Zhigang Shuai

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

405 papers	23,646 citations	82 h-index	139 g-index
432 ext. papers	26,553 ext. citations	7.5 avg, IF	7.15 L-index

#	Paper	IF	Citations
405	A Novel Strategy toward Thermally Activated Delayed Fluorescence from a Locally Excited State.. *Journal of Physical Chemistry Letters*, **2022**, 2653-2660	6.4	3
404	Computational modeling of AIE luminogens **2022**, 639-667		
403	Sunlight-coordinated high-performance Moisture Power in Natural Condition.. *Advanced Materials*, **2021**, e2103897	24	9
402	Catechol Moiety Integrated Tri-Aryl Type AIEgen for Visual and Quantitative Boronic Acid Detection. *Chemistry - A European Journal*, **2021**, 28, e202103351	4.8	0
401	Time-dependent density matrix renormalization group coupled with n-mode representation potentials for the excited state radiationless decay rate: Formalism and application to azulene *Chinese Journal of Chemical Physics*, **2021**, 34, 565-582	0.9	3
400	Effect of Strong Intermolecular Interaction in 2D Inorganic Molecular Crystals. *Journal of the American Chemical Society*, **2021**, 143, 20192-20201	16.4	3
399	Emerging technologies for a more sustainable future. *Pure and Applied Chemistry*, **2021**,	2.1	1
398	Heavy-Atom-Free Room-Temperature Phosphorescent Rylene Imide for High-Performing Organic Photovoltaics. *Advanced Science*, **2021**, e2103975	13.6	3
397	AIEgens with cyano-modification in different sites: Potential Meta-site effect in mechanochromism behavior. *Dyes and Pigments*, **2021**, 198, 109939	4.6	
396	Enhanced Reverse Intersystem Crossing Promoted by Triplet Exciton-Photon Coupling. *Journal of the American Chemical Society*, **2021**, 143, 17786-17792	16.4	2
395	Front Cover: Molecular mechanism of aggregation-induced emission. *Aggregate*, **2021**, 2, e134	22.9	
394	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. *Journal of Physical Chemistry Letters*, **2021**, 12, 2712-2720	6.4	13
393	Aggregation-Enhanced Thermally Activated Delayed Fluorescence Efficiency for Two-Coordinate Carbene-Metal-Amide Complexes: A QM/MM Study. *Journal of Physical Chemistry Letters*, **2021**, 12, 2944-2953	6.4	12
392	Intrinsic hydroquinone-functionalized aggregation-induced emission core shows redox and pH sensitivity. *Communications Chemistry*, **2021**, 4,	6.3	2
391	Creating Side Transport Pathways in Organic Solar Cells by Introducing Delayed Fluorescence Molecules. *Chemistry of Materials*, **2021**, 33, 4578-4585	9.6	4
390	Supramolecular engineering of charge transfer in wide bandgap organic semiconductors with enhanced visible-to-NIR photoresponse. *Nature Communications*, **2021**, 12, 3667	17.4	8
389	Evaluating the anharmonicity contributions to the molecular excited state internal conversion rates with finite temperature TD-DMRG. *Journal of Chemical Physics*, **2021**, 154, 214109	3.9	7

388	Intermolecular Charge-Transfer-Induced Strong Optical Emission from Herringbone H-Aggregates. *Nano Letters*, **2021**, 21, 5394-5400	11.5	5
387	A general charge transport picture for organic semiconductors with nonlocal electron-phonon couplings. *Nature Communications*, **2021**, 12, 4260	17.4	9
386	Ferroelectricity in 2D metal phosphorus trichalcogenides and van der Waals heterostructures for photocatalytic water splitting. *Journal of Materials Chemistry A*, **2021**, 9, 2734-2741	13	8
385	Simultaneous studies of pressure effect on charge transport and photophysical properties in organic semiconductors: A theoretical investigation. *Chinese Chemical Letters*, **2021**, 32, 1233-1236	8.1	1
384	Theory of Long-Lived Room-Temperature Phosphorescence in Organic Aggregates. *Accounts of Chemical Research*, **2021**, 54, 940-949	24.3	46
383	Influences of dynamic and static disorder on the carrier mobility of BTBT-C12 derivatives: a multiscale computational study. *Nanoscale*, **2021**, 13, 3252-3262	7.7	3
