

Pengyu Ren

List of Publications by Year in descending order

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142
papers

12,479
citations

41344

49
h-index

25787

108
g-index

175
all docs

175
docs citations

175
times ranked

9862
citing authors

#	ARTICLE	IF	CITATIONS
1	High-Order Ab Initio Valence Force Field with Chemical Pattern-Based Parameter Assignment. Journal of Computational Biophysics and Chemistry, 2022, 21, 431-447.	1.7	2
2	Recent progress in general force fields of small molecules. Current Opinion in Structural Biology, 2022, 72, 187-193.	5.7	15
3	Computationally driven discovery of SARS-CoV-2 M ^{pro} inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	7.4	21
4	Trapping Ca ⁺ inside a Molecular Cavity: Computational study of the potential energy surfaces for Ca ⁺ -[n]cycloparaphenylene, n=5-12. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
5	Atomic Polarizabilities for Interactive Dipole Induction Models. Journal of Chemical Information and Modeling, 2022, 62, 79-87.	5.4	8
6	Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 3607-3621.	5.3	12
7	Automation of AMOEBA polarizable force field for small molecules: Poltype 2. Journal of Computational Chemistry, 2022, 43, 1530-1542.	3.3	18
8	Molecular dynamics free energy simulations of ATP:Mg ²⁺ and ADP:Mg ²⁺ using the polarisable force field AMOEBA. Molecular Simulation, 2021, 47, 439-448.	2.0	8
9	Thermodynamics of ion binding and occupancy in potassium channels. Chemical Science, 2021, 12, 8920-8930.	7.4	25
10	High-resolution mining of the SARS-CoV-2 main protease conformational space: supercomputer-driven unsupervised adaptive sampling. Chemical Science, 2021, 12, 4889-4907.	7.4	31
11	Design of intrinsically disordered proteins that undergo phase transitions with lower critical solution temperatures. APL Materials, 2021, 9, .	5.1	29
12	Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields Using GPUs and Multi-GPU Systems. Journal of Chemical Theory and Computation, 2021, 17, 2034-2053.	5.3	40
13	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. Journal of Chemical Theory and Computation, 2021, 17, 2323-2341.	5.3	10
14	Advanced Electrostatic Model for Monovalent Ions Based on Ab Initio Energy Decomposition. Journal of Chemical Information and Modeling, 2021, 61, 2806-2817.	5.4	7
15	Interfacial Water Many-Body Effects Drive Structural Dynamics and Allosteric Interactions in SARS-CoV-2 Main Protease Dimerization Interface. Journal of Physical Chemistry Letters, 2021, 12, 6218-6226.	4.6	13
16	E2EDNA: Simulation Protocol for DNA Aptamers with Ligands. Journal of Chemical Information and Modeling, 2021, 61, 4139-4144.	5.4	8
17	Imaging sub-diffuse optical properties of cancerous and normal skin tissue using machine learning-aided spatial frequency domain imaging. Journal of Biomedical Optics, 2021, 26, .	2.6	8
18	Implementation of Geometry-Dependent Charge Flux into the Polarizable AMOEBA+ Potential. Journal of Physical Chemistry Letters, 2020, 11, 419-426.	4.6	43

