Roland Faller

List of Publications by Year
in descending order

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172 papers	5,241 citations	93792 39 h-index	124990 64 g-index
182 all docs	182 docs citations	182 times ranked	6183 citing authors

#	Article	IF	Citations
1	A molecular dynamics investigation of N-glycosylation effects on T-cell receptor kinetics. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5614-5623.	2.0	1
2	Interplay of distributions of multiple guest molecules in block copolymer micelles: A dissipative particle dynamics study. Journal of Colloid and Interface Science, 2022, 607, 1142-1152.	5.0	4
3	SARS-CoV-2 spike binding to ACE2 is stronger and longer ranged due to glycan interaction. Biophysical Journal, 2022, 121, 79-90.	0.2	23
4	An unprecedented fully reduced {Mo^V₆₀} polyoxometalate: from an all-inorganic molecular light-absorber model to improved photoelectronic performance. Chemical Science, 2022, 13, 4573-4580.	3.7	22
5	Using molecular dynamics simulations to interrogate T cell receptor non-equilibrium kinetics. Computational and Structural Biotechnology Journal, 2022, 20, 2124-2133.	1.9	9
6	Impact of Surface Polarity on Lipid Assembly under Spatial Confinement. Langmuir, 2022, 38, 7545-7557.	1.6	0
7	A computational algorithm to assess the physiochemical determinants of T cell receptor dissociation kinetics. Computational and Structural Biotechnology Journal, 2022, 20, 3473-3481.	1.9	1
8	Computing inelastic neutron scattering spectra from molecular dynamics trajectories. Scientific Reports, 2021, 11, 7938.	1.6	7
9	Contributions of the international plant science community to the fight against infectious diseases in humansâ€”part 2: Affordable drugs in edible plants for endemic and reâ€emerging diseases. Plant Biotechnology Journal, 2021, 19, 1921-1936.	4.1	31
10	Contributions of the international plant science community to the fight against human infectious diseases â€“ part 1: epidemic and pandemic diseases. Plant Biotechnology Journal, 2021, 19, 1901-1920.	4.1	44
11	Determining structure and action mechanism of LBF14 by molecular simulation. Journal of Biomolecular Structure and Dynamics, 2021, , 1-12.	2.0	2
12	Comparing the Expense and Accuracy of Methods to Simulate Atomic Vibrations in Rubrene. Journal of Chemical Theory and Computation, 2021, , .	2.3	3
13	Aggregation and pressure effects of asphaltene and resin molecules at oilâ€“water interfaces: a coarse-grained molecular dynamics and free energy study. Soft Materials, 2020, 18, 113-127.	0.8	7
14	Harnessed Dopant Block Copolymers Assist Decorating Membrane Pores: A Dissipative Particle Dynamics Study. Macromolecular Rapid Communications, 2020, 41, e1900561.	2.0	7
15	Development and simulation of fully glycosylated molecular models of ACE2-Fc fusion proteins and their interaction with the SARS-CoV-2 spike protein binding domain. PLoS ONE, 2020, 15, e0237295.	1.1	36
16	Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials. Journal of Chemical Theory and Computation, 2020, 16, 3494-3503.	2.3	12
17	Confining Liquids inside Carbon Nanotubes: Accelerated Molecular Dynamics with Spliced, Soft-Core Potentials and Simulated Annealing. Journal of Chemical Theory and Computation, 2020, 16, 2692-2702.	2.3	0
18	New Means to Control Molecular Assembly. Journal of Physical Chemistry C, 2020, 124, 6405-6412.	1.5	9

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19	Editorial: tailor-made approaches on use of multiscale modeling for research on soft materials â€“ capabilities, restrictions and future possibilities. Soft Materials, 2020, 18, 111-112.	0.8	0
20	Porous Organic Frameworks Featured by Distinct Confining Fields for the Selective Hydrogenation of Biomassâ€Derived Ketones. Advanced Materials, 2020, 32, e1908243.	11.1	22