382	Molecular Design Strategy for Simultaneously Strong Luminescence and High Mobility: Multichannel CH-□Interaction. *Journal of Physical Chemistry Letters*, **2021**, 12, 938-946	6.4	4
381	Theoretical Characterizations of TADF Materials: Roles of □and the Singlet-Triplet Excited States Interconversion. *Journal of Physical Chemistry A*, **2021**, 125, 1468-1475	2.8	14
380	Abnormal Seebeck effect in doped conducting polymers. *Applied Physics Letters*, **2021**, 118, 123301	3.4	1
379	Future directions of chemical theory and computation. *Pure and Applied Chemistry*, **2021**,	2.1	1
378	High Mobility Organic Lasing Semiconductor with Crystallization-Enhanced Emission for Light-Emitting Transistors. *Angewandte Chemie*, **2021**, 133, 20436-20441	3.6	1
377	Brightening up Circularly Polarized Luminescence of Monosubstituted Polyacetylene by Conformation Control: Mechanism, Switching, and Sensing. *Angewandte Chemie*, **2021**, 133, 22089-22097	3.6	3
376	Quantum-electrodynamical time-dependent density functional theory within Gaussian atomic basis. *Journal of Chemical Physics*, **2021**, 155, 064107	3.9	8
375	Brightening up Circularly Polarized Luminescence of Monosubstituted Polyacetylene by Conformation Control: Mechanism, Switching, and Sensing. *Angewandte Chemie - International Edition*, **2021**, 60, 21918-21926	16.4	15
374	High Mobility Organic Lasing Semiconductor with Crystallization-Enhanced Emission for Light-Emitting Transistors. *Angewandte Chemie - International Edition*, **2021**, 60, 20274-20279	16.4	6
373	Intermolecular charge-transfer aggregates enable high-efficiency near-infrared emissions by nonadiabatic coupling suppression. *Science China Chemistry*, **2021**, 64, 1786	7.9	4
372	Chebyshev Matrix Product States with Canonical Orthogonalization for Spectral Functions of Many-Body Systems. *Journal of Physical Chemistry Letters*, **2021**, 12, 9344-9352	6.4	2
371	A computational scheme for evaluating the phosphorescence quantum efficiency: applied to blue-emitting tetradentate Pt(II) complexes. *Materials Horizons*, **2021**,	14.4	5

370	Synergistic Optimization Enables Large-Area Flexible Organic Solar Cells to Maintain over 98% PCE of the Small-Area Rigid Devices. *Advanced Materials*, **2020**, 32, e2005153	24	38
369	Thermal Vibration Correlation Function Formalism for Molecular Excited State Decay Rates. *Chinese Journal of Chemistry*, **2020**, 38, 1223-1232	4.9	41
368	Finite-Temperature TD-DMRG for the Carrier Mobility of Organic Semiconductors. *Journal of Physical Chemistry Letters*, **2020**, 11, 4930-4936	6.4	13
367	Biradical-Featured Stable Organic-Small-Molecule Photothermal Materials for Highly Efficient Solar-Driven Water Evaporation. *Advanced Materials*, **2020**, 32, e1908537	24	53
366	Theoretical and Experimental Investigations on the Aggregation-Enhanced Emission from Dark State: Vibronic Coupling Effect. *Advanced Electronic Materials*, **2020**, 6, 2000255	6.4	14
365	Organic Laser Molecule with High Mobility, High Photoluminescence Quantum Yield, and Deep-Blue Lasing Characteristics. *Journal of the American Chemical Society*, **2020**, 142, 6332-6339	16.4	53
364	Computational Study on the Charge Transport and Optical Spectra of Anthracene Derivatives in Aggregates. *ChemPhysChem*, **2020**, 21, 952-957	3.2	6
363	Numerical assessment for accuracy and GPU acceleration of TD-DMRG time evolution schemes. *Journal of Chemical Physics*, **2020**, 152, 024127	3.9	21
362	Finite Temperature Dynamical Density Matrix Renormalization Group for Spectroscopy in Frequency Domain. *Journal of Physical Chemistry Letters*, **2020**, 11, 3761-3768	6.4	12
361	A general automatic method for optimal construction of matrix product operators using bipartite graph theory. *Journal of Chemical Physics*, **2020**, 153, 084118	3.9	9
360	Toward Quantitative Prediction of Fluorescence Quantum Efficiency by Combining Direct Vibrational Conversion and Surface Crossing: BODIPYs as an Example. *Journal of Physical Chemistry Letters*, **2020**, 11, 7790-7797	6.4	25
