering Chemistry Research, 2011, 50, 546-556.	1.8	35
68	Interface of Grafted and Ungrafted Silica Nanoparticles with a Polystyrene Matrix: Atomistic Molecular Dynamics Simulations. Macromolecules, 2011, 44, 2316-2327.	2.2	239
69	Monte Carlo simulations of a coarse grained model for an athermal all-polystyrene nanocomposite system. European Polymer Journal, 2011, 47, 699-712.	2.6	64
70	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.	1.2	16
71	A Study of the Entanglement in Systems with Periodic Boundary Conditions. Progress of Theoretical Physics Supplement, 2011, 191, 172-181.	0.2	27
72	Temperature Accelerated Dynamics in Glass-Forming Materials. Journal of Physical Chemistry B, 2010, 114, 7844-7853.	1.2	8

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73	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. Journal of Supercritical Fluids, 2010, 55, 503-509.	1.6	7
74	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
75	Crystallization and Melting Simulations of Oligomeric Î±1 Isotactic Polypropylene. Macromolecules, 2010, 43, 5455-5469.	2.2	35
76	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.	1.2	17
77	Efficient Parallel Decomposition of Dynamical Sampling in Glass-Forming Materials Based on an â€œOn the Flyâ€•Definition of Metabasins. Journal of Chemical Theory and Computation, 2010, 6, 1307-1322.	2.3	12
78	Progress and Outlook in Monte Carlo Simulations. Industrial & Engineering Chemistry Research, 2010, 49, 3047-3058.	1.8	102
79	Simulation studies of methane, carbon dioxide, hydrogen and deuterium in ITQ-1 and NaX zeolites. Molecular Simulation, 2009, 35, 79-89.	0.9	18
80	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.	1.2	18
81	Benefit of Microscopic Diffusion Measurement for the Characterization of Nanoporous Materials. Chemical Engineering and Technology, 2009, 32, 1494-1511.	0.9	28
82	Diffusion in micropores. Microporous and Mesoporous Materials, 2009, 125, 1-2.	2.2	0
83	Onset of Entanglements Revisited. Dynamical Analysis. Macromolecules, 2009, 42, 7485-7494.	2.2	66
84	Onset of Entanglements Revisited. Topological Analysis. Macromolecules, 2009, 42, 7474-7484.	2.2	53
85	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.	1.2	19
86	Prediction of Sorption of CO₂ in Glassy Atactic Polystyrene at Elevated Pressures Through a New Computational Scheme. Macromolecules, 2009, 42, 1759-1769.	2.2	50
87	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.	1.2	23
88	Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data. Macromolecules, 2008, 41, 2959-2962.	2.2	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. Journal of Physical Chemistry B, 2008, 112, 10628-10637.	1.2	9
90	On the Role of Inherent Structures in Glass-Forming Materials: I. The Vitrification Process. Journal of Physical Chemistry B, 2008, 112, 10619-10627.	1.2	22

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91	A second-order Markov process for modeling diffusive motion through spatial discretization. Journal of Chemical Physics, 2008, 128, 024504.	1.2	6
92	Dynamical integration of a Markovian web: A first passage time approach. Journal of Chemical Physics, 2007, 127, 084903.	1.2	42
93	Formation of rodlike structures of water between oppositely charged ions in decane and polyethylene. Journal of Chemical Physics, 2007, 127, 191101.	1.2	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.	1.2	28
95	Monte Carlo simulations of equilibrium solubilities and structure of water in n-alkanes and polyethylene. Journal of Chemical Physics, 2007, 126, 224902.	1.2	25
96	Coarse Grained End Bridging Monte Carlo Simulations of Poly(ethylene terephthalate) Melt. Macromolecules, 2007, 40, 710-722.	2.2	63
97	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.	2.2	190
98	Monte Carlo Simulation of Short Chain Branched Polyolefins in the Molten State. Macromolecules, 2007, 40, 9640-9650.	2.2	86
99	Segmental and Chain Dynamics of Isotactic Polypropylene Melts. Macromolecules, 2007, 40, 2235-2245.	2.2	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.	2.2	8
101	Hierarchical modelling of polymeric materials. Chemical Engineering Science, 2007, 62, 5697-5714.	1.9	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.	2.2	249
103	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.	1.2	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.	1.2	51
105	Topological Analysis of Linear Polymer Melts:Â A Statistical Approach. Macromolecules, 2006, 39, 4592-4604.	2.2	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.	5.6	56
107	Principles of Molecular Simulation of Gas Transport in Polymers. , 2006, , 49-94.		34
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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. Magnetic Resonance Imaging, 2005, 23, 233-237.	1.0	14
112	Molecular simulation of structure, thermodynamic and transport properties of polymeric membrane materials for hydrocarbon separation. Fluid Phase Equilibria, 2005, 228-229, 15-20.	1.4	16
113	Hierarchical modeling of amorphous polymers. Computer Physics Communications, 2005, 169, 82-88.	3.0	22
114	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.	2.2	38
115	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
116	Microscopic Origins for the Favorable Solvation of Carbonate Ether Copolymers in CO2. Journal of the American Chemical Society, 2005, 127, 12338-12342.	6.6	28
117	Detailed Atomistic Molecular Dynamics Simulation ofcis-1,4-Poly(butadiene). Macromolecules, 2005, 38, 1478-1492.	2.2	118
118	Coarse graining using pretabulated potentials: Liquid benzene. Journal of Chemical Physics, 2005, 122, 244111.	1.2	23
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120	Multiscale Modeling of Polymers. , 2005, , 2757-2761.		2
121	Multiscale Modeling of Polymers. , 2005, , 2757-2761.		0
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123	Detailed Atomistic Simulation of the Segmental Dynamics and Barrier Properties of Amorphous Poly(ethylene terephthalate) and Poly(ethylene isophthalate). Macromolecules, 2004, 37, 2978-2995.	2.2	109
124	Experimental and Self-Consistent-Field Theoretical Study of Styrene Block Copolymer Self-Adhesive Materials. Macromolecules, 2004, 37, 5093-5109.	2.2	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. Macromolecules, 2004, 37, 1102-1112.	2.2	46
126	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.	1.2	104