21	Porous Aromatic Framework Nanosheets Anchored with Lewis Pairs for Efficient and Recyclable Heterogeneous Catalysis. Advanced Science, 2020, 7, 2000067.	5.6	22
22	Effects of N-Glycosylation on the Structure, Function, and Stability of a Plant-Made Fc-Fusion Anthrax Decoy Protein. Frontiers in Plant Science, 2019, 10, 768.	1.7	29
23	ACPYPE update for nonuniform 1â€“4 scale factors: Conversion of the GLYCAM06 force field from AMBER to GROMACS. SoftwareX, 2019, 10, 100241.	1.2	41
24	Direct probe of the nuclear modes limiting charge mobility in molecular semiconductors. Materials Horizons, 2019, 6, 182-191.	6.4	53
25	Computational modelling of atomic layer etching of chlorinated germanium surfaces by argon. Physical Chemistry Chemical Physics, 2019, 21, 5898-5902.	1.3	6
26	Computational and Experimental Studies on Novel Materials for Fission Gas Capture. Minerals, Metals and Materials Series, 2019, , 1039-1050.	0.3	0
27	Molecular investigation of gas adsorption, separation, and transport on carbon nanoscrolls: A combined grand canonical Monte Carlo and molecular dynamics study. Carbon, 2018, 132, 401-410.	5.4	13
28	Put Your Backbone into It: Excited-State Structural Relaxation of PffBT4T-2DT Conducting Polymer in Solution. Journal of Physical Chemistry C, 2018, 122, 7020-7026.	1.5	7
29	Multiscale modeling on biological systems. Biochemical and Biophysical Research Communications, 2018, 498, 263.	1.0	2
30	Atomistic modeling of La³⁺ doping segregation effect on nanocrystalline yttria-stabilized zirconia. Physical Chemistry Chemical Physics, 2018, 20, 13215-13223.	1.3	8
31	Molecular dynamics simulations on heterogeneity and percolation of epoxy nanofilm during glass transition process. Materials Chemistry and Physics, 2018, 213, 239-248.	2.0	16
32	Patterning of Wrinkled Polymer Surfaces by Single-Step Electron Irradiation. Langmuir, 2018, 34, 5290-5296.	1.6	8
33	Controllable Multigeometry Nanoparticles via Cooperative Assembly of Amphiphilic Diblock Copolymer Blends with Asymmetric Architectures. ACS Nano, 2018, 12, 1413-1419.	7.3	23
34	Molecular simulation study of aluminumâ€“noble gas interfacial thermal accommodation coefficients. AICHE Journal, 2018, 64, 338-345.	1.8	11
35	Polymorphism controls the degree of charge transfer in a molecularly doped semiconducting polymer. Materials Horizons, 2018, 5, 655-660.	6.4	92
36	Molecular Dynamics Modeling of Methylene Blueâ”DOPC Lipid Bilayer Interactions. Langmuir, 2018, 34, 4314-4323.	1.6	19

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37	Helium interactions with alumina formed by atomic layer deposition show potential for mitigating problems with excess helium in spent nuclear fuel. Journal of Nuclear Materials, 2018, 499, 301-311.	1.3	8
38	Directional Statistics of Preferential Orientations of Two Shapes in Their Aggregate and Its Application to Nanoparticle Aggregation. Technometrics, 2018, 60, 332-344.	1.3	5
39	Structural Analysis of Human Glycoprotein Butyrylcholinesterase using Atomistic Molecular Dynamics: The Importance of Glycosylation Site ASN241. Biophysical Journal, 2018, 114, 47a.	0.2	0
40	Energetic design of grain boundary networks for toughening of nanocrystalline oxides. Journal of the European Ceramic Society, 2018, 38, 4260-4267.	2.8	22
41	Computational and Experimental Studies on Novel Materials for Fission Gas Capture. Minerals, Metals and Materials Series, 2018, , 1039-1050.	0.3	0
42	Molecular dynamics simulations of ternary lipid bilayers containing plant sterol and glucosylceramide. Chemistry and Physics of Lipids, 2017, 203, 24-32.	1.5	13
43	Modeling organic electronic materials: bridging length and time scales. Molecular Simulation, 2017, 43, 730-742.	0.9	8
44	Identifying Atomic Scale Structure in Undoped/Doped Semicrystalline P3HT Using Inelastic Neutron Scattering. Macromolecules, 2017, 50, 2424-2435.	2.2	52
