Doros N Theodorou

List of Publications by Year in Descending Order

253 papers	13,139 citations	59 h-index	106 g-index
271 ext. papers	13,883 ext. citations	4.3 avg, IF	6.57 L-index

#	Paper	IF	Citations
253	Multiscale simulations of polyzwitterions in aqueous bulk solutions and brush array configurations. *Soft Matter*, **2021**,	3.6	4
252	Thermodynamic analysis of oligomeric blends by applying the Kirkwood-Buff theory of solutions. *Journal of Physics: Conference Series*, **2021**, 2090, 012079	0.3	0
251	Potential of Mean Force between Bare or Grafted Silica/Polystyrene Surfaces from Self-Consistent Field Theory. *Polymers*, **2021**, 13,	4.5	5
250	RuSseL: A Self-Consistent Field Theory Code for Inhomogeneous Polymer Interphases. *Computation* , **2021**, 9, 57	2.2	2
249	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	3.4	1
248	Molecular simulations of dopamine in a lipid bilayer **2021**,		1
247	Molecular Dynamics Simulations of Polyethylene Bilayers. *Journal of Physics: Conference Series*, **2021**, 1730, 012039	0.3	
246	Structure and thermodynamics of grafted silica/polystyrene dilute nanocomposites investigated through self-consistent field theory. *Soft Matter*, **2021**, 17, 4077-4097	3.6	6
245	Molecular dynamics simulations of stretch-induced crystallization in layered polyethylene. *Polymer Crystallization*, **2021**, 4, e10172	0.9	
244	In silico study of levodopa in hydrated lipid bilayers at the atomistic level. *Journal of Molecular Graphics and Modelling*, **2021**, 107, 107972	2.8	1
243	A three-dimensional finite element methodology for addressing heterogeneous polymer systems with simulations based on self-consistent field theory **2021**,		2
242	Molecular Simulations and Mechanistic Analysis of the Effect of CO Sorption on Thermodynamics, Structure, and Local Dynamics of Molten Atactic Polystyrene. *Macromolecules*, **2020**, 53, 3669-3689	5.5	8
241	Molecular Dynamics Test of the Stress-Thermal Rule in Polyethylene and Polystyrene Entangled Melts. *Macromolecules*, **2020**, 53, 789-802	5.5	3
240	Free energy calculations by molecular simulations of deformed polymer glasses. *Computer Physics Communications*, **2020**, 249, 107008	4.2	4
239	Atomistic simulations of long-chain polyethylene melts flowing past gold surfaces: structure and wall-slip. *Molecular Physics*, **2020**, 118, e1706775	1.7	5
238	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	3.4	15
237	Kinetic concepts and local failure in the interfacial shear strength of epoxy-graphene nanocomposites. *Physical Review E*, **2020**, 102, 030501	2.4	2

236	Molecular Modeling Investigations of Sorption and Diffusion of Small Molecules in Glassy Polymers. *Membranes*, **2019**, 9,	3.8	24
235	Multiscale Simulations of Graphite-Capped Polyethylene Melts: Brownian Dynamics/Kinetic Monte Carlo Compared to Atomistic Calculations and Experiment. *Macromolecules*, **2019**, 52, 7503-7523	5.5	13
234	Molecular dynamics simulations of EPON-862/DETDA epoxy networks: structure, topology, elastic constants, and local dynamics. *Soft Matter*, **2019**, 15, 721-733	3.6	24
233	Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1414	7.9	2
232	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	5.5	12
231	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	6.1	2
230	Thermodynamic Analysis of n-Hexane-Ethanol Binary Mixtures Using the Kirkwood-Buff Theory. *Journal of Physical Chemistry B*, **2019**, 123, 247-257	3.4	7
229	Multiscale Molecular Simulations of Polymer-Matrix Nanocomposites: or What Molecular Simulations Have Taught us About the Fascinating Nanoworld. *Archives of Computational Methods in Engineering*, **2018**, 25, 591-645	7.8	33
228	Computational Studies of Nanographene Systems: Extended Discotics, Covalently Linked Supermolecules, and Functionalized Supramolecular Assemblies. *Journal of Physical Chemistry C*, **2018**, 122, 18715-18731	3.8	4
227	Thermodynamic analysis of Lennard-Jones binary mixtures using Kirkwood-Buff theory. *Fluid Phase Equilibria*, **2018**, 470, 25-37	2.5	11
226	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	5.5	13
225	Slip Spring-Based Mesoscopic Simulations of Polymer Networks: Methodology and the Corresponding Computational Code. *Polymers*, **2018**, 10,	4.5	12
224	Tacticity Effect on the Conformational Properties of Polypropylene and Poly(ethylene-propylene) Copolymers. *Macromolecules*, **2018**, 51, 6878-6891	5.5	10
223	Exploring the interactions of irbesartan and irbesartan-2-hydroxypropyl-cyclodextrin complex with model membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2017**, 1859, 1089-1098	3.8	22
222	Slip-Spring Model for the Linear and Nonlinear Viscoelastic Properties of Molten Polyethylene Derived from Atomistic Simulations. *Macromolecules*, **2017**, 50, 4524-4541	5.5	38
221	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	5.5	12
220	Equation of State Based Slip Spring Model for Entangled Polymer Dynamics. *Macromolecules*, **2017**, 50, 3004-3029	5.5	32
219	Molecular Simulations of Free and Graphite Capped Polyethylene Films: Estimation of the Interfacial Free Energies. *Macromolecules*, **2017**, 50, 8827-8844	5.5	38

