Teresa Head-Gordon

List of Publications by Citations

177 papers	11,859 citations	49 h-index	105 g-index
194 ext. papers	13,819 ext. citations	6.9 avg, IF	6.66 L-index

#	Paper	IF	Citations
177	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. *Journal of Chemical Physics*, **2004**, 120, 9665-78	3.9	1424
176	Current status of the AMOEBA polarizable force field. *Journal of Physical Chemistry B*, **2010**, 114, 2549-64	3.4	914
175	Analytic MP2 frequencies without fifth-order storage. Theory and application to bifurcated hydrogen bonds in the water hexamer. *Chemical Physics Letters*, **1994**, 220, 122-128	2.5	750
174	Improvements to the APBS biomolecular solvation software suite. *Protein Science*, **2018**, 27, 112-128	6.3	577
173	Water structure from scattering experiments and simulation. *Chemical Reviews*, **2002**, 102, 2651-70	68.1	435
172	What can x-ray scattering tell us about the radial distribution functions of water?. *Journal of Chemical Physics*, **2000**, 113, 9149-9161	3.9	351
171	Theoretical study of blocked glycine and alanine peptide analogs. *Journal of the American Chemical Society*, **1991**, 113, 5989-5997	16.4	329
170	A high-quality x-ray scattering experiment on liquid water at ambient conditions. *Journal of Chemical Physics*, **2000**, 113, 9140-9148	3.9	258
169	Systematic improvement of a classical molecular model of water. *Journal of Physical Chemistry B*, **2013**, 117, 9956-72	3.4	235
168	Tetrahedral structure or chains for liquid water. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 7973-7	11.5	201
167	The structure of ambient water. *Molecular Physics*, **2010**, 108, 1415-1433	1.7	183
166	Water structure as a function of temperature from X-ray scattering experiments and ab initio molecular dynamics. *Physical Chemistry Chemical Physics*, **2003**, 5, 1981	3.6	173
165	Representability problems for coarse-grained water potentials. *Journal of Chemical Physics*, **2007**, 126, 144509	3.9	172
164	Excitation energy transfer in condensed media. *Journal of Chemical Physics*, **2001**, 114, 3065-3072	3.9	166
163	Hydration dynamics near a model protein surface. *Biophysical Journal*, **2004**, 86, 1852-62	2.9	160
162	Toy model for protein folding. *Physical Review E*, **1993**, 48, 1469-1477	2.4	156
161	Small-angle scattering and the structure of ambient liquid water. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 14003-7	11.5	153

160	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. *Journal of Physical Chemistry B*, **2015**, 119, 9423-9437	3.4	149
159	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. *Journal of Physical Chemistry B*, **2017**, 121, 4023-4039	3.4	147
158	Structure and dynamics of the Abeta(21-30) peptide from the interplay of NMR experiments and molecular simulations. *Journal of the American Chemical Society*, **2008**, 130, 6145-58	16.4	142
157	Optimizing Protein-Solvent Force Fields to Reproduce Intrinsic Conformational Preferences of Model Peptides. *Journal of Chemical Theory and Computation*, **2011**, 7, 1220-30	6.4	127
156	New developments in force fields for biomolecular simulations. *Current Opinion in Structural Biology*, **2018**, 49, 129-138	8.1	118
155	Optimizing solute-water van der Waals interactions to reproduce solvation free energies. *Journal of Physical Chemistry B*, **2012**, 116, 4524-34	3.4	116
154	Minimalist models for protein folding and design. *Current Opinion in Structural Biology*, **2003**, 13, 160-7	8.1	116
153	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
152	Differences in ß-strand populations of monomeric Aß40 and Aß42. *Biophysical Journal*, **2013**, 104, 2714-24	2.9	114
151	Homogeneous and heterogeneous tertiary structure ensembles of amyloid-ß peptides. *Biochemistry*, **2011**, 50, 7612-28	3.2	114
150	Molecular view of water dynamics near model peptides. *Journal of Physical Chemistry B*, **2005**, 109, 12966-75	3.4	114
149	Coarse-grained sequences for protein folding and design. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 10712-7	11.5	102
148	Finding Our Way in the Dark Proteome. *Journal of the American Chemical Society*, **2016**, 138, 9730-42	16.4	93
147	Computational optimization of electric fields for better catalysis design. *Nature Catalysis*, **2018**, 1, 649-655	36.5	93
146	Collective aspects of protein folding illustrated by a toy model. *Physical Review E*, **1995**, 52, 2872-2877	2.4	90
145	Determining the Role of Hydration Forces in Protein Folding. *Journal of Physical Chemistry B*, **1999**, 103, 5413-5426	3.4	86
144	Determining the critical nucleus and mechanism of fibril elongation of the Alzheimer's Abeta(1-40) peptide. *Journal of Molecular Biology*, **2007**, 365, 535-50	6.5	81
143	Computational Design of Synthetic Enzymes. *Chemical Reviews*, **2019**, 119, 6613-6630	68.1	79

