Haitao Sun

List of Publications by Year
in descending order

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57 papers	3,382 citations	218677 26 h-index	144013 57 g-index
57 all docs	57 docs citations	57 times ranked	3741 citing authors

#	Article	IF	Citations
1	Donor Engineering for NIR-II Molecular Fluorophores with Enhanced Fluorescent Performance. Journal of the American Chemical Society, 2018, 140, 1715-1724.	13.7	379
2	Reliable Prediction with Tuned Range-Separated Functionals of the Singletâ€“Triplet Gap in Organic Emitters for Thermally Activated Delayed Fluorescence. Journal of Chemical Theory and Computation, 2015, 11, 3851-3858.	5.3	362
3	Rational Design of Molecular Fluorophores for Biological Imaging in the NIRâ€II Window. Advanced Materials, 2017, 29, 1605497.	21.0	356
4	Repurposing Cyanine NIRâ€I Dyes Accelerates Clinical Translation of Nearâ€Infraredâ€II (NIRâ€II) Bioimaging. Advanced Materials, 2018, 30, e1802546.	21.0	249
5	Albumin-chaperoned cyanine dye yields superbright NIR-II fluorophore with enhanced pharmacokinetics. Science Advances, 2019, 5, eaaw0672.	10.3	171
6	Electronic Energy Gaps for Ï€-Conjugated Oligomers and Polymers Calculated with Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 1035-1047.	5.3	142
7	Ionization Energies, Electron Affinities, and Polarization Energies of Organic Molecular Crystals: Quantitative Estimations from a Polarizable Continuum Model (PCM)-Tuned Range-Separated Density Functional Approach. Journal of Chemical Theory and Computation, 2016, 12, 2906-2916.	5.3	124
8	Rational design of a super-contrast NIR-II fluorophore affords high-performance NIR-II molecular imaging guided microsurgery. Chemical Science, 2019, 10, 326-332.	7.4	124
9	Influence of the Delocalization Error and Applicability of Optimal Functional Tuning in Density Functional Calculations of Nonlinear Optical Properties of Organic Donorâ€“Acceptor Chromophores. ChemPhysChem, 2013, 14, 2450-2461.	2.1	119
10	Impact of Dielectric Constant on the Singletâ€“Triplet Gap in Thermally Activated Delayed Fluorescence Materials. Journal of Physical Chemistry Letters, 2017, 8, 2393-2398.	4.6	118
11	Orthogonal Self-Assembly of a Two-Step Fluorescence-Resonance Energy Transfer System with Improved Photosensitization Efficiency and Photooxidation Activity. Journal of the American Chemical Society, 2021, 143, 399-408.	13.7	104
12	Developing a Bright NIRâ€II Fluorophore with Fast Renal Excretion and Its Application in Molecular Imaging of Immune Checkpoint PDâ€L1. Advanced Functional Materials, 2018, 28, 1804956.	14.9	85
13	Charge-Transfer Versus Charge-Transfer-Like Excitations Revisited. Journal of Chemical Theory and Computation, 2015, 11, 3305-3320.	5.3	75
14	Propylenedioxy Thiophene Donor to Achieve NIR-II Molecular Fluorophores with Enhanced Brightness. Chemistry of Materials, 2020, 32, 2061-2069.	6.7	72
15	Visible-Light-Driven Rotation of Molecular Motors in Discrete Supramolecular Metallacycles. Journal of the American Chemical Society, 2021, 143, 442-452.	13.7	72
16	Rotaxane-Branched Dendrimers with Enhanced Photosensitization. Journal of the American Chemical Society, 2020, 142, 16748-16756.	13.7	68
17	Conformational Relaxation and Thermally Activated Delayed Fluorescence in Anthraquinone-Based Intramolecular Charge-Transfer Compound. Journal of Physical Chemistry C, 2018, 122, 3727-3737.	3.1	65
18	Quantitative Estimation of Exciton Binding Energy of Polythiophene-Derived Polymers Using Polarizable Continuum Model Tuned Range-Separated Density Functional. Journal of Physical Chemistry C, 2016, 120, 8048-8055.	3.1	56