218	Diffusion of Aromatics in Silicalite-1: Experimental and Theoretical Evidence of Entropic Barriers. *Journal of Physical Chemistry C*, **2016**, 120, 21410-21426	3.8	19
217	Melting Point and Solid□liquid Coexistence Properties of ∃ Isotactic Polypropylene as Functions of Its Molar Mass: A Molecular Dynamics Study. *Macromolecules*, **2016**, 49, 4663-4673	5.5	14
216	Molecular Modeling and Simulation of Polymer Nanocomposites at Multiple Length Scales. *IEEE Nanotechnology Magazine*, **2016**, 15, 416-422	2.6	12
215	Mesoscopic Simulations of Crosslinked Polymer Networks. *Journal of Physics: Conference Series*, **2016**, 738, 012063	0.3	7
214	Atomistic and Coarse-grained Simulations of Hexabenzocoronene Crystals. *Journal of Physics: Conference Series*, **2016**, 738, 012019	0.3	1
213	Molecular Dynamics Study of Polyethylene under Extreme Confinement. *Journal of Physics: Conference Series*, **2016**, 738, 012012	0.3	18
212	Molecular modeling and simulation of atactic polystyrene/amorphous silica nanocomposites. *Journal of Physics: Conference Series*, **2016**, 738, 012021	0.3	2
211	Multiscale simulations of PS-SiO2 nanocomposites: from melt to glassy state. *Soft Matter*, **2016**, 12, 7585-7605	3.605	22
210	Monte Carlo simulations of structure and entanglements in polymer melts. *Molecular Simulation*, **2015**, 41, 993-995	2	2
209	Application of bi-Helmholtz nonlocal elasticity and molecular simulations to the dynamical response of carbon nanotubes **2015**,		17
208	Multiscale simulations of hexa-peri-hexabenzocoronene and hexa-n-dodecyl-hexa-peri-hexabenzocoronene **2015**,		1
207	Molecular dynamics simulations of alkyl substituted nanographene crystals** Dedicated to Professor Jean-Pierre Hansen, with deepest appreciation of his outstanding contributions to liquid and soft matter theory.View all notes. *Molecular Physics*, **2015**, 113, 2776-2790	1.7	8
206	Local Segmental Dynamics and Stresses in Polystyrene□C60 Mixtures. *Macromolecules*, **2014**, 47, 387-404	5.5	72
205	Determination of the Mechanical Properties of a Poly(methyl methacrylate) Nanocomposite with Functionalized Graphene Sheets through Detailed Atomistic Simulations. *Macromolecules*, **2014**, 47, 8072-8088	5.5	71
204	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	17
203	Self-Consistent-Field Study of Adsorption and Desorption Kinetics of Polyethylene Melts on Graphite and Comparison with Atomistic Simulations. *Macromolecules*, **2014**, 47, 6964-6981	5.5	16
202	Atomistic simulations of cavitation in a model polyethylene network. *Polymer Science - Series C*, **2013**, 55, 212-218	1.1	9
201	Structure of Polymer Layers Grafted to Nanoparticles in Silica□Polystyrene Nanocomposites. *Macromolecules*, **2013**, 46, 4670-4683	5.5	88

