Zhigang Shuai

List of Publications by Year
in descending order

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418 papers	29,610 citations	3933 88 h-index	6996 154 g-index
432 all docs	432 docs citations	432 times ranked	22212 citing authors

#	Article	IF	Citations
1	Efficient Degradation of Toxic Organic Pollutants with Ni2O3/TiO2-xBx under Visible Irradiation. Journal of the American Chemical Society, 2004, 126, 4782-4783.	13.7	1,105
2	Electronic Structure and Carrier Mobility in Graphdiyne Sheet and Nanoribbons: Theoretical Predictions. ACS Nano, 2011, 5, 2593-2600.	14.6	833
3	White light emission from a single organic molecule with dual phosphorescence at room temperature. Nature Communications, 2017, 8, 416.	12.8	621
4	Rational Molecular Design for Achieving Persistent and Efficient Pure Organic Room-Temperature Phosphorescence. CheM, 2016, 1, 592-602.	11.7	610
5	First-principles prediction of charge mobility in carbon and organic nanomaterials. Nanoscale, 2012, 4, 4348.	5.6	551
6	Tunable Band Gap Photoluminescence from Atomically Thin Transition-Metal Dichalcogenide Alloys. ACS Nano, 2013, 7, 4610-4616.	14.6	543
7	Structures, Electronic States, Photoluminescence, and Carrier Transport Properties of 1,1-Disubstituted 2,3,4,5-Tetraphenylsiloles. Journal of the American Chemical Society, 2005, 127, 6335-6346.	13.7	490
8	Toward Quantitative Prediction of Molecular Fluorescence Quantum Efficiency:â€‰ Role of Duschinsky Rotation. Journal of the American Chemical Society, 2007, 129, 9333-9339.	13.7	414
9	Computational methods for design of organic materials with high charge mobility. Chemical Society Reviews, 2010, 39, 423-434.	38.1	412
10	Efficient and Long-Lived Room-Temperature Organic Phosphorescence: Theoretical Descriptors for Molecular Designs. Journal of the American Chemical Society, 2019, 141, 1010-1015.	13.7	389
11	Title is missing!. Advanced Functional Materials, 2002, 12, 631-641.	14.9	366
12	Theory of Excited State Decays and Optical Spectra: Application to Polyatomic Molecules. Journal of Physical Chemistry A, 2010, 114, 7817-7831.	2.5	363
13	A facile strategy for realizing room temperature phosphorescence and single molecule white light emission. Nature Communications, 2018, 9, 2963.	12.8	339
14	Carrier Mobility in Graphyne Should Be Even Larger than That in Graphene: A Theoretical Prediction. Journal of Physical Chemistry Letters, 2013, 4, 1443-1448.	4.6	328
15	Charge separation in localized and delocalized electronic states in polymeric semiconductors. Nature, 1998, 392, 903-906.	27.8	321
16	Spinâ^'Orbit Coupling and Intersystem Crossing in Conjugated Polymers:Â A Configuration Interaction Description. Journal of Physical Chemistry A, 2001, 105, 3899-3907.	2.5	315
17	Structures, Electronic States, and Electroluminescent Properties of a Zinc(II) 2-(2-Hydroxyphenyl)benzothiazolate Complex. Journal of the American Chemical Society, 2003, 125, 14816-14824.	13.7	296
18	Theoretical Predictions of Size-Dependent Carrier Mobility and Polarity in Graphene. Journal of the American Chemical Society, 2009, 131, 17728-17729.	13.7	291

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19	Excited-State Electronic Structure of Conjugated Oligomers and Polymers:â€‰ A Quantum-Chemical Approach to Optical Phenomena. Accounts of Chemical Research, 1999, 32, 267-276.	15.6	286
20	Influences of Crystal Structures and Molecular Sizes on the Charge Mobility of Organic Semiconductors: Oligothiophenes. Chemistry of Materials, 2008, 20, 3205-3211.	6.7	284
21	Highly Efficient Thermally Activated Delayed Fluorescence via Jâ€Aggregates with Strong Intermolecular Charge Transfer. Advanced Materials, 2019, 31, e1808242.	21.0	278