142	Stabilization of Helixes in Glycine and Alanine Dipeptides in a Reaction Field Model of Solvent. *Journal of the American Chemical Society*, **1994**, 116, 1528-1532	16.4	76
141	Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 9811-32	3.4	66
140	Efficient derivation of cortical glutamatergic neurons from human pluripotent stem cells: a model system to study neurotoxicity in Alzheimer disease. *Neurobiology of Disease*, **2014**, 62, 62-72	7.5	65
139	Use of the rVV10 Nonlocal Correlation Functional in the B97M-V Density Functional: Defining B97M-rV and Related Functionals. *Journal of Physical Chemistry Letters*, **2017**, 8, 35-40	6.4	62
138	Assessing Ion-Water Interactions in the AMOEBA Force Field Using Energy Decomposition Analysis of Electronic Structure Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 5422-5437	6.4	62
137	molecular dynamics simulations of liquid water using high quality meta-GGA functionals. *Chemical Science*, **2017**, 8, 3554-3565	9.4	60
136	Experimental Inferential Structure Determination of Ensembles for Intrinsically Disordered Proteins. *Journal of the American Chemical Society*, **2016**, 138, 4530-8	16.4	52
135	The influence of protein dynamics on the success of computational enzyme design. *Journal of the American Chemical Society*, **2009**, 131, 14111-5	16.4	52
134	Hydration water dynamics near biological interfaces. *Journal of Physical Chemistry B*, **2009**, 113, 4082-92	3.4	51
133	Evidence for Anomalous Hydration Dynamics near a Model Hydrophobic Peptide *Journal of Physical Chemistry B*, **2004**, 108, 19885-19893	3.4	51
132	Advanced potential energy surfaces for condensed phase simulation. *Annual Review of Physical Chemistry*, **2014**, 65, 149-74	15.7	50
131	Protofibril assemblies of the arctic, Dutch, and Flemish mutants of the Alzheimer Abeta1-40 peptide. *Biophysical Journal*, **2008**, 94, 2007-16	2.9	50
130	Cool walking: a new Markov chain Monte Carlo sampling method. *Journal of Computational Chemistry*, **2003**, 24, 68-76	3.5	49
129	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. *Journal of Chemical Physics*, **2018**, 149, 180901	3.9	49
128	An efficient and stable hybrid extended Lagrangian/self-consistent field scheme for solving classical mutual induction. *Journal of Chemical Physics*, **2015**, 143, 174104	3.9	45
127	Effects of co-solvents on peptide hydration water structure and dynamics. *Physical Chemistry Chemical Physics*, **2010**, 12, 393-405	3.6	45
126	The Quest for Accurate Liquid Water Properties from First Principles. *Journal of Physical Chemistry Letters*, **2018**, 9, 5009-5016	6.4	44
125	Comparison of structure determination methods for intrinsically disordered amyloid- peptides. *Journal of Physical Chemistry B*, **2014**, 118, 6405-16	3.4	44

