Shunyang Wang

List of Publications by Year
in descending order

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71 papers	7,858 citations	136950 32 h-index	91884 69 g-index
83 all docs	83 docs citations	83 times ranked	9262 citing authors

#	Article	IF	Citations
1	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.	3.7	6
2	Accumulation and Pulse Electron Paramagnetic Resonance Spectroscopic Investigation of the 4-Oxidobenzyl Radical Generated in the RadicalS-Adenosyl-<scp>l</scp>-methionine Enzyme HydG. Biochemistry, 2022, 61, 107-116.	2.5	7
3	Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites. Analytical Chemistry, 2022, , .	6.5	5
4	Evaluating the Accuracy of the QCEIMS Approach for Computational Prediction of Electron Ionization Mass Spectra of Purines and Pyrimidines. Metabolites, 2022, 12, 68.	2.9	4
5	Improving Force Field Accuracy by Training against Condensed-Phase Mixture Properties. Journal of Chemical Theory and Computation, 2022, 18, 3577-3592.	5.3	9
6	Open Force Field Evaluator: An Automated, Efficient, and Scalable Framework for the Estimation of Physical Properties from Molecular Simulation. Journal of Chemical Theory and Computation, 2022, 18, 3566-3576.	5.3	19
7	Source of Rate Acceleration for Carbocation Cyclization in Biomimetic Supramolecular Cages. Journal of the American Chemical Society, 2022, 144, 11413-11424.	13.7	15
8	Exploration and validation of force field design protocols through QM-to-MM mapping. Physical Chemistry Chemical Physics, 2022, 24, 17014-17027.	2.8	4
9	<scp>TeraChem</scp>: A graphical processing unit<scp>â€accelerated</scp> electronic structure package for <scp>largeâ€scale</scp> ab initio molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1494.	14.6	143
10	Reversible O-Acetyl Migration within the Sialic Acid Side Chain and Its Influence on Protein Recognition. ACS Chemical Biology, 2021, 16, 1951-1960.	3.4	19
11	Quantum Chemistry Calculations for Metabolomics. Chemical Reviews, 2021, 121, 5633-5670.	47.7	47
12	Resurrected Ancestors Reveal Origins of Metamorphism in XCL1. Trends in Biochemical Sciences, 2021, 46, 433-434.	7.5	0
13	Identification and characterization of metamorphic proteins: Current and future perspectives. Biopolymers, 2021, 112, e23473.	2.4	6
14	Development and Benchmarking of Open Force Field v1.0.0â€”the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
15	Quantum Chemical Study of a Radical Relay Mechanism for the HydG-Catalyzed Synthesis of a Fe(II)(CO)₂(CN)cysteine Precursor to the H-Cluster of [FeFe] Hydrogenase. Biochemistry, 2021, 60, 3016-3026.	2.5	4
16	The automated optimisation of a coarse-grained force field using free energy data. Physical Chemistry Chemical Physics, 2021, 23, 24842-24851.	2.8	3
17	Development and Validation of AMBER-FB15-Compatible Force Field Parameters for Phosphorylated Amino Acids. Journal of Physical Chemistry B, 2021, 125, 11927-11942.	2.6	8
18	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15

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19	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.	5.3	15
20	Sequence-Based Prediction of Metamorphic Behavior in Proteins. Biophysical Journal, 2020, 119, 1380-1390.	0.5	20
21	Data-driven analysis of the number of Lennardâ€“Jones types needed in a force field. Communications Chemistry, 2020, 3, .	4.5	6
22	Linkage between Proximal and Distal Movements of P450cam Induced by Putidaredoxin. Biochemistry, 2020, 59, 2012-2021.	2.5	6
23	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.	2.5	17
24	Driving torsion scans with wavefront propagation. Journal of Chemical Physics, 2020, 152, 244116.	3.0	22
25	Bond-Order Time Series Analysis for Detecting Reaction Events in Ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 1606-1617.	5.3	12
26	Non-bonded force field model with advanced restrained electrostatic potential charges (RESP2). Communications Chemistry, 2020, 3, .	4.5	98
27	Carâ€“Parrinello Monitor for More Robust Bornâ€“Oppenheimer Molecular Dynamics. Journal of Chemical Theory and Computation, 2019, 15, 4454-4467.	5.3	5
28	Systematic Optimization of Water Models Using Liquid/Vapor Surface Tension Data. Journal of Physical Chemistry B, 2019, 123, 7061-7073.	2.6	31
29	Capillary Effects on Groundwater Response to Earth Tides. Water Resources Research, 2019, 55, 6886-6895.	4.2	18
30	Binding Thermodynamics of Hostâ€“Guest Systems with SMIRNOFF99Frosst 1.0.5 from the Open Force Field Initiative. Journal of Chemical Theory and Computation, 2019, 15, 6225-6242.	5.3	21
31	Conformational Response of N-Terminally Truncated Cytochrome P450 3A4 to Ligand Binding in Solution. Biochemistry, 2019, 58, 3903-3910.	2.5	12
32	An Intermediate Conformational State of Cytochrome P450cam-CN in Complex with Putidaredoxin. Biochemistry, 2019, 58, 2353-2361.	2.5	12
33	Force Field Development and Nanoreactor Chemistry. Challenges and Advances in Computational Chemistry and Physics, 2019, , 127-159.	0.6	1
34	Quantum chemical studies of redox properties and conformational changes of a four-center iron CO₂ reduction electrocatalyst. Chemical Science, 2018, 9, 2645-2654.	7.4	6
35	Advanced models for water simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1355.	14.6	42
36	Assimilating Radial Distribution Functions To Build Water Models with Improved Structural Properties. Journal of Chemical Information and Modeling, 2018, 58, 1766-1778.	5.4	22