22	Size-Tunable Emission from 1,3-Diphenyl-5-(2-anthryl)-2-pyrazoline Nanoparticles. Journal of the American Chemical Society, 2003, 125, 6740-6745.	13.7	271
23	Excited states structure and processes: Understanding organic light-emitting diodes at the molecular level. Physics Reports, 2014, 537, 123-156.	25.6	264
24	Intersystem Crossing Processes in Nonplanar Aromatic Heterocyclic Molecules. Journal of Physical Chemistry A, 2007, 111, 10490-10499.	2.5	261
25	Solution-Processed, High-Performance Nanoribbon Transistors Based on Dithioperylene. Journal of the American Chemical Society, 2011, 133, 1-3.	13.7	255
26	Singlet and Triplet Exciton Formation Rates in Conjugated Polymer Light-Emitting Diodes. Physical Review Letters, 2000, 84, 131-134.	7.8	254
27	An Ultra Closely Ï€â€Stacked Organic Semiconductor for High Performance Fieldâ€Effect Transistors. Advanced Materials, 2007, 19, 2613-2617.	21.0	247
28	Nuclear tunneling effects of charge transport in rubrene, tetracene, and pentacene. Physical Review B, 2009, 79, .	3.2	247
29	Dynamic Ultralong Organic Phosphorescence by Photoactivation. Angewandte Chemie - International Edition, 2018, 57, 8425-8431.	13.8	241
30	A Cyclic Triphenylamine Dimer for Organic Field-Effect Transistors with High Performance. Journal of the American Chemical Society, 2006, 128, 15940-15941.	13.7	225
31	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	222
32	Excited state radiationless decay process with Duschinsky rotation effect: Formalism and implementation. Journal of Chemical Physics, 2007, 126, 114302.	3.0	213
33	From charge transport parameters to charge mobility in organic semiconductors through multiscale simulation. Chemical Society Reviews, 2014, 43, 2662.	38.1	210
34	Sulfurâ€Bridged Annuleneâ€TCNQ Coâ€Crystal: A Selfâ€Assembled â€˜â€˜Molecular Level Heterojunctionâ€™â€™ with Air Stable Ambipolar Charge Transport Behavior. Advanced Materials, 2012, 24, 2603-2607.	21.0	207
35	Extended Squaraine Dyes with Large Two-Photon Absorption Cross-Sections. Journal of the American Chemical Society, 2006, 128, 14444-14445.	13.7	205
36	Highly sensitive switching of solid-state luminescence by controlling intersystem crossing. Nature Communications, 2018, 9, 3044.	12.8	203

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37	Correlation Function Formalism for Triplet Excited State Decay: Combined Spinâ€“Orbit and Nonadiabatic Couplings. Journal of Chemical Theory and Computation, 2013, 9, 1132-1143.	5.3	198
38	1,3-Dithiole-2-thione derivatives featuring an anthracene unit: new selective chemodosimeters for Hg(ii) ion. Chemical Communications, 2005, , 2161.	4.1	194
39	Theoretical modelling of carrier transports in molecular semiconductors: molecular design of triphenylamine dimer systems. Nanotechnology, 2007, 18, 424029.	2.6	180
40	Molecular mechanism of aggregationâ€induced emission. Aggregate, 2021, 2, e91.	9.9	179
41	Unravelling Doping Effects on PEDOT at the Molecular Level: From Geometry to Thermoelectric Transport Properties. Journal of the American Chemical Society, 2015, 137, 12929-12938.	13.7	176
42	Organic light-emitting diodes: theoretical understanding of highly efficient materials and development of computational methodology. National Science Review, 2017, 4, 224-239.	9.5	176
43	Fullerene/Sulfur-Bridged Annulene Cocrystals: Two-Dimensional Segregated Heterojunctions with Ambipolar Transport Properties and Photoresponsivity. Journal of the American Chemical Society, 2013, 135, 558-561.	13.7	174
44	Theoretical investigation of the lowest singlet and triplet states in poly(paraphenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 462 Td (vir	3.0	169