124	Solvation in modified water models: towards understanding hydrophobic effects. *Molecular Physics*, **2006**, 104, 3593-3605	1.7	44
123	Toward minimalist models of larger proteins: A ubiquitin-like protein. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 368-379	4.2	44
122	Matching simulation and experiment: a new simplified model for simulating protein folding. *Journal of Computational Biology*, **2000**, 7, 469-81	1.7	44
121	A coarse-grained alpha-carbon protein model with anisotropic hydrogen-bonding. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 626-38	4.2	43
120	Influence of denatured and intermediate states of folding on protein aggregation. *Protein Science*, **2005**, 14, 993-1003	6.3	42
119	Hydrophobic potential of mean force as a solvation function for protein structure prediction. *Structure*, **2007**, 15, 727-40	5.2	41
118	Intermediates and the folding of proteins L and G. *Protein Science*, **2004**, 13, 958-70	6.3	41
117	Conformational Ensembles of an Intrinsically Disordered Protein Consistent with NMR, SAXS, and Single-Molecule FRET. *Journal of the American Chemical Society*, **2020**, 142, 15697-15710	16.4	41
116	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. *Journal of Chemical Physics*, **2016**, 145, 124106	3.9	38
115	Computational Optimization of Electric Fields for Improving Catalysis of a Designed Kemp Eliminase. *ACS Catalysis*, **2018**, 8, 219-227	13.1	38
114	The Importance of the Scaffold for de Novo Enzymes: A Case Study with Kemp Eliminase. *Journal of the American Chemical Society*, **2017**, 139, 5793-5800	16.4	37
113	Aqueous peptides as experimental models for hydration water dynamics near protein surfaces. *Physical Chemistry Chemical Physics*, **2008**, 10, 4903-8	3.6	36
112	Perturbational view of inherent structures in water. *Physical Review E*, **1993**, 47, 2484-2490	2.4	36
111	Exploring the rich energy landscape of sulfate-water clusters SO4(2-) (H2O)(n=3-7): an electronic structure approach. *Journal of Physical Chemistry A*, **2011**, 115, 11438-54	2.8	35
110	Dielectric relaxation of aqueous solutions of hydrophilic versus amphiphilic peptides. *Journal of Physical Chemistry B*, **2008**, 112, 179-86	3.4	35
109	The role of electrostatics in the binding of small ligands to enzymes. *The Journal of Physical Chemistry*, **1987**, 91, 3342-3349		35
108	Consequences of chain networks on thermodynamic, dielectric and structural properties for liquid water. *Physical Chemistry Chemical Physics*, **2007**, 9, 83-91	3.6	34
107	Coexistence of Multilayered Phases of Confined Water: The Importance of Flexible Confining Surfaces. *ACS Nano*, **2018**, 12, 448-454	16.7	33

106	Assessing many-body contributions to intermolecular interactions of the AMOEBA force field using energy decomposition analysis of electronic structure calculations. *Journal of Chemical Physics*, **2017**, 147, 161721	3.9	31
105	Evidence of functional protein dynamics from X-ray crystallographic ensembles. *PLoS Computational Biology*, **2010**, 6, e1000911	5	31
104	Assessing thermodynamic-dynamic relationships for waterlike liquids. *Journal of Chemical Physics*, **2009**, 130, 214510	3.9	31
103	Contrasting disease and nondisease protein aggregation by molecular simulation. *Accounts of Chemical Research*, **2008**, 41, 1037-47	24.3	31
102	A New Solvent Model for Hydrophobic Association in Water I. Thermodynamics. *Journal of the American Chemical Society*, **1995**, 117, 501-507	16.4	31
101	PED in 2021: a major update of the protein ensemble database for intrinsically disordered proteins. *Nucleic Acids Research*, **2021**, 49, D404-D411	20.1	31
100	Accurate Classical Polarization Solution with No Self-Consistent Field Iterations. *Journal of Physical Chemistry Letters*, **2017**, 8, 1714-1723	6.4	30
99	Advanced models for water simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1355	7.9	30
98	Fluctuations of Electric Fields in the Active Site of the Enzyme Ketosteroid Isomerase. *Journal of the American Chemical Society*, **2019**, 141, 12487-12492	16.4	29
97	Evolution of the potential energy landscape with static pulling force for two model proteins. *Journal of Physical Chemistry B*, **2012**, 116, 8394-411	3.4	29
96	Learning to Make Chemical Predictions: the Interplay of Feature Representation, Data, and Machine Learning Methods. *CheM*, **2020**, 6, 1527-1542	16.2	28
95	Disordered structural ensembles of vasopressin and oxytocin and their mutants. *Journal of Physical Chemistry B*, **2015**, 119, 896-905	3.4	28
94	The importance of hydration for the kinetics and thermodynamics of protein folding: simplified lattice models. *Folding & Design*, **1998**, 3, 523-34		28
93	Solution X-ray scattering as a probe of hydration-dependent structuring of aqueous solutions. *Journal of Computer - Aided Molecular Design*, **1999**, 17, 97-118		28
92	Development of an Advanced Force Field for Water Using Variational Energy Decomposition Analysis. *Journal of Chemical Theory and Computation*, **2019**, 15, 5001-5013	6.4	27
91	Instantaneous normal modes as an unforced reaction coordinate for protein conformational transitions. *Biophysical Journal*, **2010**, 98, 2356-64	2.9	27
90	Structure and water dynamics of aqueous peptide solutions in the presence of co-solvents. *Physical Chemistry Chemical Physics*, **2010**, 12, 382-92	3.6	27
89	Direct Exchange Mechanism for Interlayer Ions in Non-Swelling Clays. *Environmental Science & Technology*, **2017**, 51, 393-400	10.3	26

