Shunyang Wang

List of Publications by Year in Descending Order

70 papers	4,977 citations	29 h-index	70 g-index
83 ext. papers	6,520 ext. citations	6.4 avg, IF	5.78 L-index

#	Paper	IF	Citations
70	Accumulation and Pulse Electron Paramagnetic Resonance Spectroscopic Investigation of the 4-Oxidobenzyl Radical Generated in the Radical -Adenosyl-l-methionine Enzyme HydG.. *Biochemistry*, **2022**,	3.2	2
69	Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites.. *Analytical Chemistry*, **2022**,	7.8	1
68	Proposed Mechanism for the Biosynthesis of the [FeFe] Hydrogenase H-Cluster: Central Roles for the Radical SAM Enzymes HydG and HydE.. *ACS Bio & Med Chem Au*, **2022**, 2, 11-21		0
67	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *Journal of Chemical Physics*, **2021**, 155, 204801	3.9	3
66	The automated optimisation of a coarse-grained force field using free energy data. *Physical Chemistry Chemical Physics*, **2021**, 23, 24842-24851	3.6	2
65	Development and Validation of AMBER-FB15-Compatible Force Field Parameters for Phosphorylated Amino Acids. *Journal of Physical Chemistry B*, **2021**, 125, 11927-11942	3.4	1
64	Reversible -Acetyl Migration within the Sialic Acid Side Chain and Its Influence on Protein Recognition. *ACS Chemical Biology*, **2021**, 16, 1951-1960	4.9	5
63	Quantum Chemistry Calculations for Metabolomics. *Chemical Reviews*, **2021**, 121, 5633-5670	68.1	18
62	Resurrected Ancestors Reveal Origins of Metamorphism in XCL1. *Trends in Biochemical Sciences*, **2021**, 46, 433-434	10.3	
61	TeraChem: A graphical processing unit-accelerated electronic structure package for large-scale ab initio molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2021**, 11, e1494	7.9	49
60	Identification and characterization of metamorphic proteins: Current and future perspectives. *Biopolymers*, **2021**, 112, e23473	2.2	1
59	Development and Benchmarking of Open Force Field v1.0.0-the Parsley Small-Molecule Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 6262-6280	6.4	12
58	Quantum Chemical Study of a Radical Relay Mechanism for the HydG-Catalyzed Synthesis of a Fe(II)(CO)(CN)cysteine Precursor to the H-Cluster of [FeFe] Hydrogenase. *Biochemistry*, **2021**, 60, 3016-3026	3.2	3
57	Linkage between Proximal and Distal Movements of P450cam Induced by Putidaredoxin. *Biochemistry*, **2020**, 59, 2012-2021	3.2	4
56	A combined NMR, MD and DFT conformational analysis of 9-O-acetyl sialic acid-containing GM3 ganglioside glycan and its 9-N-acetyl mimic. *Glycobiology*, **2020**, 30, 787-801	5.8	9
55	Driving torsion scans with wavefront propagation. *Journal of Chemical Physics*, **2020**, 152, 244116	3.9	10
54	Bond-Order Time Series Analysis for Detecting Reaction Events in Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 1606-1617	6.4	4

53	Data-Driven Mapping of Gas-Phase Quantum Calculations to General Force Field Lennard-Jones Parameters. *Journal of Chemical Theory and Computation*, **2020**, 16, 1115-1127	6.4	8
52	Sequence-Based Prediction of Metamorphic Behavior in Proteins. *Biophysical Journal*, **2020**, 119, 1380-1390	3.9	6
51	Data-driven analysis of the number of Lennard-Jones types needed in a force field. *Communications Chemistry*, **2020**, 3,	6.3	1
50	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). *Communications Chemistry*, **2020**, 3,	6.3	33
49	Conformational Response of N-Terminally Truncated Cytochrome P450 3A4 to Ligand Binding in Solution. *Biochemistry*, **2019**, 58, 3903-3910	3.2	8
48	An Intermediate Conformational State of Cytochrome P450cam-CN in Complex with Putidaredoxin. *Biochemistry*, **2019**, 58, 2353-2361	3.2	8
47	Force Field Development and Nanoreactor Chemistry. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 127-159	0.7	
46	Car-Parrinello Monitor for More Robust Born-Oppenheimer Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2019**, 15, 4454-4467	6.4	5
45	Systematic Optimization of Water Models Using Liquid/Vapor Surface Tension Data. *Journal of Physical Chemistry B*, **2019**, 123, 7061-7073	3.4	18
44	Capillary Effects on Groundwater Response to Earth Tides. *Water Resources Research*, **2019**, 55, 6886-6895	5.4	12
43	Binding Thermodynamics of Host-Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. *Journal of Chemical Theory and Computation*, **2019**, 15, 6225-6242	6.4	11
42	Quantum chemical studies of redox properties and conformational changes of a four-center iron CO reduction electrocatalyst. *Chemical Science*, **2018**, 9, 2645-2654	9.4	4
41	Assimilating Radial Distribution Functions To Build Water Models with Improved Structural Properties. *Journal of Chemical Information and Modeling*, **2018**, 58, 1766-1778	6.1	12
40	Polarizable Molecular Simulations Reveal How Silicon-Containing Functional Groups Govern the Desalination Mechanism in Nanoporous Graphene. *Journal of Chemical Theory and Computation*, **2018**, 14, 4279-4290	6.4	6
39	Advanced models for water simulations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1355	7.9	30
38	An Estimation of Hybrid Quantum Mechanical Molecular Mechanical Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches. *Journal of Chemical Theory and Computation*, **2017**, 13, 679-695	6.4	14
37	A Chemical Biology Solution to Problems with Studying Biologically Important but Unstable 9-O-Acetyl Sialic Acids. *ACS Chemical Biology*, **2017**, 12, 214-224	4.9	27
36	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