45	Promoting-mode free formalism for excited state radiationless decay process with Duschinsky rotation effect. Science in China Series B: Chemistry, 2008, 51, 1153-1158.	0.8	168
46	Aggregation induced blue-shifted emission â€“ the molecular picture from a QM/MM study. Physical Chemistry Chemical Physics, 2014, 16, 5545-5552.	2.8	162
47	Improving the efficiency of solution processable organic photovoltaic devices by a star-shaped molecular geometry. Journal of Materials Chemistry, 2008, 18, 4085.	6.7	160
48	Balanced Carrier Transports of Electrons and Holes in Silole-Based CompoundsA Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 7138-7143.	2.5	159
49	Multifunctional bipolar triphenylamine/oxadiazole derivatives: highly efficient blue fluorescence, red phosphorescence host and two-color based white OLEDs. Chemical Communications, 2009, , 77-79.	4.1	159
50	Thermal Vibration Correlation Function Formalism for Molecular Excited State Decay Rates. Chinese Journal of Chemistry, 2020, 38, 1223-1232.	4.9	157
51	Multiscale study of charge mobility of organic semiconductor with dynamic disorders. Physical Chemistry Chemical Physics, 2010, 12, 3309.	2.8	152
52	Theory of Long-Lived Room-Temperature Phosphorescence in Organic Aggregates. Accounts of Chemical Research, 2021, 54, 940-949.	15.6	150
53	Biradicalâ€Featured Stable Organicâ€Smallâ€Molecule Photothermal Materials for Highly Efficient Solarâ€Driven Water Evaporation. Advanced Materials, 2020, 32, e1908537.	21.0	149
54	Tuning the Energy Level and Photophysical and Electroluminescent Properties of Heavy Metal Complexes by Controlling the Ligation of the Metal with the Carbon of the Carbazole Unit. Advanced Functional Materials, 2007, 17, 651-661.	14.9	146

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55	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.	13.7	145
56	Polymorphism-Dependent and Switchable Emission of Butterfly-Like Bis(diarylmethylene)dihydroanthracenes. Chemistry of Materials, 2015, 27, 6601-6607.	6.7	144
57	Tripletâ€“Polaronâ€Interactionâ€Induced Upconversion from Triplet to Singlet: a Possible Way to Obtain Highly Efficient OLEDs. Advanced Materials, 2016, 28, 4740-4746.	21.0	140
58	Dynamic Monte Carlo Simulation for Highly Efficient Polymer Blend Photovoltaics. Journal of Physical Chemistry B, 2010, 114, 36-41.	2.6	137
59	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.	3.1	134
60	Chargeâ€Transfer Complex Crystal Based on Extendedâ€Ïâ€Conjugated Acceptor and Sulfurâ€Bridged Annulene: Chargeâ€Transfer Interaction and Remarkable High Ambipolar Transport Characteristics. Advanced Materials, 2014, 26, 4093-4099.	21.0	132
61	Evaluation of Charge Mobility in Organic Materials: From Localized to Delocalized Descriptions at a Firstâ€Principles Level. Advanced Materials, 2011, 23, 1145-1153.	21.0	127
62	Electrostatic Interaction-Induced Room-Temperature Phosphorescence in Pure Organic Molecules from QM/MM Calculations. Journal of Physical Chemistry Letters, 2016, 7, 2893-2898.	4.6	126
63	Theoretical study of thiophene oligomers: Electronic excitations, relaxation energies, and nonlinear optical properties. Journal of Chemical Physics, 1993, 98, 8819-8828.	3.0	122
64	Investigation of Exciton Coupling in Oligothiophenes by Circular Dichroism Spectroscopy. Advanced Materials, 1998, 10, 1343-1348.	21.0	119
65	Intrinsic and Extrinsic Charge Transport in CH3NH3PbI3 Perovskites Predicted from First-Principles. Scientific Reports, 2016, 6, 19968.	3.3	119