88	The combined force field-sampling problem in simulations of disordered amyloid-β peptides. *Journal of Chemical Physics*, **2019**, 150, 104108	3.9	25
87	An Analytical Electrostatic Model for Salt Screened Interactions between Multiple Proteins. *Journal of Chemical Theory and Computation*, **2006**, 2, 541-55	6.4	25
86	Protein engineering study of protein L by simulation. *Journal of Computational Biology*, **2002**, 9, 35-54	1.7	25
85	A physical approach to protein structure prediction. *Biophysical Journal*, **2002**, 82, 36-49	2.9	25
84	An efficient solvent model for study of hydrophobic phenomena. *Chemical Physics Letters*, **1994**, 227, 215-220	2.5	25
83	Family of Oxygen-Oxygen Radial Distribution Functions for Water. *Journal of Physical Chemistry Letters*, **2015**, 6, 2938-43	6.4	24
82	Interplay of water and a supramolecular capsule for catalysis of reductive elimination reaction from gold. *Nature Communications*, **2020**, 11, 415	17.4	23
81	Electrostatics Generated by a Supramolecular Capsule Stabilizes the Transition State for Carbon-Carbon Reductive Elimination from Gold(III) Complex. *Journal of Physical Chemistry Letters*, **2018**, 9, 3814-3818	6.4	23
80	Performance of the AMOEBA Water Model in the Vicinity of QM Solutes: A Diagnosis Using Energy Decomposition Analysis. *Journal of Chemical Theory and Computation*, **2017**, 13, 1963-1979	6.4	22
79	Performance of extended Lagrangian schemes for molecular dynamics simulations with classical polarizable force fields and density functional theory. *Journal of Chemical Physics*, **2017**, 146, 124115	3.9	22
78	A New and Efficient Poisson-Boltzmann Solver for Interaction of Multiple Proteins. *Journal of Chemical Theory and Computation*, **2010**, 6, 2214-2224	6.4	22
77	Separable cooperative and localized translational motions of water confined by a chemically heterogeneous environment. *Physical Chemistry Chemical Physics*, **2007**, 9, 1962-71	3.6	22
76	Redesigning the hydrophobic core of a model beta-sheet protein: destabilizing traps through a threading approach. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 582-91	4.2	22
75	Extended Experimental Inferential Structure Determination Method in Determining the Structural Ensembles of Disordered Protein States. *Communications Chemistry*, **2020**, 3,	6.3	21
74	From Intermolecular Interaction Energies and Observable Shifts to Component Contributions and Back Again: A Tale of Variational Energy Decomposition Analysis. *Annual Review of Physical Chemistry*, **2021**, 72, 641-666	15.7	21
73	Protein folding by distributed computing and the denatured state ensemble. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 16684-9	11.5	20
72	A New Method for Treating Drude Polarization in Classical Molecular Simulation. *Journal of Chemical Theory and Computation*, **2017**, 13, 5207-5216	6.4	19
71	The role of side chain entropy and mutual information for improving the de novo design of Kemp eliminases KE07 and KE70. *Physical Chemistry Chemical Physics*, **2016**, 18, 19386-96	3.6	19