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19	Accurate description of molecular dipole surface with charge flux implemented for molecular mechanics. Journal of Chemical Physics, 2020, 153, .	3.0	6
20	Reconciling NMR Structures of the HIV-1 Nucleocapsid Protein NCp7 Using Extensive Polarizable Force Field Free-Energy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 2013-2020.	5.3	4
21	Three- and five-site fixed-charge water models compatible with AMOEBA force field. Journal of Computational Chemistry, 2020, 41, 1034-1044.	3.3	3
22	Self-assembled nucleo-tripeptide hydrogels provide local and sustained doxorubicin release. Biomaterials Science, 2020, 8, 3130-3137.	5.4	19
23	Virial-based Berendsen barostat on GPUs using AMOEBA in Tinker-OpenMM. Results in Chemistry, 2019, 1, 100004.	2.0	5
24	Measuring DNA Hybridization Kinetics in Live Cells Using a Time-Resolved 3D Single-Molecule Tracking Method. Journal of the American Chemical Society, 2019, 141, 15747-15750.	13.7	15
25	Molecular Dynamics Study of the Hybridization between RNA and Modified Oligonucleotides. Journal of Chemical Theory and Computation, 2019, 15, 6422-6432.	5.3	17
26	Computational and Experimental Studies of Inhibitor Design for Aldolase A. Journal of Physical Chemistry B, 2019, 123, 6034-6041.	2.6	9
27	AMOEBA+ Classical Potential for Modeling Molecular Interactions. Journal of Chemical Theory and Computation, 2019, 15, 4122-4139.	5.3	89
28	Computational insights into the binding of IN17 inhibitors to MELK. Journal of Molecular Modeling, 2019, 25, 151.	1.8	5
29	Design and Characterization of Nucleopeptides for Hydrogel Self-Assembly. ACS Applied Bio Materials, 2019, 2, 2812-2821.	4.6	28
30	Polarizable Force Fields for Biomolecular Simulations: Recent Advances and Applications. Annual Review of Biophysics, 2019, 48, 371-394.	10.0	253
31	Helical antimicrobial peptides assemble into protofibril scaffolds that present ordered dsDNA to TLR9. Nature Communications, 2019, 10, 1012.	12.8	53
32	Modulating multi-functional ERK complexes by covalent targeting of a recruitment site in vivo. Nature Communications, 2019, 10, 5232.	12.8	17
33	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	8
34	Distinct Mechanisms of Nuclease-Directed DNA-Structure-Induced Genetic Instability in Cancer Genomes. Cell Reports, 2018, 22, 1200-1210.	6.4	36
35	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. Journal of Chemical Theory and Computation, 2018, 14, 2084-2108.	5.3	178
36	Investigating the Association Mechanism between Rafoxanide and Povidone. Langmuir, 2018, 34, 13971-13978.	3.5	9

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37	Tinker 8: Software Tools for Molecular Design. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5273-5289.	5.3	403
38	A physically grounded damped dispersion model with particle mesh Ewald summation. <i>Journal of Chemical Physics</i> , 2018, 149, 084115.	3.0	18
39	Elucidating the Phosphate Binding Mode of Phosphate-Binding Protein: The Critical Effect of Buffer Solution. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6371-6376.	2.6	20
40	Many-body effect determines the selectivity for Ca ²⁺ and Mg ²⁺ in proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E7495-E7501.	7.1	73
41	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. <i>Chemical Science</i> , 2018, 9, 956-972.	7.4	190
42	Capturing RNA Folding Free Energy with Coarse-Grained Molecular Dynamics Simulations. <i>Scientific Reports</i> , 2017, 7, 45812.	3.3	42
43	Capturing Many-Body Interactions with Classical Dipole Induction Models. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2751-2761.	5.3	26
44	LNA Thymidine Monomer Enables Differentiation of the Four Single-Nucleotide Variants by Melting Temperature. <i>Journal of the American Chemical Society</i> , 2017, 139, 7110-7116.	13.7	14
45	Tinker-OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. <i>Journal of Computational Chemistry</i> , 2017, 38, 2047-2055.	3.3	89
46	Discovery of a potent inhibitor of MELK that inhibits expression of the anti-apoptotic protein Mcl-1 and TNBC cell growth. <i>Bioorganic and Medicinal Chemistry</i> , 2017, 25, 2609-2616.	3.0	26
47	Polarizable Multipole-Based Force Field for Aromatic Molecules and Nucleobases. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 666-678.	5.3	36
48	Study of interactions between metal ions and protein model compounds by energy decomposition analyses and the AMOEBA force field. <i>Journal of Chemical Physics</i> , 2017, 147, 161733.	3.0	48
49	Accurate immune repertoire sequencing reveals malaria infection driven antibody lineage diversification in young children. <i>Nature Communications</i> , 2017, 8, 531.	12.8	41
50	Biocompatible and blood- brain barrier permeable carbon dots for inhibition of A β 2 fibrillation and toxicity, and BACE1 activity. <i>Nanoscale</i> , 2017, 9, 12862-12866.	5.6	64
51	Estimating and modeling charge transfer from the SAPT induction energy. <i>Journal of Computational Chemistry</i> , 2017, 38, 2222-2231.	3.3	21
52	Ionic Solution: What Goes Right and Wrong with Continuum Solvation Modeling. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11169-11179.	2.6	9
53	An optimized charge penetration model for use with the AMOEBA force field. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 276-291.	2.8	65
54	Truncated Conjugate Gradient: An Optimal Strategy for the Analytical Evaluation of the Many-Body Polarization Energy and Forces in Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 180-190.	5.3	34