45	Mechanism of the fcc-to-hcp phase transformation in solid Ar. Journal of Chemical Physics, 2017, 146, 214502.	1.2	17
46	Development and Application of a Coarse-Grained Model for PNIPAM by Iterative Boltzmann Inversion and Its Combination with Lattice Boltzmann Hydrodynamics. Journal of Physical Chemistry B, 2017, 121, 10394-10406.	1.2	14
47	Ligand exchange based molecular doping in 2D hybrid molecule-nanoparticle arrays: length determines exchange efficiency and conductance. Molecular Systems Design and Engineering, 2017, 2, 440-448.	1.7	8
48	Controllable multicompartment morphologies from cooperative self-assembly of copolymerâ€“copolymer blends. Soft Matter, 2017, 13, 5877-5887.	1.2	15
49	Tunable Permeability of Cross-Linked Microcapsules from pH-Responsive Amphiphilic Diblock Copolymers: A Dissipative Particle Dynamics Study. Langmuir, 2017, 33, 7288-7297.	1.6	29
50	Structural analysis of human glycoprotein butyrylcholinesterase using atomistic molecular dynamics: The importance of glycosylation site ASN241. PLoS ONE, 2017, 12, e0187994.	1.1	15
51	Reactive Molecular Dynamics Simulations of the Silanization of Silica Substrates by Methoxysilanes and Hydroxysilanes. Langmuir, 2016, 32, 7045-7055.	1.6	8
52	A quantum chemistry study of curvature effects on boron nitride nanotubes/nanosheets for gas adsorption. Physical Chemistry Chemical Physics, 2016, 18, 19944-19949.	1.3	19
53	Applications: general discussion. Faraday Discussions, 2016, 191, 565-595.	1.6	0
54	Understanding the Interaction of Pluronics L61 and L64 with a DOPC Lipid Bilayer: An Atomistic Molecular Dynamics Study. Langmuir, 2016, 32, 10026-10033.	1.6	17

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55	Particles at interfaces: general discussion. Faraday Discussions, 2016, 191, 407-434.	1.6	1
56	Response to Extreme Temperatures of Mesoporous Silica MCM-41: Porous Structure Transformation Simulation and Modification of Gas Adsorption Properties. Langmuir, 2016, 32, 11422-11431.	1.6	13
57	The raspberry model for protein-like particles: Ellipsoids and confinement in cylindrical pores. European Physical Journal: Special Topics, 2016, 225, 1643-1662.	1.2	9
58	The Mechanisms for Preferential Attachment of Nanoparticles in Liquid Determined Using Liquid Cell Electron Microscopy, Machine Learning, and Molecular Dynamics. Microscopy and Microanalysis, 2016, 22, 812-813.	0.2	1
59	Understanding the Role of Solvation Forces on the Preferential Attachment of Nanoparticles in Liquid. ACS Nano, 2016, 10, 181-187.	7.3	51
60	Direct Phase Equilibrium Simulations of NIPAM Oligomers in Water. Journal of Physical Chemistry B, 2016, 120, 3434-3440.	1.2	42
61	Molecular modeling of lipid probes and their influence on the membrane. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2353-2361.	1.4	26
62	Molecular simulation of adsorption and separation of pure noble gases and noble gas mixtures on single wall carbon nanotubes. Computational Materials Science, 2016, 114, 160-166.	1.4	23
63	Refinement of a coarse-grained model of poly(2,6-dimethyl-1,4-phenylene ether) and its application to blends of PPE and PS. Molecular Simulation, 2016, 42, 312-320.	0.9	3
64	Molecular dynamics simulations on the interaction of the transmembrane NavAb channel with cholesterol and lipids in the membrane. Journal of Biomolecular Structure and Dynamics, 2016, 34, 318-326.	2.0	5
65	Molecular dynamics of different polymer blends containing poly(2,6-dimethyl-1,4-phenylene ether). Physical Chemistry Chemical Physics, 2015, 17, 4714-4723.	1.3	8
66	Reactive modeling of the initial stages of alkoxysilane polycondensation: effects of precursor molecule structure and solution composition. Soft Matter, 2015, 11, 6780-6789.	1.2	19
67	Multiscale molecular modeling of tertiary supported lipid bilayers. Proceedings of SPIE, 2015, , .	0.8	0
68	Design Principles for Nanoparticles Enveloped by a Polymer-Tethered Lipid Membrane. ACS Nano, 2015, 9, 9942-9954.	7.3	22