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37	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.	5.3	8
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.	5.3	19
39	A Chemical Biology Solution to Problems with Studying Biologically Important but Unstable 9-O-Acetyl Sialic Acids. ACS Chemical Biology, 2017, 12, 214-224.	3.4	37
40	Building a More Predictive Protein Force Field: A Systematic and Reproducible Route to AMBER-FB15. Journal of Physical Chemistry B, 2017, 121, 4023-4039.	2.6	192
41	OpenMM 7: Rapid development of high performance algorithms for molecular dynamics. PLoS Computational Biology, 2017, 13, e1005659.	3.2	1,561
42	Geometry optimization made simple with translation and rotation coordinates. Journal of Chemical Physics, 2016, 144, 214108.	3.0	137
43	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	2.6	77
44	Large earthquakes create vertical permeability by breaching aquitards. Water Resources Research, 2016, 52, 5923-5937.	4.2	75
45	Training and Validation of a Liquid-Crystalline Phospholipid Bilayer Force Field. Journal of Chemical Theory and Computation, 2016, 12, 5960-5967.	5.3	14
46	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.	5.3	55
47	Automated Discovery and Refinement of Reactive Molecular Dynamics Pathways. Journal of Chemical Theory and Computation, 2016, 12, 638-649.	5.3	95
48	Efficient implementation of effective core potential integrals and gradients on graphical processing units. Journal of Chemical Physics, 2015, 143, 014114.	3.0	17
49	Tensor Hypercontraction Second-Order MÃ¸llerâ€“Plesset Perturbation Theory: Grid Optimization and Reaction Energies. Journal of Chemical Theory and Computation, 2015, 11, 3042-3052.	5.3	47
50	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. Journal of Physical Chemistry B, 2015, 119, 9423-9437.	2.6	183
51	Why many semiempirical molecular orbital theories fail for liquid water and how to fix them. Journal of Computational Chemistry, 2015, 36, 934-939.	3.3	16
52	United polarizable multipole water model for molecular mechanics simulation. Journal of Chemical Physics, 2015, 143, 014504.	3.0	36
53	MDTraj: A Modern Open Library for the Analysis of Molecular Dynamics Trajectories. Biophysical Journal, 2015, 109, 1528-1532.	0.5	1,576
54	What Can Density Functional Theory Tell Us about Artificial Catalytic Water Splitting?. Inorganic Chemistry, 2014, 53, 6386-6397.	4.0	126

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55	Discovering chemistry with an ab initio nanoreactor. Nature Chemistry, 2014, 6, 1044-1048.	13.6	286
56	Building Force Fields: An Automatic, Systematic, and Reproducible Approach. Journal of Physical Chemistry Letters, 2014, 5, 1885-1891.	4.6	400
57	Modeling Organochlorine Compounds and the Ïƒ-Hole Effect Using a Polarizable Multipole Force Field. Journal of Physical Chemistry B, 2014, 118, 6456-6465.	2.6	69
58	Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972.	2.6	279
59	Calculations of the Electric Fields in Liquid Solutions. Journal of Physical Chemistry B, 2013, 117, 16236-16248.	2.6	83
60	A pathway to diphosphorus from the dissociation of photoexcited tetraphosphorus. RSC Advances, 2013, 3, 23166.	3.6	14
61	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 461-469.	5.3	583
62	Systematic Parametrization of Polarizable Force Fields from Quantum Chemistry Data. Journal of Chemical Theory and Computation, 2013, 9, 452-460.	5.3	164
63	Basinâ€scale transport of heat and fluid induced by earthquakes. Geophysical Research Letters, 2013, 40, 3893-3897.	4.0	41
64	A Polarizable QM/MM Explicit Solvent Model for Computational Electrochemistry in Water. Journal of Chemical Theory and Computation, 2012, 8, 610-617.	5.3	71
65	Simulation of Solution Phase Electron Transfer in a Compact Donorâ€“Acceptor Dyad. Journal of Physical Chemistry B, 2011, 115, 12135-12144.	2.6	27
66	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.	3.1	83
67	Direct-Coupling O₂ Bond Forming a Pathway in Cobalt Oxide Water Oxidation Catalysts. Journal of Physical Chemistry Letters, 2011, 2, 2200-2204.	4.6	177
68	Communication: Hybrid ensembles for improved force matching. Journal of Chemical Physics, 2010, 133, 231101.	3.0	19
69	The Diabatic Picture of Electron Transfer, Reaction Barriers, and Molecular Dynamics. Annual Review of Physical Chemistry, 2010, 61, 149-170.	10.8	280
70	Electronic Properties of Disordered Organic Semiconductors via QM/MM Simulations. Accounts of Chemical Research, 2010, 43, 995-1004.	15.6	90
71	Acidâ€”Base Mechanism for Ruthenium Water Oxidation Catalysts. Inorganic Chemistry, 2010, 49, 4543-4553.	4.0	139