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19	The Density of States and the Transport Effective Mass in a Highly Oriented Semiconducting Polymer: Electronic Delocalization in 1D. Advanced Materials, 2015, 27, 7759-7765.	21.0	52
20	Thieno[3,4-c]pyrrole-4,6(5H)-dione Polymers with Optimized Energy Level Alignments for Fused-Ring Electron Acceptor Based Polymer Solar Cells. Chemistry of Materials, 2017, 29, 5636-5645.	6.7	43
21	Engineering naphthalimide-cyanine integrated near-infrared dye into ROS-responsive nanohybrids for tumor PDT/PTT/chemotherapy. Bioactive Materials, 2022, 14, 42-51.	15.6	41
22	A Fluorogenic ONOO^{â€“}-Triggered Carbon Monoxide Donor for Mitigating Brain Ischemic Damage. Journal of the American Chemical Society, 2022, 144, 2114-2119.	13.7	39
23	Theoretical predication for transition energies of thermally activated delayed fluorescence molecules. Chinese Chemical Letters, 2016, 27, 1445-1452.	9.0	37
24	A genetic engineering strategy for editing near-infrared-II fluorophores. Nature Communications, 2022, 13, .	12.8	33
25	Applicability of optimal functional tuning in density functional calculations of ionization potentials and electron affinities of adenineâ€“thymine nucleobase pairs and clusters. Physical Chemistry Chemical Physics, 2015, 17, 4337-4345.	2.8	32
26	Theoretical study of excited states of <scp>DNA</scp> base dimers and tetramers using optimally tuned rangeâ€separated density functional theory. Journal of Computational Chemistry, 2016, 37, 684-693.	3.3	30
27	Prediction of excitedâ€state properties of oligoacene crystals using polarizable continuum modelâ€tuned rangeâ€separated hybrid functional approach. Journal of Computational Chemistry, 2017, 38, 569-575.	3.3	28
28	Theoretical exploitation of acceptors based on benzobis(thiadiazole) and derivatives for organic NIR-II fluorophores. Physical Chemistry Chemical Physics, 2018, 20, 19759-19767.	2.8	24
29	Methyl Thioether Functionalization of a Polymeric Donor for Efficient Solar Cells Processed from Non-Halogenated Solvents. Chemistry of Materials, 2019, 31, 3025-3033.	6.7	23
30	High brightness NIR-II nanofluorophores based on fused-ring acceptor molecules. Nano Research, 2020, 13, 2570-2575.	10.4	23
31	Nearâ€Unity Triplet Generation Promoted via Spiroâ€Conjugation. Angewandte Chemie - International Edition, 2022, 61, .	13.8	20
32	Accurate Prediction for Dynamic Hybrid Local and Charge Transfer Excited States from Optimally Tuned Range-Separated Density Functionals. Journal of Physical Chemistry C, 2019, 123, 5616-5625.	3.1	19
33	Prediction of Excited-State Properties of Oligoacene Crystals Using Fragment-Based Quantum Mechanical Method. Journal of Physical Chemistry A, 2019, 123, 5407-5417.	2.5	18
34	Facile construction of well-defined radical metallacycles through coordination-driven self-assembly. Materials Chemistry Frontiers, 2021, 5, 1863-1871.	5.9	17
35	Effects of Fluorination on Fused Ring Electron Acceptor for Active Layer Morphology, Exciton Dissociation, and Charge Recombination in Organic Solar Cells. ACS Applied Materials & Interfaces, 2020, 12, 56231-56239.	8.0	15
36	Photoelectron spectroscopy and computational investigations of the electronic structures and noncovalent interactions of cyclodextrin-closo-dodecaborate anion complexes Ï‡-CDÂ·B₁₂X₁₂^{2â^’} (Ï‡ = Î±, Î², Î³; X = H, F). Physical Chemistry Chemical Physics, 2020, 22, 7193-7200.	2.8	14