69	Reactive Molecular Dynamics Simulations of Siliceous Solids Polycondensed from Tetra- and Trihydroxysilane. Journal of Non-Crystalline Solids, 2015, 429, 183-189.	1.5	10
70	Molecular Dynamics Study of the Local Structure of Photovoltaic Polymer PCDTBT. Journal of Chemical & Engineering Data, 2014, 59, 2982-2986.	1.0	4
71	Parallel Optimization of a Reactive Force Field for Polycondensation of Alkoxysilanes. Journal of Physical Chemistry B, 2014, 118, 10966-10978.	1.2	37
72	Modeling of Polystyrene under Confinement: Exploring the Limits of Iterative Boltzmann Inversion. Macromolecules, 2013, 46, 7957-7976.	2.2	23

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73	Molecular dynamics simulation of dipalmitoylphosphatidylcholine modified with a MTSL nitroxide spin label in a lipid membrane. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2770-2777.	1.4	8
74	Normal and shear interactions between high grafting density polymer brushes grown by atom transfer radical polymerization. Soft Matter, 2013, 9, 5753.	1.2	21
75	Molecular transport of proteins through nanoporous membranes fabricated by interferometric lithography. Physical Chemistry Chemical Physics, 2013, 15, 965-971.	1.3	13
76	Simulating realistic imaging conditions for in situ liquid microscopy. Ultramicroscopy, 2013, 135, 36-42.	0.8	20
77	Compression of High Grafting Density Opposing Polymer Brushes Using Molecular Dynamics Simulations in Explicit Solvent. Journal of Physical Chemistry B, 2013, 117, 4134-4141.	1.2	10
78	Conformational, Dynamical. and Tensional Study of Tethered Bilayer Lipid Membranes in Coarse-Grained Molecular Simulations. Langmuir, 2012, 28, 15907-15915.	1.6	23
79	Simulations of PEGylated and Tethered Lipid Bilayers. Biophysical Journal, 2012, 102, 503a.	0.2	0
80	Mesoscale simulations of biomolecular transport through nanofilters with tapered and cylindrical geometries. Physical Chemistry Chemical Physics, 2012, 14, 15066.	1.3	6
81	Molecular Dynamics Study of a MARTINI Coarse-Grained Polystyrene Brush in Good Solvent: Structure and Dynamics. Macromolecules, 2012, 45, 563-571.	2.2	30
82	Pressure and Surface Tension Control Self-Assembled Structures in Mixtures of Pegylated and Non-Pegylated Lipids. Langmuir, 2012, 28, 2275-2280.	1.6	17
83	Role of Unsaturated Lipid and Ergosterol in Ethanol Tolerance of Model Yeast Biomembranes. Biophysical Journal, 2012, 102, 507-516.	0.2	115
84	A Molecular Dynamics Technique to Extract Forces in Soft Matter Systems Under Compression With Constant Solvent Chemical Potential. Journal of Chemical Theory and Computation, 2012, 8, 1072-1077.	2.3	7
85	Coarse-Grained Modeling of Polystyrene in Various Environments by Iterative Boltzmann Inversion. Macromolecules, 2012, 45, 9205-9219.	2.2	72
86	Multi-Scale Modeling of Bulk Heterojunctions for Organic Photovoltaic Applications. , 2012, , .		2
87	Structural properties of polystyrene oligomers in different environments: a molecular dynamics study. Physical Chemistry Chemical Physics, 2011, 13, 18107.	1.3	3
88	Lipid Domain Depletion at Small Localized Bends Imposed by a Step Geometry. Langmuir, 2011, 27, 2783-2788.	1.6	17
89	Crystalline, Ordered and Disordered Lipid Membranes: Convergence of Stress Profiles due to Ergosterol. Journal of the American Chemical Society, 2011, 133, 3720-3723.	6.6	17
90	Bilayer Structure and Lipid Dynamics in a Model Stratum Corneum with Oleic Acid. Journal of Physical Chemistry B, 2011, 115, 3164-3171.	1.2	64

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91	Computational Modeling of Curvature Effects in Supported Lipid Bilayers. Current Nanoscience, 2011, 7, 716-720.	0.7	12
92	The Impact of Texas Red on Lipid Bilayer Properties. Journal of Physical Chemistry B, 2011, 115, 8500-8505.	1.2	58