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127	Understanding and predicting structureâ€“property relations in polymeric materials through molecular simulations. Molecular Physics, 2004, 102, 147-166.	0.8	52
128	On the separation between torsionâ€“vibration and conformational relaxation processes in the incoherent intermediate scattering function of polyethylene. Chemical Physics, 2003, 292, 371-382.	0.9	14
129	Chain and local dynamics of polyisoprene as probed by experiments and computer simulations. Journal of Chemical Physics, 2003, 119, 6883-6894.	1.2	85
130	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.	2.2	198
131	Atomistic Monte Carlo Simulation of Polybutadiene Isomers:Âcis-1,4-Polybutadiene and 1,2-Polybutadiene. Macromolecules, 2003, 36, 6925-6938.	2.2	50
132	Microscopic calculation of the static electric susceptibility of polyethylene. Journal of Chemical Physics, 2003, 119, 11458-11466.	1.2	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. Physical Review Letters, 2002, 88, 105503.	2.9	218
135	Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm. Journal of Chemical Physics, 2002, 117, 5465-5479.	1.2	130
136	Atomistic molecular dynamics simulation of diffusion in binary liquid n-alkane mixtures. Journal of Chemical Physics, 2002, 116, 7656-7665.	1.2	49
137	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.	1.2	85
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139	Atomic structure of a high polymer melt. Europhysics Letters, 2002, 57, 506-511.	0.7	42
140	Mushrooms and Brushes in Thin Films of Diblock Copolymer/Homopolymer Mixtures. Macromolecules, 2002, 35, 1116-1132.	2.2	24
141	Entanglement Network of the Polypropylene/Polyamide Interface. 3. Deformation to Fracture. Macromolecules, 2002, 35, 508-521.	2.2	32
142	Parallel tempering method for reconstructing isotropic and anisotropic porous media. Journal of Chemical Physics, 2002, 117, 5876-5884.	1.2	24
143	Segmental Dynamics of Atactic Polypropylene As Revealed by Molecular Simulations and Quasielastic Neutron Scattering. Macromolecules, 2002, 35, 7110-7124.	2.2	35
144	Linking the atomistic scale and the mesoscale: molecular orbital and solid state packing calculations on poly(p-phenylene). Polymer, 2002, 43, 185-193.	1.8	9

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147	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.	1.2	29
148	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.	1.2	56
149	Prediction of Permeation Properties of CO2 and N2 through Silicalite via Molecular Simulations. Journal of Physical Chemistry B, 2001, 105, 777-788.	1.2	182
150	Coarse-Grained Molecular Simulation of Penetrant Diffusion in a Glassy Polymer Using Reverse and Kinetic Monte Carlo. Macromolecules, 2001, 34, 8541-8553.	2.2	61
151	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.	1.2	36
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153	Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities. Chemical Engineering Science, 2001, 56, 2789-2801.	1.9	42
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155	Calculation of the chemical potential of chain molecules using the staged particle deletion scheme. Journal of Chemical Physics, 2001, 115, 8231-8237.	1.2	41
156	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
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. Macromolecular Theory and Simulations, 2000, 9, 500-515.	0.6	26
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159	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
160	Molecular Simulation of Phase Equilibria for Waterâ^'n-Butane and Waterâ^'n-Hexane Mixtures. Journal of Physical Chemistry B, 2000, 104, 4958-4963.	1.2	47
161	Dynamics ofn-Butaneâ^'Methane Mixtures in Silicalite, Using Quasielastic Neutron Scattering and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2000, 104, 5541-5552.	1.2	77
162	Entanglement Network of the Polypropylene/Polyamide Interface. 2. Network Generation. Macromolecules, 2000, 33, 1397-1410.	2.2	22

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164	Entanglement Network of the Polypropylene/Polyamide Interface. 1. Self-Consistent Field Model. Macromolecules, 2000, 33, 1385-1396.	2.2	28
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