359	Experimentally Observed Reverse Intersystem Crossing-Boosted Lasing. *Angewandte Chemie*, **2020**, 132, 21861-21866	3.6	2
358	Experimentally Observed Reverse Intersystem Crossing-Boosted Lasing. *Angewandte Chemie - International Edition*, **2020**, 59, 21677-21682	16.4	25
357	Simultaneously and Selectively Imaging a Cytoplasm Membrane and Mitochondria Using a Dual-Colored Aggregation-Induced Emission Probe. *Analytical Chemistry*, **2020**, 92, 14494-14500	7.8	16
356	A novel molecular descriptor for highly efficient (?TADF > 90%) transition metal TADF Au(III) complexes. *Journal of Materials Chemistry A*, **2020**, 8, 18721-18725	13	11
355	Applying Marcus theory to describe the carrier transports in organic semiconductors: Limitations and beyond. *Journal of Chemical Physics*, **2020**, 153, 080902	3.9	21
354	Computational screen-out strategy for electrically pumped organic laser materials. *Nature Communications*, **2020**, 11, 4485	17.4	27
353	Toward Achieving Single-Molecule White Electroluminescence from Dual Emission of Fluorescence and Phosphorescence. *Chemistry of Materials*, **2020**, 32, 4038-4044	9.6	26

352	Long Persistent Luminescence Enabled by Dissociation of Triplet Intermediate States in an Organic Guest/Host System. *Journal of Physical Chemistry Letters*, **2020**, 11, 3582-3588	6.4	7
351	Festschrift in Honor of Prof. Jean-Luc Brédas on His 65th Birthday. *Chemistry of Materials*, **2019**, 31, 6307-6308	9.6	0
350	High-Performance Organic Thermoelectric Materials: Theoretical Insights and Computational Design. *Advanced Electronic Materials*, **2019**, 5, 1800882	6.4	24
349	Highly Efficient Thermally Activated Delayed Fluorescence via J-Aggregates with Strong Intermolecular Charge Transfer. *Advanced Materials*, **2019**, 31, e1808242	24	164
348	Reducing Lattice Thermal Conductivity of the Thermoelectric SnSe Monolayer: Role of Phonon–Electron Coupling. *Journal of Physical Chemistry C*, **2019**, 123, 12001-12006	3.8	11
347	Boosting the Seebeck Coefficient for Organic Coordination Polymers: Role of Doping-Induced Polaron Band Formation. *Journal of Physical Chemistry Letters*, **2019**, 10, 2493-2499	6.4	9
346	Superexchange Induced Charge Transport in Organic Donor–Acceptor Cocrystals and Copolymers: A Theoretical Perspective. *Chemistry of Materials*, **2019**, 31, 6424-6434	9.6	20
345	Hydrogen Bonding-Induced Morphology Dependence of Long-Lived Organic Room-Temperature Phosphorescence: A Computational Study. *Journal of Physical Chemistry Letters*, **2019**, 10, 6948-6954	6.4	45
344	Strong Solid-State Fluorescence Induced by Restriction of the Coordinate Bond Bending in Two-Coordinate Copper(I)-Carbene Complexes. *Inorganic Chemistry*, **2019**, 58, 14403-14409	5.1	22
343	Pressure-induced emission enhancement in hexaphenylsilole: a computational study. *Journal of Materials Chemistry C*, **2019**, 7, 1388-1398	7.1	19
342	Highly Efficient Organic Room-Temperature Phosphorescent Luminophores through Tuning Triplet States and Spin-Orbit Coupling with Incorporation of a Secondary Group. *Journal of Physical Chemistry Letters*, **2019**, 10, 7141-7147	6.4	14
341	Efficient and Long-Lived Room-Temperature Organic Phosphorescence: Theoretical Descriptors for Molecular Designs. *Journal of the American Chemical Society*, **2019**, 141, 1010-1015	16.4	228
340	Understanding Carrier Transport in Organic Semiconductors: Computation of Charge Mobility Considering Quantum Nuclear Tunneling and Delocalization Effects. *Journal of Chemical Theory and Computation*, **2019**, 15, 1477-1491	6.4	22
339	The isotope effect on charge transport for bithiophene and di(n-hexyl)-bithiophene: impacts of deuteration position, deuteration number and side chain substitution position. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	1
338	General Approach To Compute Phosphorescent OLED Efficiency. *Journal of Physical Chemistry C*, **2018**, 122, 6340-6347	3.8	57
337	From Molecular Packing Structures to Electronic Processes: Theoretical Simulations for Organic Solar Cells. *Advanced Energy Materials*, **2018**, 8, 1702743	21.8	73
