Pengyu Ren

List of Publications by Year
in descending order

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142 papers	12,479 citations	41258 49 h-index	25716 108 g-index
175 all docs	175 docs citations	175 times ranked	9862 citing authors

#	Article	IF	Citations
1	High-OrderAb InitioValence Force Field with Chemical Pattern-Based Parameter Assignment. Journal of Computational Biophysics and Chemistry, 2022, 21, 431-447.	1.0	2
2	Recent progress in general force fields of small molecules. Current Opinion in Structural Biology, 2022, 72, 187-193.	2.6	15
3	Computationally driven discovery of SARS-CoV-2 M^{pro}inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	3.7	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, , .	1.3	0
5	Atomic Polarizabilities for Interactive Dipole Induction Models. Journal of Chemical Information and Modeling, 2022, 62, 79-87.	2.5	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.	2.3	12
7	Automation of <scp>AMOEBA</scp> polarizable force field for small molecules: Poltype 2. Journal of Computational Chemistry, 2022, 43, 1530-1542.	1.5	18
8	Molecular dynamics free energy simulations of ATP:Mg²⁺ and ADP:Mg²⁺ using the polarisable force field AMOEBA. Molecular Simulation, 2021, 47, 439-448.	0.9	8
9	Thermodynamics of ion binding and occupancy in potassium channels. Chemical Science, 2021, 12, 8920-8930.	3.7	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.	3.7	31
11	Design of intrinsically disordered proteins that undergo phase transitions with lower critical solution temperatures. APL Materials, 2021, 9, .	2.2	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.	2.3	40
13	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. Journal of Chemical Theory and Computation, 2021, 17, 2323-2341.	2.3	10
14	Advanced Electrostatic Model for Monovalent Ions Based on Ab Initio Energy Decomposition. Journal of Chemical Information and Modeling, 2021, 61, 2806-2817.	2.5	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.	2.1	13
16	E2EDNA: Simulation Protocol for DNA Aptamers with Ligands. Journal of Chemical Information and Modeling, 2021, 61, 4139-4144.	2.5	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, .	1.4	8
18	Implementation of Geometry-Dependent Charge Flux into the Polarizable AMOEBA+ Potential. Journal of Physical Chemistry Letters, 2020, 11, 419-426.	2.1	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, .	1.2	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.	2.3	4
21	Threeâ€site and fiveâ€site fixedâ€charge water models compatible with AMOEBA force field. Journal of Computational Chemistry, 2020, 41, 1034-1044.	1.5	3
22	Self-assembled nucleo-tripeptide hydrogels provide local and sustained doxorubicin release. Biomaterials Science, 2020, 8, 3130-3137.	2.6	19
23	Virial-based Berendsen barostat on GPUs using AMOEBA in Tinker-OpenMM. Results in Chemistry, 2019, 1, 100004.	0.9	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.	6.6	15
25	Molecular Dynamics Study of the Hybridization between RNA and Modified Oligonucleotides. Journal of Chemical Theory and Computation, 2019, 15, 6422-6432.	2.3	17
26	Computational and Experimental Studies of Inhibitor Design for Aldolase A. Journal of Physical Chemistry B, 2019, 123, 6034-6041.	1.2	9
27	AMOEBA+ Classical Potential for Modeling Molecular Interactions. Journal of Chemical Theory and Computation, 2019, 15, 4122-4139.	2.3	89
28	Computational insights into the binding of IN17 inhibitors to MELK. Journal of Molecular Modeling, 2019, 25, 151.	0.8	5
29	Design and Characterization of Nucleopeptides for Hydrogel Self-Assembly. ACS Applied Bio Materials, 2019, 2, 2812-2821.	2.3	28
30	Polarizable Force Fields for Biomolecular Simulations: Recent Advances and Applications. Annual Review of Biophysics, 2019, 48, 371-394.	4.5	253
31	Helical antimicrobial peptides assemble into protofibril scaffolds that present ordered dsDNA to TLR9. Nature Communications, 2019, 10, 1012.	5.8	53
32	Modulating multi-functional ERK complexes by covalent targeting of a recruitment site in vivo. Nature Communications, 2019, 10, 5232.	5.8	17
33	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	8
34	Distinct Mechanisms of Nuclease-Directed DNA-Structure-Induced Genetic Instability in Cancer Genomes. Cell Reports, 2018, 22, 1200-1210.	2.9	36
35	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. Journal of Chemical Theory and Computation, 2018, 14, 2084-2108.	2.3	178
36	Investigating the Association Mechanism between Rafoxanide and Povidone. Langmuir, 2018, 34, 13971-13978.	1.6	9