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55	Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30261-30269.	2.8	44
56	General van der Waals potential for common organic molecules. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 4911-4919.	3.0	30
57	Calculating protein-ligand binding affinities with MMPBSA: Method and error analysis. <i>Journal of Computational Chemistry</i> , 2016, 37, 2436-2446.	3.3	169
58	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles. <i>Journal of Computational Chemistry</i> , 2016, 37, 494-506.	3.3	26
59	The impact of physiological crowding on the diffusivity of membrane bound proteins. <i>Soft Matter</i> , 2016, 12, 2127-2134.	2.7	35
60	Using docking and alchemical free energy approach to determine the binding mechanism of eEF2K inhibitors and prioritizing the compound synthesis. <i>Frontiers in Molecular Biosciences</i> , 2015, 2, 9.	3.5	15
61	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2609-2618.	5.3	93
62	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 623-634.	5.3	45
63	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II. Toward Massively Parallel Computations Using Smooth Particle Mesh Ewald. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2589-2599.	5.3	53
64	Development of an AMOEBA water model using GEM distributed multipoles. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	20
65	United polarizable multipole water model for molecular mechanics simulation. <i>Journal of Chemical Physics</i> , 2015, 143, 014504.	3.0	36
66	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5326-5339.	5.3	26
67	Quantification of a Pharmacodynamic ERK End Point in Melanoma Cell Lysates: Toward Personalized Precision Medicine. <i>ACS Medicinal Chemistry Letters</i> , 2015, 6, 47-52.	2.8	14
68	The Molecular Mechanism of Eukaryotic Elongation Factor 2 Kinase Activation. <i>Journal of Biological Chemistry</i> , 2014, 289, 23901-23916.	3.4	32
69	Classical Electrostatics for Biomolecular Simulations. <i>Chemical Reviews</i> , 2014, 114, 779-814.	47.7	229
70	Hydration Free Energy from Orthogonal Space Random Walk and Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2792-2801.	5.3	13
71	Reversible Covalent Inhibition of eEF2K by Carbonitriles. <i>ChemBioChem</i> , 2014, 15, 2435-2442.	2.6	23
72	Hydration gibbs free energies of open and closed shell trivalent lanthanide and actinide cations from polarizable molecular dynamics. <i>Journal of Molecular Modeling</i> , 2014, 20, 2471.	1.8	35

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73	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: I. Toward Massively Parallel Direct Space Computations. Journal of Chemical Theory and Computation, 2014, 10, 1638-1651.	5.3	76
74	Synthesis and biological evaluation of pyrido[2,3-d]pyrimidine-2,4-dione derivatives as eEF-2K inhibitors. Bioorganic and Medicinal Chemistry, 2014, 22, 4910-4916.	3.0	55
75	Anisotropic Coarse-Grained Model for Proteins Based On Gay-Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2014, 10, 731-750.	5.3	44
76	Identification and Validation of Novel PERK Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 1467-1475.	5.4	12
77	β Sheets Not Required: Combined Experimental and Computational Studies of Self-Assembly and Gelation of the Ester-Containing Analogue of an Fmoc-Dipeptide Hydrogelator. Langmuir, 2014, 30, 5287-5296.	3.5	53
78	Modeling Organochlorine Compounds and the β -Hole Effect Using a Polarizable Multipole Force Field. Journal of Physical Chemistry B, 2014, 118, 6456-6465.	2.6	69
79	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	5.3	524
80	Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972.	2.6	279
81	Investigation of the Mechanism of Antimicrobial Lipopeptides using Coarse-Grained Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 602a.	0.5	0
82	Calculations of the Electric Fields in Liquid Solutions. Journal of Physical Chemistry B, 2013, 117, 16236-16248.	2.6	83
83	Multiscale modeling of RNA 3D structures. , 2013, , .		0
84	RNA 3D Structure Prediction by Using a Coarse-Grained Model and Experimental Data. Journal of Physical Chemistry B, 2013, 117, 3135-3144.	2.6	74
85	Elucidating binding modes of zuonin A enantiomers to JNK1 via in silico methods. Journal of Molecular Graphics and Modelling, 2013, 45, 38-44.	2.4	2
86	Large Domain Motions in Ago Protein Controlled by the Guide DNA-Strand Seed Region Determine the Ago-DNA-mRNA Complex Recognition Process. PLoS ONE, 2013, 8, e54620.	2.5	16
87	Prediction and Coarse-Grained Modeling of RNA Structures. , 2013, , 53-68.		4
88	Exploring the Relationship between Sequences, Structures, Dynamical Behaviors and Functions of New Type Protein Drugs: DARPinS. Current Pharmaceutical Design, 2013, 19, 2308-2317.	1.9	1
89	Role of Bivalent Cations in Structural Stabilities of New Drug Targets α -Vacciniarelated Kinases (VRK) from Molecular Dynamics Simulations. Current Pharmaceutical Design, 2013, 19, 2269-2281.	1.9	1
90	Abstract 4542: Towards the identification of PKR-like endoplasmic reticulum kinase (PERK) inhibitors.. , 2013, , .		0