66	Synthesis and Photovoltaic Properties of a Solution-Processable Organic Molecule Containing Triphenylamine and DCM Moieties. Journal of Physical Chemistry C, 2007, 111, 8661-8666.	3.1	117
67	Isoindigoâ€Based Polymers with Small Effective Masses for Highâ€Mobility Ambipolar Fieldâ€Effect Transistors. Advanced Materials, 2017, 29, 1702115.	21.0	115
68	Multilevel Conductance Switching of Memory Device through Photoelectric Effect. Journal of the American Chemical Society, 2012, 134, 20053-20059.	13.7	114
69	Unraveling the aggregation effect on amorphous phase AIE luminogens: a computational study. Nanoscale, 2016, 8, 15173-15180.	5.6	112
70	Single Crystalline Submicrotubes from Small Organic Molecules. Chemistry of Materials, 2005, 17, 6430-6435.	6.7	110
71	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, 9094-9104.	2.5	110
72	Effect of length and size of heterojunction on the transport properties of carbon-nanotube devices. Applied Physics Letters, 2007, 91, 133511.	3.3	109

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73	Toward Quantitative Prediction of Charge Mobility in Organic Semiconductors: Tunneling Enabled Hopping Model. Advanced Materials, 2012, 24, 3568-3572.	21.0	109
74	Thin film field-effect transistors of 2,6-diphenyl anthracene (DPA). Chemical Communications, 2015, 51, 11777-11779.	4.1	107
75	Vibration correlation function formalism of radiative and non-radiative rates for complex molecules. Chemical Physics, 2010, 370, 215-222.	1.9	104
76	Negative differential resistance induced by intermolecular interaction in a bimolecular device. Applied Physics Letters, 2007, 91, .	3.3	101
77	Triplet formation and decay in conjugated polymer devices. Chemical Physics Letters, 2002, 360, 195-201.	2.6	99
78	Polyaniline/Fe₃O₄ Nanoparticle Composite: Synthesis and Reaction Mechanism. Journal of Physical Chemistry B, 2009, 113, 5052-5058.	2.6	98
79	Tunable Electronic Properties of Two-Dimensional Transition Metal Dichalcogenide Alloys: A First-Principles Prediction. Journal of Physical Chemistry Letters, 2014, 5, 285-291.	4.6	98
80	Theoretical investigation of the negative differential resistance in squashed C60 molecular device. Applied Physics Letters, 2008, 92, .	3.3	97
81	Understanding the Charge Transport and Polarities in Organic Donorâ€“Acceptor Mixedâ€Stack Crystals: Molecular Insights from the Superâ€Exchange Couplings. Advanced Materials, 2015, 27, 1443-1449.	21.0	97
82	Static and dynamic third-harmonic generation in long polyacetylene and polyparaphenylene vinylene chains. Physical Review B, 1991, 44, 5962-5965.	3.2	95
83	Intramolecular Electron Transfer within the Substituted Tetrathiafulvaleneâ'Quinone Dyads:Â Facilitated by Metal Ion and Photomodulation in the Presence of Spiropyran. Journal of the American Chemical Society, 2007, 129, 6839-6846.	13.7	95
84	Influence of alkyl side-chain length on the carrier mobility in organic semiconductors: herringbone vs. piâ€“pi stacking. Journal of Materials Chemistry C, 2016, 4, 4546-4555.	5.5	94
85	First Synthesis of 2,3,6,7-Tetrabromonaphthalene Diimide. Organic Letters, 2007, 9, 3917-3920.	4.6	93
86	Modeling thermoelectric transport in organic materials. Physical Chemistry Chemical Physics, 2012, 14, 16505.	2.8	93
87	From Molecular Packing Structures to Electronic Processes: Theoretical Simulations for Organic Solar Cells. Advanced Energy Materials, 2018, 8, 1702743.	19.5	93
88	Chain-Length Dependence of Singlet and Triplet Exciton Formation Rates in Organic Light-Emitting Diodes. Advanced Functional Materials, 2004, 14, 684-692.	14.9	92
89	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.	13.7	90