336	MOlecular MAterials Property Prediction Package (MOMAP) 1.0: a software package for predicting the luminescent properties and mobility of organic functional materials. *Molecular Physics*, **2018**, 116, 1078-1090	1.7	110
335	From Alloy-Like to Cascade Blended Structure: Designing High-Performance All-Small-Molecule Ternary Solar Cells. *Journal of the American Chemical Society*, **2018**, 140, 1549-1556	16.4	113

334	Lattice thermal conductivity of monolayer AsP from first-principles molecular dynamics. *Physical Chemistry Chemical Physics*, **2018**, 20, 14024-14030	3.6	20
333	Asymmetric photon transport in organic semiconductor nanowires through electrically controlled exciton diffusion. *Science Advances*, **2018**, 4, eaap9861	14.3	39
332	Dynamic Ultralong Organic Phosphorescence by Photoactivation. *Angewandte Chemie*, **2018**, 130, 8561-8567	3.6	39
331	Highly sensitive switching of solid-state luminescence by controlling intersystem crossing. *Nature Communications*, **2018**, 9, 3044	17.4	146
330	Roles of Long-Range Hopping, Quantum Nuclear Effect, and Exciton Delocalization in Exciton Transport in Organic Semiconductors: A Multiscale Study. *Journal of Physical Chemistry C*, **2018**, 122, 18365-18375	3.8	10
329	A facile strategy for realizing room temperature phosphorescence and single molecule white light emission. *Nature Communications*, **2018**, 9, 2963	17.4	216
328	Time-Dependent Density Matrix Renormalization Group Algorithms for Nearly Exact Absorption and Fluorescence Spectra of Molecular Aggregates at Both Zero and Finite Temperature. *Journal of Chemical Theory and Computation*, **2018**, 14, 5027-5039	6.4	52
327	Theoretical insights into molecular blending on charge transport properties in organic semiconductors based on quantum nuclear tunneling model. *Journal of Photonics for Energy*, **2018**, 8, 1	1.2	1
326	Theoretical Studies on the Deformation Potential, Electron-Phonon Coupling, and Carrier Transports of Layered Systems. *Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica*, **2018**, 34, 961-976	3.8	13
325	Janus monolayer of WSeTe, a new structural phase transition material driven by electrostatic gating. *Nanoscale*, **2018**, 10, 21629-21633	7.7	41
324	High performance thermoelectric materials based on metal organic coordination polymers through first-principles band engineering. *Journal of Computational Chemistry*, **2018**, 39, 2582-2588	3.5	8
323	Suppressing charge recombination in small-molecule ternary organic solar cells by modulating donor-acceptor interfacial arrangements. *Physical Chemistry Chemical Physics*, **2018**, 20, 24570-24576	3.6	9
322	Effect of donor length on electronic structures and charge transport polarity for DTDPP-based D-A copolymers: a computational study based on a super-exchange model. *Journal of Materials Chemistry A*, **2018**, 6, 11985-11993	13	15
321	Dynamic Ultralong Organic Phosphorescence by Photoactivation. *Angewandte Chemie - International Edition*, **2018**, 57, 8425-8431	16.4	158
320	Organic light-emitting diodes: theoretical understanding of highly efficient materials and development of computational methodology. *National Science Review*, **2017**, 4, 224-239	10.8	94
319	Doping optimization of organic-inorganic hybrid perovskite CH3NH3PbI3 for high thermoelectric efficiency. *Synthetic Metals*, **2017**, 225, 108-114	3.6	27
318	Theoretical Investigations on the Roles of Intramolecular Structure Distortion versus Irregular Intermolecular Packing in Optical Spectra of 6T Nanoparticles. *Chemistry of Materials*, **2017**, 29, 2513-2520	9.6	17
317	Super-exchange-induced high performance charge transport in donor-acceptor copolymers. *Journal of Materials Chemistry C*, **2017**, 5, 3247-3253	7.1	34

316	Role of the Dark 2A State in Donor-Acceptor Copolymers as a Pathway for Singlet Fission: A DMRG Study. *Journal of Physical Chemistry Letters*, **2017**, 8, 2175-2181	6.4	25