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91	Computational Insights for the Discovery of Non-ATP Competitive Inhibitors of MAP Kinases. <i>Current Pharmaceutical Design</i> , 2012, 18, 1173-1185.	1.9	19
92	Biomolecular electrostatics and solvation: a computational perspective. <i>Quarterly Reviews of Biophysics</i> , 2012, 45, 427-491.	5.7	152
93	Manipulating JNK Signaling with (â ²⁺)-Zuonin A. <i>ACS Chemical Biology</i> , 2012, 7, 1873-1883.	3.4	20
94	Some insights into the binding mechanism of Aurora B kinase gained by molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2012, 18, 4591-4601.	1.8	4
95	From in Silico Discovery to Intracellular Activity: Targeting JNKâ€“Protein Interactions with Small Molecules. <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 721-725.	2.8	25
96	Probing the Effect of Conformational Constraint on Phosphorylated Ligand Binding to an SH2 Domain Using Polarizable Force Field Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1716-1727.	2.6	42
97	Experimental and Computational Studies Reveal an Alternative Supramolecular Structure for Fmoc-Dipeptide Self-Assembly. <i>Biomacromolecules</i> , 2012, 13, 3562-3571.	5.4	79
98	Pharmaceutical Applications of the Polarizable Amoeba Potential, Including Protein-Ligand Binding Affinity and Drug Solubility, using the Force Field X Software. <i>Biophysical Journal</i> , 2012, 102, 409a-410a.	0.5	0
99	Molecular dynamics simulations of Ago silencing complexes reveal a large repertoire of admissible â€“seed-lessâ€™ targets. <i>Scientific Reports</i> , 2012, 2, 569.	3.3	62
100	Modeling Structural Coordination and Ligand Binding in Zinc Proteins with a Polarizable Potential. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1314-1324.	5.3	100
101	A Review of Physics-Based Coarse-Grained Potentials for the Simulations of Protein Structure and Dynamics. <i>Annual Reports in Computational Chemistry</i> , 2012, 8, 129-148.	1.7	19
102	Automation of AMOEBA polarizable force field parameterization for small molecules. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1138.	1.4	134
103	The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1721-1736.	5.3	77
104	Toward accurate solvation dynamics of lanthanides and actinides in water using polarizable force fields: from gas-phase energetics to hydration free energies. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	62
105	Computational Insights for the Discovery of Non-ATP Competitive Inhibitors of MAP Kinases. <i>Current Drug Metabolism</i> , 2012, 18, 1173-1185.	1.2	1
106	Examining Docking Interactions on ERK2 with Modular Peptide Substrates. <i>Biochemistry</i> , 2011, 50, 9500-9510.	2.5	34
107	Solution NMR Insights into Docking Interactions Involving Inactive ERK2. <i>Biochemistry</i> , 2011, 50, 3660-3672.	2.5	39
108	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3143-3161.	5.3	385

