

# 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	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
2	All-Electron Gaussian-Based $G_0W_0$ for Valence and Core Excitation Energies of Periodic Systems. Journal of Chemical Theory and Computation, 2021, 17, 727-741.	5.3	32
3	Ab Initio Full Cell $G_0W_0+DMFT$ for Correlated Materials. Physical Review X, 2021, 11, .	5.3	33
4	Efficient Implementation of Ab Initio Quantum Embedding in Periodic Systems: Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 119-129.	5.3	64
5	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
6	Recent developments in the PySCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
7	Photoenzymatic Hydrogenation of Heteroaromatic Olefins Using $NADH$ Reductases with Photoredox Catalysts. Angewandte Chemie - International Edition, 2020, 59, 10484-10488.	13.8	67
8	Photoenzymatic Hydrogenation of Heteroaromatic Olefins Using $NADH$ Reductases with Photoredox Catalysts. Angewandte Chemie, 2020, 132, 10570-10574.	2.0	13
9	Large Increase in External Quantum Efficiency by Dihedral Angle Tuning in a SkyBlue Thermally Activated Delayed Fluorescence Emitter. Advanced Optical Materials, 2019, 7, 1900476.	7.3	25
10	Coupled-cluster impurity solvers for dynamical mean-field theory. Physical Review B, 2019, 100, .	3.2	37
11	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
12	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
13	Unraveling the Fate of Host Excitons in Host-Guest Phosphorescent Organic Light-Emitting Diodes. Journal of Physical Chemistry C, 2019, 123, 10311-10318.	3.1	10
14	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
15	Self-Attractive Hartree Decomposition: Partitioning Electron Density into Smooth Localized Fragments. Journal of Chemical Theory and Computation, 2018, 14, 92-103.	5.3	7
16	Charge Transfer in Molecular Materials. , 2018, , 1-31.		4
17	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
18	A structural and mechanistic study of $\beta$ -clamp-mediated cysteine perfluoroarylation. Scientific Reports, 2017, 7, 7954.	3.3	20

#	ARTICLE	IF	CITATIONS
19	Shorter Exciton Lifetimes via an External Heavy-Atom Effect: Alleviating the Effects of Bimolecular Processes in Organic Light-Emitting Diodes. <i>Advanced Materials</i> , 2017, 29, 1701987.	21.0	90
20	Charge Recombination in Phosphorescent Organic Light-Emitting Diode Host-Guest Systems through QM/MM Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 19987-19994.	3.1	19
21	Salt Effect Accelerates Site-Selective Cysteine Bioconjugation. <i>ACS Central Science</i> , 2016, 2, 637-646.	11.3	36
22	Many-electron expansion: A density functional hierarchy for strongly correlated systems. <i>Physical Review B</i> , 2016, 93, .	3.2	13
23	Prediction of Excited-State Energies and Singlet-Triplet Gaps of Charge-Transfer States Using a Restricted Open-Shell Kohn-Sham Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3353-3359.	5.3	74
24	Œ-Clamp-mediated cysteine conjugation. <i>Nature Chemistry</i> , 2016, 8, 120-128.	13.6	236
25	Thermally Activated Delayed Fluorescence Materials Based on Homoconjugation Effect of Donor-Acceptor Triptycenes. <i>Journal of the American Chemical Society</i> , 2015, 137, 11908-11911.	13.7	331