93	Characterization of polymerâ€“fullerene mixtures for organic photovoltaics by systematically coarse-grained molecular simulations. Fluid Phase Equilibria, 2011, 302, 21-25.	1.4	51
94	A comparative MD study of the local structure of polymer semiconductors P3HT and PBTTT. Physical Chemistry Chemical Physics, 2010, 12, 14735.	1.3	69
95	Folding and unfolding characteristics of short beta strand peptides under different environmental conditions and starting configurations. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2010, 1804, 2003-2015.	1.1	6
96	Molecular Simulation Study of the Structure of High Density Polymer Brushes in Good Solvent. Macromolecules, 2010, 43, 9131-9138.	2.2	47
97	Coarse-Grained Computer Simulations of Polymer/Fullerene Bulk Heterojunctions for Organic Photovoltaic Applications. Journal of Chemical Theory and Computation, 2010, 6, 526-537.	2.3	166
98	Membrane Curvature Modeling and Lipid Organization in Supported Lipid Bilayers. Biophysical Journal, 2010, 98, 78a-79a.	0.2	0
99	Molecular Modeling of Biomembranes: A How-to Approach. , 2010, , 35-58.		2
100	What Is the Difference Between a Supported and a Free Bilayer? Insights from Molecular Modeling on Different Scales. Behavior Research Methods, 2010, 11, 127-157.	2.3	2
101	Influence of Ethanol on Lipid/Sterol Membranes: Phase Diagram Construction from AFM Imaging. Langmuir, 2010, 26, 10415-10418.	1.6	32
102	Silica xerogel/aerogel-supported lipid bilayers: Consequences of surface corrugation. Biochimica Et Biophysica Acta - Biomembranes, 2010, 1798, 719-729.	1.4	26
103	Structure and Phase Behavior of Cholesterol Containing Membranes in the Presence of Ethanol. Biophysical Journal, 2010, 98, 491a.	0.2	0
104	What is the Difference Between a Supported and a Free Lipid Bilayer?. Biophysical Journal, 2010, 98, 283a.	0.2	0
105	Coarse-grained modeling of lipids. Chemistry and Physics of Lipids, 2009, 159, 59-66.	1.5	83
106	Density imbalances and free energy of lipid transfer in supported lipid bilayers. Journal of Chemical Physics, 2009, 131, 175104.	1.2	32
107	Structural Determination of High Density, ATRP Grown Polystyrene Brushes by Neutron Reflectivity. Macromolecules, 2009, 42, 9523-9527.	2.2	26
108	Using Ergosterol To Mitigate the Deleterious Effects of Ethanol on Bilayer Structure. Journal of Physical Chemistry B, 2009, 113, 2388-2397.	1.2	35

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109	Computational Studies of Texas Redâ^'1,2-Dihexadecanoyl-sn-glycero-3-phosphoethanolamineâ€"Model Building and Applications. Journal of Physical Chemistry B, 2009, 113, 8758-8766.	1.2	30
110	Water Replacement Hypothesis in Atomic Detailâ€"Factors Determining the Structure of Dehydrated Bilayer Stacks. Biophysical Journal, 2009, 97, 490-499.	0.2	56
111	Multiscale Modeling of Supported Lipid Bilayers. , 2009, , 101-120.		4
112	Asymmetric nature of lateral pressure profiles in supported lipid membranes and its implications for membrane protein functions. Soft Matter, 2009, 5, 3258.	1.2	32
113	Confined polymer systems: synergies between simulations and neutron scattering experiments. Soft Matter, 2009, 5, 4612.	1.2	20
114	Coarse-grained simulations of supported and unsupported lipid monolayers. Soft Matter, 2009, 5, 4526.	1.2	20
115	Multiscale Modeling of supported bilayers. Biophysical Journal, 2009, 96, 607a.	0.2	0
116	Examining the Contributions of Lipid Shape and Headgroup Charge on Bilayer Behavior. Biophysical Journal, 2008, 95, 2636-2646.	0.2	121
117	Behavioral Differences between Phosphatidic Acid and Phosphatidylcholine in the Presence of the Nicotinic Acetylcholine Receptor. Biophysical Journal, 2008, 95, 5637-5647.	0.2	10
118	Drying and Rehydration of DLPC/DSPC Symmetric and Asymmetric Supported Lipid Bilayers: a Combined AFM and Fluorescence Microscopy Study. Langmuir, 2008, 24, 10371-10381.	1.6	22