70	Systematic Optimization of Water Models Using Liquid/Vapor Surface Tension Data. *Journal of Physical Chemistry B*, **2019**, 123, 7061-7073	3.4	18
69	How hot? Systematic convergence of the replica exchange method using multiple reservoirs. *Journal of Computational Chemistry*, **2010**, 31, 620-7	3.5	18
68	Improvements to the AMOEBA Force Field by Introducing Anisotropic Atomic Polarizability of the Water Molecule. *Journal of Chemical Theory and Computation*, **2018**, 14, 6722-6733	6.4	18
67	Multiresolution 3D-DenseNet for Chemical Shift Prediction in NMR Crystallography. *Journal of Physical Chemistry Letters*, **2019**, 10, 4558-4565	6.4	17
66	Reliable protein structure refinement using a physical energy function. *Journal of Computational Chemistry*, **2011**, 32, 709-17	3.5	17
65	Can electric fields drive chemistry for an aqueous microdroplet?. *Nature Communications*, **2022**, 13, 280	17.4	17
64	Diels-Alder Reactions in Water Are Determined by Microsolvation. *Nano Letters*, **2020**, 20, 606-611	11.5	17
63	Recent Advances for Improving the Accuracy, Transferability, and Efficiency of Reactive Force Fields. *Journal of Chemical Theory and Computation*, **2021**, 17, 3237-3251	6.4	17
62	Catalytic Principles from Natural Enzymes and Translational Design Strategies for Synthetic Catalysts. *ACS Central Science*, **2021**, 7, 72-80	16.8	17
61	Mechanism of Nucleation and Growth of A□0 Fibrils from All-Atom and Coarse-Grained Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 12088-12097	3.4	16
60	AutoDetect-mNP: An Unsupervised Machine Learning Algorithm for Automated Analysis of Transmission Electron Microscope Images of Metal Nanoparticles. *Jacs Au*, **2021**, 1, 316-327		16
59	Mode specific THz spectra of solvated amino acids using the AMOEBA polarizable force field. *Physical Chemistry Chemical Physics*, **2017**, 19, 5579-5590	3.6	15
58	A monte carlo method for generating side chain structural ensembles. *Structure*, **2015**, 23, 44-55	5.2	15
57	Electronic structure calculations permit identification of the driving forces behind frequency shifts in transition metal monocarbonyls. *Physical Chemistry Chemical Physics*, **2020**, 22, 781-798	3.6	15
56	Mutually polarizable QM/MM model with in situ optimized localized basis functions. *Journal of Chemical Physics*, **2019**, 150, 074103	3.9	14
55	Embedding A□2 in heterogeneous membranes depends on cholesterol asymmetries. *Biophysical Journal*, **2013**, 105, 899-910	2.9	14
54	Simulated photoelectron spectra of the cyanide-water anion via quasiclassical molecular dynamics. *Journal of Physical Chemistry A*, **2011**, 115, 5928-35	2.8	14
53	Optimal neural networks for protein-structure prediction. *Physical Review E*, **1993**, 48, 1502-1515	2.4	14