315	Theoretical Study of Conversion and Decay Processes of Excited Triplet and Singlet States in a Thermally Activated Delayed Fluorescence Molecule. *Journal of Physical Chemistry C*, **2017**, 121, 13448-13456	3.8	91
314	Real-time monitoring of hydrophobic aggregation reveals a critical role of cooperativity in hydrophobic effect. *Nature Communications*, **2017**, 8, 15639	17.4	47
313	Excitonic coupling effect on the nonradiative decay rate in molecular aggregates: Formalism and application. *Chemical Physics Letters*, **2017**, 683, 507-514	2.5	21
312	A-D-A Electron-Donating Small Molecules for Solution-Processed Organic Solar Cells: A Review. *Macromolecular Rapid Communications*, **2017**, 38, 1700470	4.8	55
311	Intrinsic Charge Transport in Stanene: Roles of Bucklings and Electron–Phonon Couplings. *Advanced Electronic Materials*, **2017**, 3, 1700143	6.4	38
310	White light emission from a single organic molecule with dual phosphorescence at room temperature. *Nature Communications*, **2017**, 8, 416	17.4	457
309	Tuning Thermal Transport in Chain-Oriented Conducting Polymers for Enhanced Thermoelectric Efficiency: A Computational Study. *Advanced Functional Materials*, **2017**, 27, 1702847	15.6	41
308	Isoindigo-Based Polymers with Small Effective Masses for High-Mobility Ambipolar Field-Effect Transistors. *Advanced Materials*, **2017**, 29, 1702115	24	91
307	Puckered Arsenene: A Promising Room-Temperature Thermoelectric Material from First-Principles Prediction. *Journal of Physical Chemistry C*, **2017**, 121, 19080-19086	3.8	42
306	GeAs2: A IV–V Group Two-Dimensional Semiconductor with Ultralow Thermal Conductivity and High Thermoelectric Efficiency. *Chemistry of Materials*, **2017**, 29, 6261-6268	9.6	57
305	Strain induced polymorphism and band structure modulation in low-temperature 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene single crystal. *Science China Chemistry*, **2017**, 60, 275-283	7.9	3
304	Electrostatic Interaction-Induced Room-Temperature Phosphorescence in Pure Organic Molecules from QM/MM Calculations. *Journal of Physical Chemistry Letters*, **2016**, 7, 2893-8	6.4	96
303	Intrinsic and Extrinsic Charge Transport in CH3NH3PbI3 Perovskites Predicted from First-Principles. *Scientific Reports*, **2016**, 7, 19968	4.9	103
302	Gibbs-Curie-Wulff Theorem in Organic Materials: A Case Study on the Relationship between Surface Energy and Crystal Growth. *Advanced Materials*, **2016**, 28, 1697-702	24	55
301	Triplet-Polaron-Interaction-Induced Upconversion from Triplet to Singlet: a Possible Way to Obtain Highly Efficient OLEDs. *Advanced Materials*, **2016**, 28, 4740-6	24	107
300	The Impact of Interlayer Electronic Coupling on Charge Transport in Organic Semiconductors: A Case Study on Titanylphthalocyanine Single Crystals. *Angewandte Chemie - International Edition*, **2016**, 55, 5206-9	16.4	38
299	Unraveling the aggregation effect on amorphous phase AIE luminogens: a computational study. *Nanoscale*, **2016**, 8, 15173-80	7.7	77

298	Understanding the efficiency drooping of the deep blue organometallic phosphors: a computational study of radiative and non-radiative decay rates for triplets. *Journal of Materials Chemistry C*, **2016**, 4, 6829-6838	7.1	66
297	Naphtho[1,2-b:5,6-b?]dithiophene-Based Small Molecules for Thick-Film Organic Solar Cells with High Fill Factors. *Chemistry of Materials*, **2016**, 28, 943-950	9.6	44
296	Nuclear quantum tunnelling and carrier delocalization effects to bridge the gap between hopping and bandlike behaviors in organic semiconductors. *Nanoscale Horizons*, **2016**, 1, 53-59	10.8	43
295	Effect of Intermolecular Excited-state Interaction on Vibrationally Resolved Optical Spectra in Organic Molecular Aggregates. *Acta Chimica Sinica*, **2016**, 74, 902	3.3	20
294	The Impact of Interlayer Electronic Coupling on Charge Transport in Organic Semiconductors: A Case Study on Titanylphthalocyanine Single Crystals. *Angewandte Chemie*, **2016**, 128, 5292-5295	3.6	5