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109	Understanding the Specificity of a Docking Interaction between JNK1 and the Scaffolding Protein JIP1. Journal of Physical Chemistry B, 2011, 115, 1491-1502.	2.6	34
110	Statistical Potentials for Hairpin and Internal Loops Improve the Accuracy of the Predicted RNA Structure. Journal of Molecular Biology, 2011, 413, 473-483.	4.2	17
111	Molecular Docking Simulations for Macromolecularly Imprinted Polymers. Industrial & Engineering Chemistry Research, 2011, 50, 13877-13884.	3.7	28
112	Virtual screening using molecular simulations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1940-1951.	2.6	171
113	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	3.3	69
114	Gay-Berne and electrostatic multipole based coarse-grain potential in implicit solvent. Journal of Chemical Physics, 2011, 135, 155104.	3.0	36
115	A Model of a MAPK-Substrate Complex in an Active Conformation: A Computational and Experimental Approach. PLoS ONE, 2011, 6, e18594.	2.5	20
116	Temperature-induced unfolding of epidermal growth factor (EGF): Insight from molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2010, 29, 2-12.	2.4	24
117	A combined molecular dynamics and experimental study of doped polypyrrole. Polymer, 2010, 51, 4985-4993.	3.8	36
118	Conformational preference of ChaK1 binding peptides: a molecular dynamics study. PMC Biophysics, 2010, 3, 2.	2.3	2
119	Phosphorylation of the Transcription Factor Ets-1 by ERK2: Rapid Dissociation of ADP and Phospho-Ets-1. Biochemistry, 2010, 49, 3619-3630.	2.5	26
120	Polarizable Molecular Dynamics Simulation of Zn(II) in Water Using the AMOEBA Force Field. Journal of Chemical Theory and Computation, 2010, 6, 2059-2070.	5.3	137
121	Coarse-Grained Model for Simulation of RNA Three-Dimensional Structures. Journal of Physical Chemistry B, 2010, 114, 13497-13506.	2.6	83
122	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	2.6	1,093
123	Trypsin-ligand binding free energy calculation with AMOEBA. , 2009, 2009, 2328-31.		9
124	Trypsin-ligand binding free energies from explicit and implicit solvent simulations with polarizable potential. Journal of Computational Chemistry, 2009, 30, 1701-1711.	3.3	96
125	Correlation of RNA Secondary Structure Statistics with Thermodynamic Stability and Applications to Folding. Journal of Molecular Biology, 2009, 391, 769-783.	4.2	23
126	Substrate specificity of human kallikreins 1 and 6 determined by phage display. Protein Science, 2008, 17, 664-672.	7.6	34

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127	A transferable coarse-grained model for hydrogen-bonding liquids. Physical Chemistry Chemical Physics, 2008, 10, 2050.	2.8	37
128	Calculation of protein-ligand binding free energy by using a polarizable potential. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6290-6295.	7.1	222
129	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. Journal of Chemical Physics, 2007, 126, 124114.	3.0	79
130	Molecular Modeling of Conformational Properties of Oligodepsipeptides. Biomacromolecules, 2007, 8, 3015-3024.	5.4	13
131	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. International Journal of Quantum Chemistry, 2007, 107, 1390-1395.	2.0	81
132	Simulation of Ca ²⁺ and Mg ²⁺ Solvation Using Polarizable Atomic Multipole Potential. Journal of Physical Chemistry B, 2006, 110, 18553-18559.	2.6	246
133	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. Journal of Chemical Physics, 2006, 125, 054511.	3.0	169
134	Generalized coarse-grained model based on point multipole and Gay-Berne potentials. Journal of Chemical Physics, 2006, 125, 064103.	3.0	86
135	Temperature and Pressure Dependence of the AMOEBA Water Model. Journal of Physical Chemistry B, 2004, 108, 13427-13437.	2.6	191
136	Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field. Journal of the American Chemical Society, 2003, 125, 15671-15682.	13.7	474
137	Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation. Journal of Physical Chemistry B, 2003, 107, 5933-5947.	2.6	1,270
138	Consistent treatment of inter- and intramolecular polarization in molecular mechanics calculations. Journal of Computational Chemistry, 2002, 23, 1497-1506.	3.3	545
139	The atomistic simulation of the gas permeability of poly(organophosphazenes). Part 1. Poly(dibutoxyphosphazenes). Computational and Theoretical Polymer Science, 2000, 10, 447-463.	1.1	60
140	Molecular simulation of the glass transition of polyphosphazenes. Computational and Theoretical Polymer Science, 1999, 9, 111-116.	1.1	55
141	The COMPASS force field: parameterization and validation for phosphazenes. Computational and Theoretical Polymer Science, 1998, 8, 229-246.	1.1	1,186
142	Hydration of divalent lanthanides, Sm ²⁺ and Eu ²⁺ : A molecular dynamics study with polarizable AMOEBA force field. Journal of Computational Chemistry, 0, , .	3.3	4