119	Characterization of domain instabilities in lipid bilayers by Karhunenâ€"Loeve analysis. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 1154-1180.	1.4	1
120	Coarse-grained modeling of interactions of lipid bilayers with supports. Journal of Chemical Physics, 2008, 129, 175102.	1.2	36
121	Interactions of Lipid Bilayers with Supports: A Coarse-Grained Molecular Simulation Study. Journal of Physical Chemistry B, 2008, 112, 7086-7094.	1.2	90
122	Comparing the density of states of binary Lennard-Jones glasses in bulk and film. Journal of Chemical Physics, 2008, 128, 124509.	1.2	8
123	Coarse Grained Simulation of Lipid Membrane and Triblock Copolymers. AIP Conference Proceedings, 2008, , .	0.3	2
124	Density of States Simulations of Various Glass Formers. AIP Conference Proceedings, 2008, , .	0.3	0
125	State-Point Dependence and Transferability of Potentials in Systematic Structural Coarse-Graining. , 2008, , 69-82.		0
126	State point dependence of systematically coarseâ€"grained potentials. Molecular Simulation, 2007, 33, 759-767.	0.9	60

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127	Phase separation in polyisoprene/polystyrene blends by a systematically coarse-grained model. Journal of Chemical Physics, 2007, 126, 144908.	1.2	28
128	Coarse-Grain Modeling of Polymers. Reviews in Computational Chemistry, 2007, , 233-262.	1.5	8
129	Phase behavior and dynamic heterogeneities in lipids: A coarse-grained simulation study of DPPCâ€“DPPE mixtures. Biochimica Et Biophysica Acta - Biomembranes, 2007, 1768, 620-627.	1.4	15
130	Coarse-grained simulations of ABA amphiphilic triblock copolymer solutions in thin films. Physical Chemistry Chemical Physics, 2007, 9, 4662.	1.3	34
131	Phase and Mixing Behavior in Two-Component Lipid Bilayers:â€‰ A Molecular Dynamics Study in DLPC/DSPC Mixtures. Journal of Physical Chemistry B, 2007, 111, 9504-9512.	1.2	22
132	Molecular-Scale Structure in Fluidâˆ’Gel Patterned Bilayers:â€‰ Stability of Interfaces and Transmembrane Distribution. Langmuir, 2007, 23, 12465-12468.	1.6	20
133	How Alcohol Chain-Length and Concentration Modulate Hydrogen Bond Formation in a Lipid Bilayer. Biophysical Journal, 2007, 92, 2366-2376.	0.2	87
134	Simulations of biomembranes and water: Important technical aspects. Fluid Phase Equilibria, 2007, 261, 18-25.	1.4	25
135	Multiscale modeling of polystyrene in various environments. Fluid Phase Equilibria, 2007, 261, 35-40.	1.4	13
136	Simulations of glasses: multiscale modeling and density of states Monte-Carlo simulations. Molecular Simulation, 2006, 32, 175-184.	0.9	9
137	Under the Influence of Alcohol: The Effect of Ethanol and Methanol on Lipid Bilayers. Biophysical Journal, 2006, 90, 1121-1135.	0.2	321
138	Systematic Coarse-Graining of a Polymer Blend:Â Polyisoprene and Polystyrene. Journal of Chemical Theory and Computation, 2006, 2, 607-615.	2.3	64
139	Crossover from Unentangled to Entangled Dynamics in a Systematically Coarse-Grained Polystyrene Melt. Macromolecules, 2006, 39, 812-820.	2.2	81
140	Karhunen-Loeve analysis for pattern description in phase separated lipid bilayer systems. Journal of Chemical Physics, 2006, 124, 234906.	1.2	5
141	Structural effects of small molecules on phospholipid bilayers investigated by molecular simulations. Fluid Phase Equilibria, 2005, 228-229, 135-140.	1.4	20
142	Systematic coarse-graining of atomistic models for simulation of polymeric systems. Computers and Chemical Engineering, 2005, 29, 2380-2385.	2.0	75
143	Investigating interactions of biomembranes and alcohols: A multiscale approach. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 1025-1032.	2.4	27
144	Molecular Dynamics of a Polymer in Mixed Solvent:Â Atactic Polystyrene in a Mixture of Cyclohexane andN,N-Dimethylformamide. Journal of Physical Chemistry B, 2005, 109, 15714-15723.	1.2	18