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37	Tinker 8: Software Tools for Molecular Design. Journal of Chemical Theory and Computation, 2018, 14, 5273-5289.	2.3	403
38	A physically grounded damped dispersion model with particle mesh Ewald summation. Journal of Chemical Physics, 2018, 149, 084115.	1.2	18
39	Elucidating the Phosphate Binding Mode of Phosphate-Binding Protein: The Critical Effect of Buffer Solution. Journal of Physical Chemistry B, 2018, 122, 6371-6376.	1.2	20
40	Many-body effect determines the selectivity for Ca ²⁺ and Mg ²⁺ in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7495-E7501.	3.3	73
41	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. Chemical Science, 2018, 9, 956-972.	3.7	190
42	Capturing RNA Folding Free Energy with Coarse-Grained Molecular Dynamics Simulations. Scientific Reports, 2017, 7, 45812.	1.6	42
43	Capturing Many-Body Interactions with Classical Dipole Induction Models. Journal of Chemical Theory and Computation, 2017, 13, 2751-2761.	2.3	26
44	LNA Thymidine Monomer Enables Differentiation of the Four Single-Nucleotide Variants by Melting Temperature. Journal of the American Chemical Society, 2017, 139, 7110-7116.	6.6	14
45	Tinkerâ€OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. Journal of Computational Chemistry, 2017, 38, 2047-2055.	1.5	89
46	Discovery of a potent inhibitor of MELK that inhibits expression of the anti-apoptotic protein Mcl-1 and TNBC cell growth. Bioorganic and Medicinal Chemistry, 2017, 25, 2609-2616.	1.4	26
47	Polarizable Multipole-Based Force Field for Aromatic Molecules and Nucleobases. Journal of Chemical Theory and Computation, 2017, 13, 666-678.	2.3	36
48	Study of interactions between metal ions and protein model compounds by energy decomposition analyses and the AMOEBA force field. Journal of Chemical Physics, 2017, 147, 161733.	1.2	48
49	Accurate immune repertoire sequencing reveals malaria infection driven antibody lineage diversification in young children. Nature Communications, 2017, 8, 531.	5.8	41
50	Biocompatible and bloodâ€“brain barrier permeable carbon dots for inhibition of AÎ² fibrillation and toxicity, and BACE1 activity. Nanoscale, 2017, 9, 12862-12866.	2.8	64
51	Estimating and modeling charge transfer from the SAPT induction energy. Journal of Computational Chemistry, 2017, 38, 2222-2231.	1.5	21
52	Ionic Solution: What Goes Right and Wrong with Continuum Solvation Modeling. Journal of Physical Chemistry B, 2017, 121, 11169-11179.	1.2	9
53	An optimized charge penetration model for use with the AMOEBA force field. Physical Chemistry Chemical Physics, 2017, 19, 276-291.	1.3	65
54	Truncated Conjugate Gradient: An Optimal Strategy for the Analytical Evaluation of the Many-Body Polarization Energy and Forces in Molecular Simulations. Journal of Chemical Theory and Computation, 2017, 13, 180-190.	2.3	34

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55	Calculating binding free energies of hostâ€“guest systems using the AMOEBA polarizable force field. Physical Chemistry Chemical Physics, 2016, 18, 30261-30269.	1.3	44
56	General van der Waals potential for common organic molecules. Bioorganic and Medicinal Chemistry, 2016, 24, 4911-4919.	1.4	30
57	Calculating proteinâ€“ligand binding affinities with MMPBSA: Method and error analysis. Journal of Computational Chemistry, 2016, 37, 2436-2446.	1.5	169
58	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general shortâ€range penetration correction up to quadrupoles. Journal of Computational Chemistry, 2016, 37, 494-506.	1.5	26
59	The impact of physiological crowding on the diffusivity of membrane bound proteins. Soft Matter, 2016, 12, 2127-2134.	1.2	35
60	Using docking and alchemical free energy approach to determine the binding mechanism of eEF2K inhibitors and prioritizing the compound synthesis. Frontiers in Molecular Biosciences, 2015, 2, 9.	1.6	15
61	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. Journal of Chemical Theory and Computation, 2015, 11, 2609-2618.	2.3	93
62	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. Journal of Chemical Theory and Computation, 2015, 11, 623-634.	2.3	45
63	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II. Toward Massively Parallel Computations Using Smooth Particle Mesh Ewald. Journal of Chemical Theory and Computation, 2015, 11, 2589-2599.	2.3	53
64	Development of an AMOEBA water model using GEM distributed multipoles. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	20