293	Influence of alkyl side-chain length on the carrier mobility in organic semiconductors: herringbone vs. pi–pi stacking. *Journal of Materials Chemistry C*, **2016**, 4, 4546-4555	7.1	64
292	Efficient ambipolar transport properties in alternate stacking donor-acceptor complexes: from experiment to theory. *Physical Chemistry Chemical Physics*, **2016**, 18, 14094-103	3.6	52
291	Using the isotope effect to probe an aggregation induced emission mechanism: theoretical prediction and experimental validation. *Chemical Science*, **2016**, 7, 5573-5580	9.4	49
290	Indirect-to-Direct Band Gap Crossover in Few-Layer Transition Metal Dichalcogenides: A Theoretical Prediction. *Journal of Physical Chemistry C*, **2016**, 120, 21866-21870	3.8	66
289	Inner Space Perturbation Theory in Matrix Product States: Replacing Expensive Iterative Diagonalization. *Journal of Chemical Theory and Computation*, **2016**, 12, 4871-4878	6.4	16
288	Rational Molecular Design for Achieving Persistent and Efficient Pure Organic Room-Temperature Phosphorescence. *CheM*, **2016**, 1, 592-602	16.2	399
287	Theoretical Insights into the Mechanism of AIE. *ACS Symposium Series*, **2016**, 35-59	0.4	2
286	Theoretical Modeling of the Optical and Electrical Processes in Polymeric Solar Cells. *Topics in Applied Physics*, **2015**, 101-142	0.5	5
285	Unravelling Doping Effects on PEDOT at the Molecular Level: From Geometry to Thermoelectric Transport Properties. *Journal of the American Chemical Society*, **2015**, 137, 12929-38	16.4	129
284	Polymorphism-Dependent and Switchable Emission of Butterfly-Like Bis(diarylmethylene)dihydroanthracenes. *Chemistry of Materials*, **2015**, 27, 6601-6607	9.6	131
283	Solvent effects on the optical spectra and excited-state decay of triphenylamine-thiadiazole with hybridized local excitation and intramolecular charge transfer. *Journal of Physical Chemistry A*, **2015**, 119, 5233-40	2.8	55
282	Mechanism of charge transport in organic semiconductors and carbon nanomaterials. *Materials Research Society Symposia Proceedings*, **2015**, 1733, 1		
281	Influences of Conjugation Extent on the Aggregation-Induced Emission Quantum Efficiency in Silole Derivatives: A Computational Study. *Chemistry - an Asian Journal*, **2015**, 10, 2154-61	4.5	26

280	Synergistic Photomodulation of Capacitive Coupling and Charge Separation Toward Functional Organic Field-Effect Transistors with High Responsivity. *Advanced Electronic Materials*, **2015**, 1, 1500159	6.4	24
279	Thin film field-effect transistors of 2,6-diphenyl anthracene (DPA). *Chemical Communications*, **2015**, 51, 11777-9	5.8	78
278	Negative isotope effect for charge transport in acenes and derivatives--a theoretical conclusion. *Physical Chemistry Chemical Physics*, **2015**, 17, 3273-80	3.6	17
277	Electronic properties and charge carrier mobilities of graphynes and graphdiynes from first principles. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 215-227	7.9	34
276	Spectroscopic Signature of the Aggregation-Induced Emission Phenomena Caused by Restricted Nonradiative Decay: A Theoretical Proposal. *Journal of Physical Chemistry C*, **2015**, 119, 5040-5047	3.8	59
275	Understanding the charge transport and polarities in organic donor-acceptor mixed-stack crystals: molecular insights from the super-exchange couplings. *Advanced Materials*, **2015**, 27, 1443-9	24	79
274	Comparative study on the methodologies for calculating the excited state in DMRG. *Scientia Sinica Chimica*, **2015**, 45, 1316-1324	1.6	2
273	Rubrene analogues with the aggregation-induced emission enhancement behaviour. *Journal of Materials Chemistry C*, **2014**, 2, 884-890	7.1	21
272	Excited states structure and processes: Understanding organic light-emitting diodes at the molecular level. *Physics Reports*, **2014**, 537, 123-156	27.7	154
271	Tunable Electronic Properties of Two-Dimensional Transition Metal Dichalcogenide Alloys: A First-Principles Prediction. *Journal of Physical Chemistry Letters*, **2014**, 5, 285-91	6.4	77