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37	Graphene Oxide-BiOCl Nanoparticle Composites as Catalysts for Oxidation of Volatile Organic Compounds in Nonthermal Plasmas. ACS Applied Nano Materials, 2020, 3, 9363-9374.	5.0	13
38	Why Can High Chargeâ€Carrier Mobilities be Achieved Along Ï€â€Conjugated Polymer Chains with Alternating Donorâ€“Acceptor Moieties?. Advanced Theory and Simulations, 2018, 1, 1800016.	2.8	12
39	Channel-resolved multiorbital double ionization of molecular Cl2 in an intense femtosecond laser field. Physical Review A, 2018, 98, .	2.5	11
40	Design of zinc porphyrinâ€perylene diimide donorâ€bridgeâ€acceptor chromophores for large secondâ€order nonlinear optical response: A theoretical exploration. International Journal of Quantum Chemistry, 2018, 118, e25536.	2.0	10
41	Benchmark study of ionization potentials and electron affinities of armchair single-walled carbon nanotubes using density functional theory. Journal of Physics Condensed Matter, 2018, 30, 215501.	1.8	10
42	Shielding Unit Engineering of NIR-II Molecular Fluorophores for Improved Fluorescence Performance and Renal Excretion Ability. Frontiers in Chemistry, 2021, 9, 739802.	3.6	10
43	pH Controlled Intersystem Crossing and Singlet Oxygen Generation of 8â€Azaadenine in Aqueous Solution. ChemPhysChem, 2019, 20, 757-765.	2.1	8
44	Gaseous cyclodextrin-closo-dodecaborate complexes Ï‡CDÂ·B₁₂X₁₂^{2â^'} (Ï‡ = Î±, Î², and Î³; X = F, Cl, Br, and I): electronic structures and intramolecular interactions. Physical Chemistry Chemical Physics, 2021, 23, 13447-13457.	2.8	8
45	New Insights about the Photostability of DNA/RNA Bases: Triplet nÏ€* State Leads to Effective Intersystem Crossing in Pyrimidinones. Journal of Physical Chemistry B, 2021, 125, 2042-2049.	2.6	8
46	Achieving Adjustable Multifunction Based on Hostâ€“Guest Interaction-Manipulated Reversible Molecular Conformational Switching. ACS Applied Materials & Interfaces, 2022, 14, 1807-1816.	8.0	7
47	Intramolecular Charge Transfer in 5-Halogen Cytidines Revealed by Femtosecond Time-Resolved Spectroscopy. Journal of Physical Chemistry B, 2020, 124, 2560-2567.	2.6	6
48	Defect-Engineered Graphene Films as Ozonation Catalysts for the Devastation of Sulfamethoxazole: Insights into the Active Sites and Oxidation Mechanism. ACS Applied Materials & Interfaces, 2021, 13, 52706-52716.	8.0	6
49	Electronic structures and binding motifs of sodium polysulfide clusters NaSnâ^' (n = 5â€“9): A joint negative ion photoelectron spectroscopy and computational investigation. Journal of Chemical Physics, 2019, 150, 244305.	3.0	4
50	Assessment of DFT methods for the prediction of detachment energies and electronic structures of complex and multiply charged anions. Computational and Theoretical Chemistry, 2021, 1202, 113295.	2.5	4
51	Dissociative Ionization and Coulomb Explosion of Molecular Bromocyclopropane in an Intense Femtosecond Laser Field. Molecules, 2018, 23, 3096.	3.8	3
52	Computational Screening of Atomically Thin Two-Dimensional Nanomaterial-Coated Cs₃Sb Heterostructures for High-Performance Photocathodes. Journal of Physical Chemistry C, 2020, 124, 26396-26403.	3.1	3
53	Tuning the optical properties of BODIPY dyes by N-rich heterocycle conjugation using a combined synthesis and computational approach. New Journal of Chemistry, 2021, 45, 19641-19645.	2.8	3
54	Nearâ€Unity Triplet Generation Promoted via Spiroâ€Conjugation. Angewandte Chemie, 2022, 134, e202113190.	2.0	3

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55	Excited State Dynamics of Methylated Guanosine Derivatives Revealed by Femtosecond Timeâ€resolved Spectroscopy. Photochemistry and Photobiology, 2022, 98, 1008-1016.	2.5	2
56	Dissociative Ionization of Molecular CF2Br2 under 800 and 400 nm Intense Femtosecond Laser Fields. Applied Sciences (Switzerland), 2021, 11, 1704.	2.5	1
57	Simulation of Negative Ion Photoelectron Spectroscopy Using a Nuclear Ensemble Approach: Implications from a Nuclear Vibration Effect. Journal of Physical Chemistry A, 2021, 125, 6621-6628.	2.5	1