200	Structure and entanglements in short chain branched polyolefin melts **2013**,		2
199	Tracking a glassy polymer on its energy landscape in the course of elastic deformation. *Molecular Physics*, **2013**, 111, 3430-3441	1.7	18
198	Temporal disconnectivity of the energy landscape in glassy systems. *Journal of Chemical Physics*, **2013**, 138, 12A545	3.9	6
197	Microscopic Description of Entanglements in Polyethylene Networks and Melts: Strong, Weak, Pairwise, and Collective Attributes. *Macromolecules*, **2012**, 45, 9475-9492	5.5	39
196	Monte Carlo Simulation of Short Chain Branched Polyolefins: Structure and Properties. *Macromolecules*, **2012**, 45, 8453-8466	5.5	22
195	Single-File Diffusion **2012**, 111-142		2
194	Constructing Molecular Models and Sampling Equilibrium Probability Distributions **2012**, 191-226		1
193	Molecular Dynamics Simulations **2012**, 227-273		
192	Infrequent Event Techniques for Simulating Diffusion in Microporous Solids **2012**, 275-301		
191	Diffusional Effects in Zeolite Catalysts **2012**, 807-837		0
190	Zeolite Membranes **2012**, 769-805		
189	Metal Organic Frameworks (MOFs) **2012**, 729-767		
188	Medium-Pore (Ten-Ring) Zeolites **2012**, 653-728		2
187	Large Pore (12-Ring) Zeolites **2012**, 607-651		1
186	Amorphous Materials and Extracrystalline (Meso/Macro) Pores **2012**, 515-560		1
185	Measurement of Elementary Diffusion Processes **2012**, 303-345		
184	Direct Macroscopic Measurement of Sorption and Tracer Exchange Rates **2012**, 427-457		
183	Imaging of Transient Concentration Profiles **2012**, 395-426		1

182	Sorption Kinetics **2012**, 143-189		3
181	Eight-Ring Zeolites **2012**, 561-606		2
180	Chromatographic and Permeation Methods of Measuring Intraparticle Diffusion **2012**, 459-513		
179	Elementary Principles of Diffusion **2012**, 1-24		
178	Diffusion as a Random Walk **2012**, 25-58		4
177	Diffusion and Non-equilibrium Thermodynamics **2012**, 59-83		
176	Diffusion Mechanisms **2012**, 85-110		2
175	Diffusion Measurement by Monitoring Molecular Displacement **2012**, 347-394		
174	On solving the master equation in spatially periodic systems. *Journal of Chemical Physics*, **2012**, 137, 034112	3.9	11
173	**2012**,		322
172	Interface of Grafted and Ungrafted Silica Nanoparticles with a Polystyrene Matrix: Atomistic Molecular Dynamics Simulations. *Macromolecules*, **2011**, 44, 2316-2327	5.5	217
171	Systematic Coarse Graining of 4-Cyano-4?-pentylbiphenyl. *Industrial & Engineering Chemistry Research*, **2011**, 50, 546-556	3.9	32
170	Monte Carlo simulations of a coarse grained model for an athermal all-polystyrene nanocomposite system. *European Polymer Journal*, **2011**, 47, 699-712	5.2	58
169	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	3.9	13
168	A Study of the Entanglement in Systems with Periodic Boundary Conditions. *Progress of Theoretical Physics Supplement*, **2011**, 191, 172-181		21
167	Diffusion via space discretization method to study the concentration dependence of self-diffusivity under confinement. *Journal of Chemical Physics*, **2010**, 132, 134108	3.9	6
166	Crystallization and Melting Simulations of Oligomeric ? Isotactic Polypropylene. *Macromolecules*, **2010**, 43, 5455-5469	5.5	30
165	Prediction of infinite dilution benzene solubility in linear polyethylene melts via the direct particle deletion method. *Journal of Physical Chemistry B*, **2010**, 114, 6233-46	3.4	14