90	Charge transfer rates in organic semiconductors beyond first-order perturbation: From weak to strong coupling regimes. Journal of Chemical Physics, 2009, 130, 024704.	3.0	89

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91	Solutionâ€Processed Solid Solution of a Novel Carbazole Derivative for Highâ€Performance Blue Phosphorescent Organic Lightâ€Emitting Diodes. Advanced Materials, 2010, 22, 4167-4171.	21.0	89
92	Synergistic Optimization Enables Largeâ€Area Flexible Organic Solar Cells to Maintain over 98% PCE of the Smallâ€Area Rigid Devices. Advanced Materials, 2020, 32, e2005153.	21.0	89
93	A Densely and Uniformly Packed Organic Semiconductor Based on Annelated Î²â€Trithiophenes for Highâ€Performance Thin Film Transistors. Advanced Functional Materials, 2009, 19, 272-276.	14.9	88
94	Side Chain Engineering of Copolymers Based on Bithiazole and Benzodithiophene for Enhanced Photovoltaic Performance. Macromolecules, 2011, 44, 4230-4240.	4.8	88
95	Theoretical Insights into the Aggregation-Induced Emission by Hydrogen Bonding: A QM/MM Study. Journal of Physical Chemistry A, 2012, 116, 3881-3888.	2.5	88
96	Gibbsâ€“Curieâ€“Wulff Theorem in Organic Materials: A Case Study on the Relationship between Surface Energy and Crystal Growth. Advanced Materials, 2016, 28, 1697-1702.	21.0	88
97	Indirect-to-Direct Band Gap Crossover in Few-Layer Transition Metal Dichalcogenides: A Theoretical Prediction. Journal of Physical Chemistry C, 2016, 120, 21866-21870.	3.1	87
98	Nonlinear optical processes in short polyenes: Configuration interaction description of twoâ€photon absorption and thirdâ€harmonic generation. Journal of Chemical Physics, 1992, 97, 1132-1137.	3.0	85
99	Low-Dimensional Aggregates from Stilbazolium-Like Dyes. Angewandte Chemie - International Edition, 2004, 43, 4060-4063.	13.8	84
100	Energy Level Alignment and Charge Carrier Mobility in Noncovalently Functionalized Graphene. Journal of Physical Chemistry Letters, 2013, 4, 2158-2165.	4.6	83
101	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.	5.3	83
102	Electron-phonon couplings and carrier mobility in graphynes sheet calculated using the Wannier-interpolation approach. Journal of Chemical Physics, 2014, 141, 034704.	3.0	82
103	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.	5.5	82
104	Brightening up Circularly Polarized Luminescence of Monosubstituted Polyacetylene by Conformation Control: Mechanism, Switching, and Sensing. Angewandte Chemie - International Edition, 2021, 60, 21918-21926.	13.8	82
105	Theoretical comparative studies of charge mobilities for molecular materials: Pet versus bnpery. Organic Electronics, 2008, 9, 635-640.	2.6	81
106	Efficient ambipolar transport properties in alternate stacking donorâ€“acceptor complexes: from experiment to theory. Physical Chemistry Chemical Physics, 2016, 18, 14094-14103.	2.8	81
107	GeAs₂: A IVâ€“V Group Two-Dimensional Semiconductor with Ultralow Thermal Conductivity and High Thermoelectric Efficiency. Chemistry of Materials, 2017, 29, 6261-6268.	6.7	80
108	Nature of photoexcitations in poly (paraphenylene vinylene) and its oligomers. Chemical Physics Letters, 1994, 228, 301-306.	2.6	79

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109	Electronic structure of Ï€-conjugated oligomers and polymers: a quantumâ€“chemical approach to transport properties. Synthetic Metals, 2001, 125, 107-116.	3.9	79
110	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.	6.7	79
111	Negative differential resistance behaviors in porphyrin molecular junctions modulated with side groups. Applied Physics Letters, 2008, 92, .	3.3	77
112	Hydrogen Bonding-Induced Morphology Dependence of Long-Lived Organic Room-Temperature Phosphorescence: A Computational Study. Journal of Physical Chemistry Letters, 2019, 10, 6948-6954.	4.6	76