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145	Simulation of the effects of chain architecture on the sorption of ethylene in polyethylene. Journal of Chemical Physics, 2004, 120, 11304-11315.	1.2	42
146	Automatic coarse graining of polymers. Polymer, 2004, 45, 3869-3876.	1.8	105
147	Structural effects of small molecules on phospholipid bilayers investigated by molecular simulations. Fluid Phase Equilibria, 2004, 225, 63-68.	1.4	39
148	Correlation of Static and Dynamic Inhomogeneities in Polymer Mixtures:Â A Computer Simulation of Polyisoprene and Polystyrene. Macromolecules, 2004, 37, 1095-1101.	2.2	33
149	Simulation of Domain Formation in DLPCâ^'DSPC Mixed Bilayers. Langmuir, 2004, 20, 7686-7693.	1.6	102
150	Properties of Poly(isoprene):Â Model Building in the Melt and in Solution. Macromolecules, 2003, 36, 5406-5414.	2.2	64
151	Molecular Simulation Study of Phospholipid Bilayers and Insights of the Interactions with Disaccharides. Biophysical Journal, 2003, 85, 2830-2844.	0.2	200
152	Modeling the Binding of Cholera Toxin to a Lipid Membrane by a Nonâ€additive Twoâ€Dimensional Hardâ€Disk Model. Soft Materials, 2003, 1, 343-352.	0.8	12
153	Density of states of a binary Lennard-Jones glass. Journal of Chemical Physics, 2003, 119, 4405-4408.	1.2	55
154	Potential of mean force between a spherical particle suspended in a nematic liquid crystal and a substrate. Journal of Chemical Physics, 2002, 117, 7781-7787.	1.2	89
155	Density-of-states Monte Carlo method for simulation of fluids. Journal of Chemical Physics, 2002, 116, 8745-8749.	1.2	159
156	Multicanonical parallel tempering. Journal of Chemical Physics, 2002, 116, 5419-5423.	1.2	82
157	Constant pressure hybrid Molecular Dynamicsâ€"Monte Carlo simulations. Journal of Chemical Physics, 2002, 116, 55.	1.2	70
158	Structure and mobility of cyclohexane as a solvent for trans-polyisoprene. Physical Chemistry Chemical Physics, 2002, 4, 2269-2272.	1.3	8
159	Modeling of poly(isoprene) melts on different scales. Polymer, 2002, 43, 621-628.	1.8	36
160	Local Structure and Dynamics oftrans-Polyisoprene Oligomers. Macromolecules, 2001, 34, 1436-1448.	2.2	45
161	Chain Stiffness Intensifies the Reptation Characteristics of Polymer Dynamics in the Melt. ChemPhysChem, 2001, 2, 180-184.	1.0	49
162	Molecular Simulation in Polymer Science: Understanding Experiments Better. Progress of Theoretical Physics Supplement, 2000, 138, 311-319.	0.2	11

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163	Local Reorientation Dynamics of Semiflexible Polymers in the Melt. Macromolecules, 2000, 33, 6602-6610.	2.2	74
164	Coarse graining of nonbonded inter-particle potentials using automatic simplex optimization to fit structural properties. Journal of Chemical Physics, 2000, 113, 6264-6275.	1.2	111
165	ORIENTATION CORRELATION IN SIMPLIFIED MODELS OF POLYMER MELTS. International Journal of Modern Physics C, 1999, 10, 355-360.	0.8	9
166	Automatic parameterization of force fields for liquids by simplex optimization. Journal of Computational Chemistry, 1999, 20, 1009-1017.	1.5	118
167	Local chain ordering in amorphous polymer melts: influence of chain stiffness. Physical Chemistry Chemical Physics, 1999, 1, 2071-2076.	1.3	63
168	Molecular Mobility in Cyclic Hydrocarbons:Â A Simulation Study. Journal of Physical Chemistry B, 1999, 103, 9731-9737.	1.2	21
169	Phase chaos in the anisotropic complex Ginzburg-Landau equation. Physical Review E, 1998, 57, R6249-R6252.	0.8	14
170	Multiscale modeling shows differences between supported and free biomembranes. SPIE Newsroom, 0, , .	0.1	0
171	Development of a ReaxFF Force Field for Aqueous Phosphoenolpyruvate as a Novel Biomimetic Carbon Capture Absorbent. Journal of Physical Chemistry C, 0, , .	1.5	2
172	Production of novel SARSâ€CoVâ€2 Spike truncations in Chinese hamster ovary cells leads to high expression and binding to antibodies. Biotechnology Journal, 0, , 2100678.	1.8	2