164	Efficient Parallel Decomposition of Dynamical Sampling in Glass-Forming Materials Based on an On the Fly Definition of Metabasins. *Journal of Chemical Theory and Computation*, **2010**, 6, 1307-1322	6.4	12
163	Progress and Outlook in Monte Carlo Simulations. *Industrial & Engineering Chemistry Research*, **2010**, 49, 3047-3058	3.9	86
162	Temperature accelerated dynamics in glass-forming materials. *Journal of Physical Chemistry B*, **2010** , 114, 7844-53	3.4	8
161	Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. *Journal of Supercritical Fluids*, **2010**, 55, 503-509	4.2	5
160	Simulation studies of methane, carbon dioxide, hydrogen and deuterium in ITQ-1 and NaX zeolites. *Molecular Simulation*, **2009**, 35, 79-89	2	17
159	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, 13761-7	3.4	17
158	Benefit of Microscopic Diffusion Measurement for the Characterization of Nanoporous Materials. *Chemical Engineering and Technology*, **2009**, 32, 1494-1511	2	26
157	Onset of Entanglements Revisited. Dynamical Analysis. *Macromolecules*, **2009**, 42, 7485-7494	5.5	62
156	Onset of Entanglements Revisited. Topological Analysis. *Macromolecules*, **2009**, 42, 7474-7484	5.5	47
155	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	3.9	17
154	Prediction of Sorption of CO2 in Glassy Atactic Polystyrene at Elevated Pressures Through a New Computational Scheme. *Macromolecules*, **2009**, 42, 1759-1769	5.5	45
153	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, 11708-15	3.4	21
152	Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data. *Macromolecules*, **2008**, 41, 2959-2962	5.5	43
151	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, 10628-37	3.4	8
150	On the role of inherent structures in glass-forming materials: I. The vitrification process. *Journal of Physical Chemistry B*, **2008**, 112, 10619-27	3.4	21
149	A second-order Markov process for modeling diffusive motion through spatial discretization. *Journal of Chemical Physics*, **2008**, 128, 024504	3.9	6
148	Computer Simulation of Sorption and Transport in Zeolites **2008**, 1662		2
147	Segmental and Chain Dynamics of Isotactic Polypropylene Melts. *Macromolecules*, **2007**, 40, 2235-2245	5.5	37

146	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	5.5	8
145	Hierarchical modelling of polymeric materials. *Chemical Engineering Science*, **2007**, 62, 5697-5714	4.4	56
144	Quasi-elastic neutron scattering and molecular dynamics simulation as complementary techniques for studying diffusion in zeolites. *Microporous and Mesoporous Materials*, **2007**, 102, 21-50	5.3	220
143	Dynamical integration of a Markovian web: a first passage time approach. *Journal of Chemical Physics*, **2007**, 127, 084903	3.9	38
142	Formation of rodlike structures of water between oppositely charged ions in decane and polyethylene. *Journal of Chemical Physics*, **2007**, 127, 191101	3.9	2
141	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	3.9	26
140	Monte Carlo simulations of equilibrium solubilities and structure of water in n-alkanes and polyethylene. *Journal of Chemical Physics*, **2007**, 126, 224902	3.9	21
139	Coarse Grained End Bridging Monte Carlo Simulations of Poly(ethylene terephthalate) Melt. *Macromolecules*, **2007**, 40, 710-722	5.5	61
138	Coarse-Grained and Reverse-Mapped United-Atom Simulations of Long-Chain Atactic Polystyrene Melts:Structure, Thermodynamic Properties, Chain Conformation, and Entanglements. *Macromolecules*, **2007**, 40, 3876-3885	5.5	165
137	Monte Carlo Simulation of Short Chain Branched Polyolefins in the Molten State. *Macromolecules*, **2007**, 40, 9640-9650	5.5	75
136	Accelerating molecular simulations by reversible mapping between local minima. *Journal of Chemical Physics*, **2006**, 125, 084107	3.9	13
135	A reversible minimum-to-minimum mapping method for the calculation of free-energy differences. *Journal of Chemical Physics*, **2006**, 124, 034109	3.9	20
134	Equilibration and Coarse-Graining Methods for Polymers **2006**, 419-448		4
133	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, 22742-53	3.4	38
132	Diffusion of long n-alkanes in silicalite. A comparison between neutron scattering experiments and hierarchical simulation results. *Journal of Physical Chemistry B*, **2006**, 110, 1964-7	3.4	47
131	Topological Analysis of Linear Polymer Melts:A Statistical Approach. *Macromolecules*, **2006**, 39, 4592-4604	5.5	239
130	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	12	52
129	Principles of Molecular Simulation of Gas Transport in Polymers **2006**, 49-94		23