65	United polarizable multipole water model for molecular mechanics simulation. Journal of Chemical Physics, 2015, 143, 014504.	1.2	36
66	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. Journal of Chemical Theory and Computation, 2015, 11, 5326-5339.	2.3	26
67	Quantification of a Pharmacodynamic ERK End Point in Melanoma Cell Lysates: Toward Personalized Precision Medicine. ACS Medicinal Chemistry Letters, 2015, 6, 47-52.	1.3	14
68	The Molecular Mechanism of Eukaryotic Elongation Factor 2 Kinase Activation. Journal of Biological Chemistry, 2014, 289, 23901-23916.	1.6	32
69	Classical Electrostatics for Biomolecular Simulations. Chemical Reviews, 2014, 114, 779-814.	23.0	229
70	Hydration Free Energy from Orthogonal Space Random Walk and Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2792-2801.	2.3	13
71	Reversible Covalent Inhibition of eEFâ€2K by Carbonitriles. ChemBioChem, 2014, 15, 2435-2442.	1.3	23
72	Hydration gibbs free energies of open and closed shell trivalent lanthanide and actinide cations from polarizable molecular dynamics. Journal of Molecular Modeling, 2014, 20, 2471.	0.8	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.	2.3	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.	1.4	55
75	Anisotropic Coarse-Grained Model for Proteins Based On Gayâ€“Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2014, 10, 731-750.	2.3	44
76	Identification and Validation of Novel PERK Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 1467-1475.	2.5	12
77	Î² 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.	1.6	53
78	Modeling Organochlorine Compounds and the Ïƒ-Hole Effect Using a Polarizable Multipole Force Field. Journal of Physical Chemistry B, 2014, 118, 6456-6465.	1.2	69
79	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	2.3	524
80	Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972.	1.2	279
81	Investigation of the Mechanism of Antimicrobial Lipopeptides using Coarse-Grained Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 602a.	0.2	0
82	Calculations of the Electric Fields in Liquid Solutions. Journal of Physical Chemistry B, 2013, 117, 16236-16248.	1.2	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.	1.2	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.	1.3	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.	1.1	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.	0.9	1
89	Role of Bivalent Cations in Structural Stabilities of New Drug Targets â€"â€"Vacciniarelated Kinases (VRK) from Molecular Dynamics Simulations. Current Pharmaceutical Design, 2013, 19, 2269-2281.	0.9	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. Current Pharmaceutical Design, 2012, 18, 1173-1185.	0.9	19
92	Biomolecular electrostatics and solvation: a computational perspective. Quarterly Reviews of Biophysics, 2012, 45, 427-491.	2.4	152
93	Manipulating JNK Signaling with (â˜)-Zuonin A. ACS Chemical Biology, 2012, 7, 1873-1883.	1.6	20
94	Some insights into the binding mechanism of Aurora B kinase gained by molecular dynamics simulation. Journal of Molecular Modeling, 2012, 18, 4591-4601.	0.8	4
95	From in Silico Discovery to Intracellular Activity: Targeting JNKâ€“Protein Interactions with Small Molecules. ACS Medicinal Chemistry Letters, 2012, 3, 721-725.	1.3	25
96	Probing the Effect of Conformational Constraint on Phosphorylated Ligand Binding to an SH2 Domain Using Polarizable Force Field Simulations. Journal of Physical Chemistry B, 2012, 116, 1716-1727.	1.2	42
97	Experimental and Computational Studies Reveal an Alternative Supramolecular Structure for Fmoc-Dipeptide Self-Assembly. Biomacromolecules, 2012, 13, 3562-3571.	2.6	79
98	Pharmaceutical Applications of the Polarizable Amoeba Potential, Including Protein-Ligand Binding Affinity and Drug Solubility, using the Force Field X Software. Biophysical Journal, 2012, 102, 409a-410a.	0.2	0
99	Molecular dynamics simulations of Ago silencing complexes reveal a large repertoire of admissible â€˜seed-lessâ€™ targets. Scientific Reports, 2012, 2, 569.	1.6	62
100	Modeling Structural Coordination and Ligand Binding in Zinc Proteins with a Polarizable Potential. Journal of Chemical Theory and Computation, 2012, 8, 1314-1324.	2.3	100
101	A Review of Physics-Based Coarse-Grained Potentials for theÂSimulations of Protein Structure and Dynamics. Annual Reports in Computational Chemistry, 2012, 8, 129-148.	0.9	19
102	Automation of AMOEBA polarizable force field parameterization for small molecules. Theoretical Chemistry Accounts, 2012, 131, 1138.	0.5	134