113	Symmetrized density-matrix renormalization-group method for excited states of Hubbard models. Physical Review B, 1996, 54, 7598-7601.	3.2	74
114	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, 5233-5240.	2.5	73
115	Quantum chemical insights into the aggregation induced emission phenomena: A QM/MM study for pyrazine derivatives. Journal of Computational Chemistry, 2012, 33, 1862-1869.	3.3	72
116	Electronic structure and nonlinear optical properties of the fullerenesC60andC70: A valence-effective-Hamiltonian study. Physical Review B, 1992, 46, 16135-16141.	3.2	71
117	Binaphthalene Molecules with Tetrathiafulvalene Units:Â CD Spectrum Modulation and New Chiral Molecular Switches by Reversible Oxidation and Reduction of Tetrathiafulvalene Units. Journal of Organic Chemistry, 2006, 71, 2123-2130.	3.2	71
118	Photoactive Gate Dielectrics. Advanced Materials, 2010, 22, 3282-3287.	21.0	71
119	Computational Evaluation of Optoelectronic Properties for Organic/Carbon Materials. Accounts of Chemical Research, 2014, 47, 3301-3309.	15.6	71
120	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.	3.1	70
121	Aâ€“Ï€â€“Dâ€“Ï€â€“A Electronâ€Donating Small Molecules for Solutionâ€Processed Organic Solar Cells: A Review. Macromolecular Rapid Communications, 2017, 38, 1700470.	3.9	70
122	General Approach To Compute Phosphorescent OLED Efficiency. Journal of Physical Chemistry C, 2018, 122, 6340-6347.	3.1	70
123	Organic thin-film transistors of phthalocyanines. Pure and Applied Chemistry, 2008, 80, 2231-2240.	1.9	69
124	Water Transport and Purification in Nanochannels Controlled by Asymmetric Wettability. Small, 2011, 7, 2225-2231.	10.0	69
125	First-principles investigation of organic semiconductors for thermoelectric applications. Journal of Chemical Physics, 2009, 131, 224704.	3.0	68
126	Janus monolayer of WSeTe, a new structural phase transition material driven by electrostatic gating. Nanoscale, 2018, 10, 21629-21633.	5.6	68

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127	The role of acoustic phonon scattering in charge transport in organic semiconductors: a first-principles deformation-potential study. Science in China Series B: Chemistry, 2009, 52, 1646-1652.	0.8	67
128	Using the isotope effect to probe an aggregation induced emission mechanism: theoretical prediction and experimental validation. Chemical Science, 2016, 7, 5573-5580.	7.4	67
129	Real-time monitoring of hydrophobic aggregation reveals a critical role of cooperativity in hydrophobic effect. Nature Communications, 2017, 8, 15639.	12.8	67
130	General model for the description of the third-order optical nonlinearitiesin conjugated systems: Application to the all-trans Î²-carotene molecule. Physical Review B, 1997, 55, 1505-1516.	3.2	66
131	Two-Photon Absorption in Quadrupolar Bis(acceptor)-Terminated Chromophores with Electron-Rich Bis(heterocycle)vinylene Bridges. Chemistry of Materials, 2007, 19, 432-442.	6.7	66
132	An Acetylene-Containing Perylene Diimide Copolymer for High Mobility n-Channel Transistor in Air. Macromolecules, 2013, 46, 2152-2158.	4.8	66
133	Making silole photovoltaically active by attaching carbazolyl donor groups to the silolyl acceptor core. Chemical Communications, 2005, , 3583.	4.1	65
134	Theoretical study of radiative and non-radiative decay processes in pyrazine derivatives. Journal of Chemical Physics, 2011, 135, 014304.	3.0	65
135	Design, Synthesis, and Properties of Asymmetrical Heteroacene and Its Application in Organic Electronics. Journal of Physical Chemistry C, 2010, 114, 10565-10571.	3.1	64