128	Self-Consistent-Field Study of Compressible Semiflexible Melts Adsorbed on a Solid Substrate and Comparison with Atomistic Simulations. *Macromolecules*, **2005**, 38, 7134-7149	5.5	47
127	Microscopic origins for the favorable solvation of carbonate ether copolymers in CO2. *Journal of the American Chemical Society*, **2005**, 127, 12338-42	16.4	26
126	Detailed Atomistic Molecular Dynamics Simulation of cis-1,4-Poly(butadiene). *Macromolecules*, **2005**, 38, 1478-1492	5.5	104
125	Coarse graining using pretabulated potentials: liquid benzene. *Journal of Chemical Physics*, **2005**, 122, 244111	3.9	23
124	Diffusion in Fluid Catalytic Cracking Catalysts on Various Displacement Scales and Its Role in Catalytic Performance. *Chemistry of Materials*, **2005**, 17, 2466-2474	9.6	68
123	Multiscale Modeling of Polymers **2005**, 2757-2761		2
122	Pulsed-field gradient nuclear magnetic resonance study of transport properties of fluid catalytic cracking catalysts. *Magnetic Resonance Imaging*, **2005**, 23, 233-7	3.3	11
121	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	13
120	Hierarchical modeling of amorphous polymers. *Computer Physics Communications*, **2005**, 169, 82-88	4.2	20
119	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	5.5	35
118	Multiscale Modeling of Polymers **2005**, 2757-2761		
117	Connectivity-Altering Monte Carlo Simulations of the End Group Effects on Volumetric Properties for Poly(ethylene oxide). *Macromolecules*, **2004**, 37, 7026-7033	5.5	49
116	Detailed Atomistic Simulation of the Segmental Dynamics and Barrier Properties of Amorphous Poly(ethylene terephthalate) and Poly(ethylene isophthalate). *Macromolecules*, **2004**, 37, 2978-2995	5.5	95
115	Experimental and Self-Consistent-Field Theoretical Study of Styrene Block Copolymer Self-Adhesive Materials. *Macromolecules*, **2004**, 37, 5093-5109	5.5	35
114	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	5.5	44
113	Transport Diffusivity of N2 and CO2 in Silicalite: Coherent Quasielastic Neutron Scattering Measurements and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 12748-12756	3.4	99
112	Understanding and predicting structure–property relations in polymeric materials through molecular simulations. *Molecular Physics*, **2004**, 102, 147-166	1.7	48
111	On the separation between torsion–vibration and conformational relaxation processes in the incoherent intermediate scattering function of polyethylene. *Chemical Physics*, **2003**, 292, 371-382	2.3	14

110	Chain and local dynamics of polyisoprene as probed by experiments and computer simulations. *Journal of Chemical Physics*, **2003**, 119, 6883-6894	3.9	78
109	Crossover from the Rouse to the Entangled Polymer Melt Regime: Signals from Long, Detailed Atomistic Molecular Dynamics Simulations, Supported by Rheological Experiments. *Macromolecules* , **2003**, 36, 1376-1387	5.5	179
108	Atomistic Monte Carlo Simulation of Polybutadiene Isomers: cis-1,4-Polybutadiene and 1,2-Polybutadiene. *Macromolecules*, **2003**, 36, 6925-6938	5.5	48
107	Microscopic calculation of the static electric susceptibility of polyethylene. *Journal of Chemical Physics*, **2003**, 119, 11458-11466	3.9	8
106	Polymers at Surfaces and Interfaces **2003**, 329-419		11
105	Linking the atomistic scale and the mesoscale: molecular orbital and solid state packing calculations on poly(p-phenylene). *Polymer*, **2002**, 43, 185-193	3.9	9
104	Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors. *Computer Physics Communications*, **2002**, 144, 1-22	4.2	28
103	A novel Monte Carlo scheme for the rapid equilibration of atomistic model polymer systems of precisely defined molecular architecture. *Physical Review Letters*, **2002**, 88, 105503	7.4	200
102	Atomistic Monte Carlo simulation of strictly monodisperse long polyethylene melts through a generalized chain bridging algorithm. *Journal of Chemical Physics*, **2002**, 117, 5465-5479	3.9	117
101	Atomistic molecular dynamics simulation of diffusion in binary liquid n-alkane mixtures. *Journal of Chemical Physics*, **2002**, 116, 7656-7665	3.9	46
100	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	3.9	78
99	Variable-Connectivity Monte Carlo Algorithms for the Atomistic Simulation of Long-Chain Polymer Systems. *Lecture Notes in Physics*, **2002**, 67-127	0.8	12
98	Atomic structure of a high polymer melt. *Europhysics Letters*, **2002**, 57, 506-511	1.6	38
97	Mushrooms and Brushes in Thin Films of Diblock Copolymer/Homopolymer Mixtures. *Macromolecules*, **2002**, 35, 1116-1132	5.5	22
96	Entanglement Network of the Polypropylene/Polyamide Interface. 3. Deformation to Fracture. *Macromolecules*, **2002**, 35, 508-521	5.5	28
95	Parallel tempering method for reconstructing isotropic and anisotropic porous media. *Journal of Chemical Physics*, **2002**, 117, 5876-5884	3.9	24
94	Segmental Dynamics of Atactic Polypropylene As Revealed by Molecular Simulations and Quasielastic Neutron Scattering. *Macromolecules*, **2002**, 35, 7110-7124	5.5	34
93	Diffusion of small molecules in disordered media: study of the effect of kinetic and spatial heterogeneities. *Chemical Engineering Science*, **2001**, 56, 2789-2801	4.4	42