103	The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. Journal of Chemical Theory and Computation, 2012, 8, 1721-1736.	2.3	77
104	Toward accurate solvation dynamics of lanthanides and actinides in water using polarizable force fields: from gas-phase energetics to hydration free energies. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	62
105	Computational Insights for the Discovery of Non-ATP Competitive Inhibitors of MAP Kinases. Current Drug Metabolism, 2012, 18, 1173-1185.	0.7	1
106	Examining Docking Interactions on ERK2 with Modular Peptide Substrates. Biochemistry, 2011, 50, 9500-9510.	1.2	34
107	Solution NMR Insights into Docking Interactions Involving Inactive ERK2. Biochemistry, 2011, 50, 3660-3672.	1.2	39
108	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. Journal of Chemical Theory and Computation, 2011, 7, 3143-3161.	2.3	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.	1.2	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.	2.0	17
111	Molecular Docking Simulations for Macromolecularly Imprinted Polymers. Industrial & Engineering Chemistry Research, 2011, 50, 13877-13884.	1.8	28
112	Virtual screening using molecular simulations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1940-1951.	1.5	171
113	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	1.5	69
114	Gay-Berne and electrostatic multipole based coarse-grain potential in implicit solvent. Journal of Chemical Physics, 2011, 135, 155104.	1.2	36
115	A Model of a MAPKâ€¢Substrate Complex in an Active Conformation: A Computational and Experimental Approach. PLoS ONE, 2011, 6, e18594.	1.1	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.	1.3	24
117	A combined molecular dynamics and experimental study of doped polypyrrole. Polymer, 2010, 51, 4985-4993.	1.8	36
118	Conformational preference of ChaK1 binding peptides: a molecular dynamics study. PMC Biophysics, 2010, 3, 2.	2.2	2
119	Phosphorylation of the Transcription Factor Ets-1 by ERK2: Rapid Dissociation of ADP and Phospho-Ets-1. Biochemistry, 2010, 49, 3619-3630.	1.2	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.	2.3	137
121	Coarse-Grained Model for Simulation of RNA Three-Dimensional Structures. Journal of Physical Chemistry B, 2010, 114, 13497-13506.	1.2	83
122	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	1.2	1,093
123	Trypsin-ligand binding free energy calculation with AMOEBA. , 2009, 2009, 2328-31.		9
124	Trypsinâ€ligand binding free energies from explicit and implicit solvent simulations with polarizable potential. Journal of Computational Chemistry, 2009, 30, 1701-1711.	1.5	96
125	Correlation of RNA Secondary Structure Statistics with Thermodynamic Stability and Applications to Folding. Journal of Molecular Biology, 2009, 391, 769-783.	2.0	23
126	Substrate specificity of human kallikreins 1 and 6 determined by phage display. Protein Science, 2008, 17, 664-672.	3.1	34

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127	A transferable coarse-grained model for hydrogen-bonding liquids. Physical Chemistry Chemical Physics, 2008, 10, 2050.	1.3	37
128	Calculation of proteinâ€“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.	3.3	222
129	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. Journal of Chemical Physics, 2007, 126, 124114.	1.2	79
130	Molecular Modeling of Conformational Properties of Oligodepsipeptides. Biomacromolecules, 2007, 8, 3015-3024.	2.6	13
131	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. International Journal of Quantum Chemistry, 2007, 107, 1390-1395.	1.0	81
132	Simulation of Ca2+and Mg2+Solvation Using Polarizable Atomic Multipole Potential. Journal of Physical Chemistry B, 2006, 110, 18553-18559.	1.2	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.	1.2	169
134	Generalized coarse-grained model based on point multipole and Gay-Berne potentials. Journal of Chemical Physics, 2006, 125, 064103.	1.2	86
135	Temperature and Pressure Dependence of the AMOEBA Water Model. Journal of Physical Chemistry B, 2004, 108, 13427-13437.	1.2	191
136	Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field. Journal of the American Chemical Society, 2003, 125, 15671-15682.	6.6	474
137	Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation. Journal of Physical Chemistry B, 2003, 107, 5933-5947.	1.2	1,270
138	Consistent treatment of inter- and intramolecular polarization in molecular mechanics calculations. Journal of Computational Chemistry, 2002, 23, 1497-1506.	1.5	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 <scp>AMOEBA</scp> force field. Journal of Computational Chemistry, 0, , .	1.5	4