Tianyu Zhu

List of Publications by Year
in descending order

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Version: 2024-02-01

25 papers	1,720 citations	471509 17 h-index	610901 24 g-index
28 all docs	28 docs citations	28 times ranked	2215 citing authors

#	Article	IF	Citations
1	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
2	Thermally Activated Delayed Fluorescence Materials Based on Homoconjugation Effect of Donorâ€“Acceptor Triptycenes. Journal of the American Chemical Society, 2015, 137, 11908-11911.	13.7	331
3	Ï€-Clamp-mediated cysteine conjugation. Nature Chemistry, 2016, 8, 120-128.	13.6	236
4	Shorter Exciton Lifetimes via an External Heavyâ€Atom Effect: Alleviating the Effects of Bimolecular Processes in Organic Lightâ€Emitting Diodes. Advanced Materials, 2017, 29, 1701987.	21.0	90
5	Extracting Design Principles for Efficient Thermally Activated Delayed Fluorescence (TADF) from a Simple Four-State Model. Chemistry of Materials, 2019, 31, 6995-7006.	6.7	84
6	Prediction of Excited-State Energies and Singletâ€“Triplet Gaps of Charge-Transfer States Using a Restricted Open-Shell Kohnâ€“Sham Approach. Journal of Chemical Theory and Computation, 2016, 12, 3353-3359.	5.3	74
7	Molecular Design of Deep Blue Thermally Activated Delayed Fluorescence Materials Employing a Homoconjugative Triptycene Scaffold and Dihedral Angle Tuning. Chemistry of Materials, 2018, 30, 1462-1466.	6.7	71
8	Photoenzymatic Hydrogenation of Heteroaromatic Olefins Using â€˜Eneâ€™â€Reductases with Photoredox Catalysts. Angewandte Chemie - International Edition, 2020, 59, 10484-10488.	13.8	67
9	Efficient Implementation of Ab Initio Quantumâ€Embedding in Periodic Systems: Density Matrixâ€Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 119-129.	5.3	64
10	Efficient Formulation of Ab Initio Quantum Embedding in Periodic Systems: Dynamical Mean-Field Theory. Journal of Chemical Theory and Computation, 2020, 16, 141-153.	5.3	40
11	Coupled-cluster impurity solvers for dynamical mean-field theory. Physical Review B, 2019, 100, .	3.2	37
12	Salt Effect Accelerates Site-Selective Cysteine Bioconjugation. ACS Central Science, 2016, 2, 637-646.	11.3	36
13	AbÂInitio Full Cell <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi><mml:mo>+</mml:mo><mml:mi>DMFT</mml:mi></mml:mrow></mml:math> for Correlated Materials. Physical Review X, 2021, 11, .	8.9	33
14	All-Electron Gaussian-Based G₀W₀ for Valence and Core Excitation Energies of Periodic Systems. Journal of Chemical Theory and Computation, 2021, 17, 727-741.	5.3	32
15	Large Increase in External Quantum Efficiency by Dihedral Angle Tuning in a Skyâ€Blue Thermally Activated Delayed Fluorescence Emitter. Advanced Optical Materials, 2019, 7, 1900476.	7.3	25
16	A structural and mechanistic study of Ï€-clamp-mediated cysteine perfluoroarylation. Scientific Reports, 2017, 7, 7954.	3.3	20
17	Charge Recombination in Phosphorescent Organic Light-Emitting Diode Hostâ€“Guest Systems through QM/MM Simulations. Journal of Physical Chemistry C, 2016, 120, 19987-19994.	3.1	19
18	Understanding the Dipole Moment of Liquid Water from a Self-Attractive Hartree Decomposition. Journal of Physical Chemistry Letters, 2021, 12, 6-12.	4.6	14

#	Article	IF	Citations
19	Many-electron expansion: A density functional hierarchy for strongly correlated systems. Physical Review B, 2016, 93, .	3.2	13
20	Photoenzymatic Hydrogenation of Heteroaromatic Olefins Using â€˜Eneâ€™â€Reductases with Photoredox Catalysts. Angewandte Chemie, 2020, 132, 10570-10574.	2.0	13
21	Unraveling the Fate of Host Excitons in Hostâ€“Guest Phosphorescent Organic Light-Emitting Diodes. Journal of Physical Chemistry C, 2019, 123, 10311-10318.	3.1	10
22	Self-Attractive Hartree Decomposition: Partitioning Electron Density into Smooth Localized Fragments. Journal of Chemical Theory and Computation, 2018, 14, 92-103.	5.3	7
23	Long-range interactions from the many-pair expansion: A different avenue to dispersion in DFT. Journal of Chemical Physics, 2017, 146, 024111.	3.0	6
24	Implementation of the Many-Pair Expansion for Systematically Improving Density Functional Calculations of Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1089-1101.	5.3	5
25	Charge Transfer in Molecular Materials. , 2018, , 1-31.		4