270	Aggregation induced blue-shifted emission--the molecular picture from a QM/MM study. *Physical Chemistry Chemical Physics*, **2014**, 16, 5545-52	3.6	138
269	From charge transport parameters to charge mobility in organic semiconductors through multiscale simulation. *Chemical Society Reviews*, **2014**, 43, 2662-79	58.5	162
268	Nonadiabatic Molecular Dynamics Modeling of the Intrachain Charge Transport in Conjugated Diketopyrrolo-pyrrole Polymers. *Journal of Physical Chemistry C*, **2014**, 118, 6631-6640	3.8	26
267	Enhancement of the p-channel performance of sulfur-bridged annulene through a donor–acceptor co-crystal approach. *Journal of Materials Chemistry C*, **2014**, 2, 8886-8891	7.1	22
266	Electron-phonon couplings and carrier mobility in graphynes sheet calculated using the Wannier-interpolation approach. *Journal of Chemical Physics*, **2014**, 141, 034704	3.9	52
265	Aggregation effects on the optical emission of 1,1,2,3,4,5-hexaphenylsilole (HPS): a QM/MM study. *Journal of Physical Chemistry A*, **2014**, 118, 9094-104	2.8	92
264	First-principles investigations on the anisotropic charge transport in 4,4?-bis((E)-2-(naphthalen-2-yl)vinyl)-1,1?-biphenyl single crystal. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	1
263	Search for Organic Thermoelectric Materials with High Mobility: The Case of 2,7-Dialkyl[1]benzothieno[3,2-b][1]benzothiophene Derivatives. *Chemistry of Materials*, **2014**, 26, 2669-2677	9.6	66

262	Theoretical Prediction of Isotope Effects on Charge Transport in Organic Semiconductors. *Journal of Physical Chemistry Letters*, **2014**, 5, 2267-73	6.4	24
261	A □licked□porphyrin cage with high binding affinity towards fullerenes. *RSC Advances*, **2014**, 4, 27389-27392	3.7	16
260	Understanding Lattice Strain-Controlled Charge Transport in Organic Semiconductors: A Computational Study. *Advanced Functional Materials*, **2014**, 24, 5531-5540	15.6	25
259	Charge-transfer complex crystal based on extended-□conjugated acceptor and sulfur-bridged annulene: charge-transfer interaction and remarkable high ambipolar transport characteristics. *Advanced Materials*, **2014**, 26, 4093-9	24	119
258	Computational evaluation of optoelectronic properties for organic/carbon materials. *Accounts of Chemical Research*, **2014**, 47, 3301-9	24.3	54
257	Interface electronic structures of reversible double-docking self-assembled monolayers on an Au(111) surface. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, 20130018	3	7
256	Naphtho[1,2-b:5,6-b?]dithiophene Based Two-Dimensional Conjugated Polymers for Highly Efficient Thick-Film Inverted Polymer Solar Cells. *Chemistry of Materials*, **2014**, 26, 6947-6954	9.6	40
255	Charge Transport: Understanding Lattice Strain-Controlled Charge Transport in Organic Semiconductors: A Computational Study (Adv. Funct. Mater. 35/2014). *Advanced Functional Materials*, **2014**, 24, 5530-5530	15.6	
254	Chemical Sciences: Contributions to Building a Sustainable Society and Sharing of International Responsibilities. *ACS Symposium Series*, **2014**, 101-139	0.4	
253	Spectral Signature of Intrachain and Interchain Polarons in Donor-Acceptor Copolymers. *Acta Chimica Sinica*, **2014**, 72, 201	3.3	6
252	Substitution effects on the electrical tranporting properties of tetrathia[22]annulene[2,1,2,1]: experimental and theoretical investigations. *Journal of Materials Chemistry C*, **2013**, 1, 5765	7.1	14
251	Theoretical study of the low-lying electronic excited states for molecular aggregates. *Science China Chemistry*, **2013**, 56, 1258-1262	7.9	15
250	From electronic excited state theory to the property predictions of organic optoelectronic materials. *Science China Chemistry*, **2013**, 56, 1277-1284	7.9	14
249	Spectroscopic Study of Electron and Hole Polarons in a High-Mobility Donor□Acceptor Conjugated Copolymer. *Journal of Physical Chemistry C*, **2013**, 117, 6835-6841	3.8	28
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