92	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	3.9	29
91	Calculation of the chemical potential of chain molecules using the staged particle deletion scheme. *Journal of Chemical Physics*, **2001**, 115, 8231-8237	3.9	41
90	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	3.9	45
89	Local Structure and Dynamics of trans-Polyisoprene Oligomers. *Macromolecules*, **2001**, 34, 1436-1448	5.5	40
88	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	3.9	28
87	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	3.9	55
86	Prediction of Permeation Properties of CO2 and N2 through Silicalite via Molecular Simulations. *Journal of Physical Chemistry B*, **2001**, 105, 777-788	3.4	162
85	Coarse-Grained Molecular Simulation of Penetrant Diffusion in a Glassy Polymer Using Reverse and Kinetic Monte Carlo. *Macromolecules*, **2001**, 34, 8541-8553	5.5	56
84	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	3.4	31
83	Directed Bridging Methods for Fast Atomistic Monte Carlo Simulations of Bulk Polymers. *Macromolecules*, **2001**, 34, 8554-8568	5.5	51
82	Atomistic Monte Carlo simulation of steady-state uniaxial elongational flow of long-chain polyethylene melts: dependence of the melt degree of orientation on stress, molecular length and elongational strain rate. *Macromolecular Theory and Simulations*, **2000**, 9, 500-515	1.5	26
81	Atomistic simulation of the birefringence of uniaxially stretched polyethylene melts. *Computational and Theoretical Polymer Science*, **2000**, 10, 1-13		34
80	Component segmental mobilities in an athermal polymer blend: Quasielastic incoherent neutron scattering versus simulation. *Journal of Chemical Physics*, **2000**, 112, 8687-8694	3.9	47
79	Molecular Simulation of Phase Equilibria for Water–Butane and Water–Hexane Mixtures. *Journal of Physical Chemistry B*, **2000**, 104, 4958-4963	3.4	44
78	Dynamics ofn-Butane–Methane Mixtures in Silicalite, Using Quasielastic Neutron Scattering and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2000**, 104, 5541-5552	3.4	69
77	Entanglement Network of the Polypropylene/Polyamide Interface. 2. Network Generation. *Macromolecules*, **2000**, 33, 1397-1410	5.5	21
76	Atomistic Molecular Dynamics Simulation of Stress Relaxation upon Cessation of Steady-State Uniaxial Elongational Flow. *Macromolecules*, **2000**, 33, 8062-8076	5.5	41
75	Entanglement Network of the Polypropylene/Polyamide Interface. 1. Self-Consistent Field Model. *Macromolecules*, **2000**, 33, 1385-1396	5.5	27

74	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	3.9	30
73	On the calculation of the chemical potential using the particle deletion scheme. *Molecular Physics*, **1999**, 96, 905-913	1.7	56
72	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	3.9	32
71	Effect of Tacticity on the Molecular Dynamics of Polypropylene Melts. *Macromolecules*, **1999**, 32, 8635-8644	5.5	39
70	Molecular Dynamics Simulation ofn-Butane–Methane Mixtures in Silicalite. *Journal of Physical Chemistry B*, **1999**, 103, 3380-3390	3.4	58
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2 Elementary Steps and Mechanisms: Sections 5.3 □5.51051-1188 8

1 On the calculation of the chemical potential using the particle deletion scheme 3