52	Convergence of the Many-Body Expansion for Energy and Forces for Classical Polarizable Models in the Condensed Phase. *Journal of Chemical Theory and Computation*, **2016**, 12, 3884-93	6.4	13
51	Effect of a Paramagnetic Spin Label on the Intrinsically Disordered Peptide Ensemble of Amyloid-β *Biophysical Journal*, **2017**, 113, 1002-1011	2.9	13
50	Toward minimalist models of larger proteins: a ubiquitin-like protein. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 368-79	4.2	13
49	A global optimization strategy for predicting alpha-helical protein tertiary structure. *Computers & Chemistry*, **2000**, 24, 489-97		12
48	Approaching the basis set limit for DFT calculations using an environment-adapted minimal basis with perturbation theory: Formulation, proof of concept, and a pilot implementation. *Journal of Chemical Physics*, **2016**, 145, 044109	3.9	12
47	Accurate prediction of chemical shifts for aqueous protein structure on "Real World" data. *Chemical Science*, **2020**, 11, 3180-3191	9.4	11
46	Inertial extended-Lagrangian scheme for solving charge equilibration models. *Physical Chemistry Chemical Physics*, **2019**, 21, 18652-18659	3.6	11
45	C-GeM: Coarse-Grained Electron Model for Predicting the Electrostatic Potential in Molecules. *Journal of Physical Chemistry Letters*, **2019**, 10, 6820-6826	6.4	11
44	Calculating the Bimolecular Rate of Protein-Protein Association with Interacting Crowders. *Journal of Chemical Theory and Computation*, **2013**, 9, 2481-9	6.4	11
43	Strong Anisotropy in Liquid Water upon Librational Excitation Using Terahertz Laser Fields. *Journal of Physical Chemistry B*, **2020**, 124, 4989-5001	3.4	11
42	Combining Iteration-Free Polarization with Large Time Step Stochastic-Isokinetic Integration. *Journal of Chemical Theory and Computation*, **2019**, 15, 2195-2205	6.4	10
41	Solvent Entropy Contributions to Catalytic Activity in Designed and Optimized Kemp Eliminases. *Journal of Physical Chemistry B*, **2018**, 122, 5300-5307	3.4	10
40	The dynamical mechanism of auto-inhibition of AMP-activated protein kinase. *PLoS Computational Biology*, **2011**, 7, e1002082	5	10
39	Improved Energy Selection of Nativelike Protein Loops from Loop Decoys. *Journal of Chemical Theory and Computation*, **2008**, 4, 515-21	6.4	10
38	Comparing generalized ensemble methods for sampling of systems with many degrees of freedom. *Journal of Chemical Physics*, **2016**, 145, 174107	3.9	10
37	Higher-Order Extended Lagrangian Born-Oppenheimer Molecular Dynamics for Classical Polarizable Models. *Journal of Chemical Theory and Computation*, **2018**, 14, 499-511	6.4	9
36	Role of hydrophilicity and length of diblock arms for determining star polymer physical properties. *Journal of Physical Chemistry B*, **2015**, 119, 944-57	3.4	9
35	Reaction field cavity optimization: A born-again Born model for ionic hydration. *Journal of Chemical Physics*, **1999**, 111, 9700-9704	3.9	9

34	A Reactive Force Field with Coarse-Grained Electrons for Liquid Water. *Journal of Physical Chemistry Letters*, **2020**, 11, 9240-9247	6.4	9
33	Structural transition of nanogel star polymers with pH by controlling PEGMA interactions with acid or base copolymers. *Molecular Physics*, **2016**, 114, 3221-3231	1.7	8
32	Energy Decomposition Analysis for Interactions of Radicals: Theory and Implementation at the MP2 Level with Application to Hydration of Halogenated Benzene Cations and Complexes between CO and Pyridine and Imidazole. *Journal of Physical Chemistry A*, **2019**, 123, 9621-9633	2.8	8
31	PB-AM: An open-source, fully analytical linear poisson-boltzmann solver. *Journal of Computational Chemistry*, **2017**, 38, 1275-1282	3.5	8
30	Hydrophobic solvation of Gay-Berne particles in modified water models. *Journal of Chemical Physics* , **2008**, 128, 104506	3.9	8
29	An isolated water droplet in the aqueous solution of a supramolecular tetrahedral cage. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 32954-32961	11.5	8
28	Challenges for density functional theory: calculation of CO adsorption on electrocatalytically relevant metals. *Physical Chemistry Chemical Physics*, **2021**, 23, 9394-9406	3.6	8
27	A facile method for expression and purification of (15)N isotope-labeled human Alzheimer amyloid peptides from E. coli for NMR-based structural analysis. *Protein Expression and Purification*, **2015**, 116, 82-9	2	7
26	A structural coarse-grained model for clays using simple iterative Boltzmann inversion. *Journal of Chemical Physics*, **2018**, 148, 222809	3.9	7
25	Water is not a dynamic polydisperse branched polymer. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 13169-13170	11.5	7
24	Driving forces for transmembrane alpha-helix oligomerization. *Biophysical Journal*, **2010**, 99, 227-37	2.9	6
23	Effect of Hydrophobic Core Topology and Composition on the Structure and Kinetics of Star Polymers: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2017**, 121, 2902-2918	3.4	5
22	An optimization approach to the problem of protein structure prediction. *Mathematical Programming*, **2004**, 101, 497-514	2.1	5
21	Critical Role of Thermal Fluctuations for CO Binding on Electrocatalytic Metal Surfaces. *Jacs Au*, **2021**, 1, 1708-1718		5
20	Molecular Properties and Chemical Transformations Near Interfaces. *Journal of Physical Chemistry B* , **2021**, 125, 9037-9051	3.4	5
19	NewtonNet: a Newtonian message passing network for deep learning of interatomic potentials and forces		5
18	Neural-network design applied to protein-secondary-structure predictions. *Physical Review E*, **1995**, 51, 3619-3627	2.4	4
17	Evaluation of simple model descriptions of the diffusional association rate for enzyme-ligand systems. *The Journal of Physical Chemistry*, **1989**, 93, 490-494		3