35	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. *PLoS Computational Biology*, **2017**, 13, e1005659	5	686
34	Large earthquakes create vertical permeability by breaching aquitards. *Water Resources Research*, **2016**, 52, 5923-5937	5.4	59
33	Training and Validation of a Liquid-Crystalline Phospholipid Bilayer Force Field. *Journal of Chemical Theory and Computation*, **2016**, 12, 5960-5967	6.4	12
32	Automated Code Engine for Graphical Processing Units: Application to the Effective Core Potential Integrals and Gradients. *Journal of Chemical Theory and Computation*, **2016**, 12, 92-106	6.4	46
31	Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways. *Journal of Chemical Theory and Computation*, **2016**, 12, 638-49	6.4	73
30	Geometry optimization made simple with translation and rotation coordinates. *Journal of Chemical Physics*, **2016**, 144, 214108	3.9	71
29	Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 9811-32	3.4	66
28	Why many semiempirical molecular orbital theories fail for liquid water and how to fix them. *Journal of Computational Chemistry*, **2015**, 36, 934-9	3.5	12
27	United polarizable multipole water model for molecular mechanics simulation. *Journal of Chemical Physics*, **2015**, 143, 014504	3.9	30
26	MDTraj: A Modern Open Library for the Analysis of Molecular Dynamics Trajectories. *Biophysical Journal*, **2015**, 109, 1528-32	2.9	834
25	Efficient implementation of effective core potential integrals and gradients on graphical processing units. *Journal of Chemical Physics*, **2015**, 143, 014114	3.9	13
24	Tensor Hypercontraction Second-Order Møller-Plesset Perturbation Theory: Grid Optimization and Reaction Energies. *Journal of Chemical Theory and Computation*, **2015**, 11, 3042-52	6.4	38
23	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. *Journal of Physical Chemistry B*, **2015**, 119, 9423-9437	3.4	149
22	What can density functional theory tell us about artificial catalytic water splitting?. *Inorganic Chemistry*, **2014**, 53, 6386-97	5.1	97
21	Discovering chemistry with an ab initio nanoreactor. *Nature Chemistry*, **2014**, 6, 1044-8	17.6	209
20	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 1885-91	6.4	294
19	Modeling organochlorine compounds and the Ehole effect using a polarizable multipole force field. *Journal of Physical Chemistry B*, **2014**, 118, 6456-65	3.4	65
18	Systematic improvement of a classical molecular model of water. *Journal of Physical Chemistry B*, **2013**, 117, 9956-72	3.4	235

17	Calculations of the electric fields in liquid solutions. *Journal of Physical Chemistry B*, **2013**, 117, 16236-48	3.4	73
16	A pathway to diphosphorus from the dissociation of photoexcited tetraphosphorus. *RSC Advances*, **2013**, 3, 23166	3.7	11
15	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. *Journal of Chemical Theory and Computation*, **2013**, 9, 461-469	6.4	440
14	Systematic Parametrization of Polarizable Force Fields from Quantum Chemistry Data. *Journal of Chemical Theory and Computation*, **2013**, 9, 452-60	6.4	124
13	Basin-scale transport of heat and fluid induced by earthquakes. *Geophysical Research Letters*, **2013**, 40, 3893-3897	4.9	34
12	A Polarizable QM/MM Explicit Solvent Model for Computational Electrochemistry in Water. *Journal of Chemical Theory and Computation*, **2012**, 8, 610-7	6.4	63
11	Simulation of solution phase electron transfer in a compact donor-acceptor dyad. *Journal of Physical Chemistry B*, **2011**, 115, 12135-44	3.4	24
10	Molecular Insight Into the Energy Levels at the Organic Donor/Acceptor Interface: A Quantum Mechanics/Molecular Mechanics Study. *Journal of Physical Chemistry C*, **2011**, 115, 14431-14436	3.8	82
9	Direct-Coupling O2 Bond Forming a Pathway in Cobalt Oxide Water Oxidation Catalysts. *Journal of Physical Chemistry Letters*, **2011**, 2, 2200-2204	6.4	159
8	Electronic properties of disordered organic semiconductors via QM/MM simulations. *Accounts of Chemical Research*, **2010**, 43, 995-1004	24.3	83
7	Acid-base mechanism for ruthenium water oxidation catalysts. *Inorganic Chemistry*, **2010**, 49, 4543-53	5.1	134
6	Communication: Hybrid ensembles for improved force matching. *Journal of Chemical Physics*, **2010**, 133, 231101	3.9	17
5	The diabatic picture of electron transfer, reaction barriers, and molecular dynamics. *Annual Review of Physical Chemistry*, **2010**, 61, 149-70	15.7	256
4	Force Field Partial Charges with Restrained Electrostatic Potential 2 (RESP2)		3
3	OpenMM 7: Rapid Development of High Performance Algorithms for Molecular Dynamics		1
2	The Automated Optimisation of a Coarse-Grained Force Field Using Free Energy Data		2
1	Capturing non-local through-bond effects when fragmenting molecules for quantum chemical torsion scans		3