List of Publications

16	Optimized Pseudopotentials and Basis Sets for Semiempirical Density Functional Theory for Electrocatalysis Applications. *Journal of Physical Chemistry Letters*, **2021**, 12, 10304-10309	6.4	3
15	Stochastic Constrained Extended System Dynamics for Solving Charge Equilibration Models. *Journal of Chemical Theory and Computation*, **2020**, 16, 5991-5998	6.4	3
14	Convergence of stochastic-extended Lagrangian molecular dynamics method for polarizable force field simulation. *Journal of Computational Physics*, **2021**, 438, 110338	4.1	3
13	Protein C-GeM: A Coarse-Grained Electron Model for Fast and Accurate Protein Electrostatics Prediction. *Journal of Chemical Information and Modeling*, **2021**, 61, 4357-4369	6.1	3
12	Studying Solvation of Small Biomolecules via Molecular Dynamics using a Polarizable Force Field. *Biophysical Journal*, **2017**, 112, 497a	2.9	2
11	Configurational Entropy of Folded Proteins and Its Importance for Intrinsically Disordered Proteins. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
10	Optimizing the Solvent Reorganization Free Energy by Metal Substitution for Nanocage Catalysis. *ACS Catalysis*, **2022**, 12, 3782-3788	13.1	2
9	Dynamical inversion of the energy landscape promotes non-equilibrium self-assembly of binary mixtures. *Chemical Science*, **2018**, 9, 1640-1646	9.4	1
8	Electronic reaction field cavity optimization: Extension to solvation of molecules **1999**,		1
7	Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew		1
6	Proton Traffic Jam: Effect of Nanoconfinement and Acid Concentration on Proton Hopping Mechanism. *Angewandte Chemie - International Edition*, **2021**, 60, 25419-25427	16.4	1
5	Linear Combination of Atomic Dipoles to Calculate the Bond and Molecular Dipole Moments of Molecules and Molecular Liquids.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12360-12369	6.4	1
4	A benchmark dataset for Hydrogen Combustion.. *Scientific Data*, **2022**, 9, 215	8.2	0
3	Tribute to William C. Swope. *Journal of Physical Chemistry B*, **2014**, 118, 6357-9	3.4	
2	FROM MONOMER STRUCTURE TO FIBRIL POLYMORPHISM: COMPUTATIONAL AND EXPERIMENTAL STUDIES OF THE ALZHEIMER'S ABETA PEPTIDE. *FASEB Journal*, **2009**, 23, 423.2	0.9	
1	Parallel implementation of approximate atomistic models of the AMOEBA polarizable model. *Chemical Physics Letters*, **2016**, 664, 191-198	2.5	