136	Coordination Complexes of 2-(4-Quinolyl)nitronyl Nitroxide with M(hfac)2[M = Mn(II), Co(II), and Cu(II)]:Â Syntheses, Crystal Structures, and Magnetic Characterization. Inorganic Chemistry, 2004, 43, 4091-4098.	4.0	62
137	An improved dynamic Monte Carlo model coupled with Poisson equation to simulate the performance of organic photovoltaic devices. Journal of Chemical Physics, 2011, 134, 124102.	3.0	62
138	Tuning Thermal Transport in Chainâ€Oriented Conducting Polymers for Enhanced Thermoelectric Efficiency: A Computational Study. Advanced Functional Materials, 2017, 27, 1702847.	14.9	62
139	Correction vector method for exact dynamic NLO coefficients in restricted configuration space. Chemical Physics Letters, 1995, 245, 224-229.	2.6	60
140	Comparison of density matrix renormalization group calculations with electron-hole models of exciton binding in conjugated polymers. Journal of Chemical Physics, 1998, 108, 7451-7458.	3.0	60
141	Geometric and electronic structures of the boron-doped photocatalyst TiO2. Journal of Physics Condensed Matter, 2006, 18, 87-96.	1.8	60
142	First-Principles Predictions of Thermoelectric Figure of Merit for Organic Materials: Deformation Potential Approximation. Journal of Chemical Theory and Computation, 2012, 8, 3338-3347.	5.3	59
143	Theory of Charge Transport in Carbon Electronic Materials. Springer Briefs in Molecular Science, 2012, , .	0.1	59
144	Absorption and Emission in Quaterthienyl Thin Films. Advanced Materials, 2003, 15, 818-822.	21.0	58

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145	Toward Achieving Single-Molecule White Electroluminescence from Dual Emission of Fluorescence and Phosphorescence. Chemistry of Materials, 2020, 32, 4038-4044.	6.7	57
146	Size-Dependent Exciton Chirality in (R)-(+)-1,1â€˜-Bi-2-naphthol Dimethyl Ether Nanoparticles. Journal of the American Chemical Society, 2004, 126, 15439-15444.	13.7	56
147	Helical Molecular Duplex Strands:Â Multiple Hydrogen-Bond-Mediated Assembly of Self-Complementary Oligomeric Hydrazide Derivatives. Journal of Organic Chemistry, 2007, 72, 4936-4946.	3.2	56
148	Organic Single Crystal Fieldâ€effect Transistors Based on 6Hâ€pyrrolo[3,2â€“b:4,5â€“bÂ´]bis[1,4]benzothiazine and its Derivatives. Advanced Materials, 2010, 22, 2458-2462.	21.0	56
149	Puckered Arsenene: A Promising Room-Temperature Thermoelectric Material from First-Principles Prediction. Journal of Physical Chemistry C, 2017, 121, 19080-19086.	3.1	56
150	Asymmetric photon transport in organic semiconductor nanowires through electrically controlled exciton diffusion. Science Advances, 2018, 4, eaap9861.	10.3	56
151	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.	4.6	56
152	Low-lying electronic excitations and nonlinear optic properties of polymers via symmetrized density matrix renormalization group method. Synthetic Metals, 1997, 85, 1019-1022.	3.9	55
153	Molecular Design of Negative Differential Resistance Device through Intermolecular Interaction. Journal of Physical Chemistry C, 2007, 111, 19098-19102.	3.1	54
154	Dibenzotetrathiafulvalene Bisimides: New Building Blocks for Organic Electronic Materials**. Advanced Materials, 2007, 19, 3037-3042.	21.0	54
155	Sunlightâ€Coordinated Highâ€Performance Moisture Power in Natural Conditions. Advanced Materials, 2022, 34, e2103897.	21.0	54
156	Effects of Intermolecular Interaction and Moleculeâ^'Electrode Couplings on Molecular Electronic Conductance. Journal of Physical Chemistry B, 2005, 109, 12304-12308.	2.6	53
157	Applying Marcus theory to describe the carrier transports in organic semiconductors: Limitations and beyond. Journal of Chemical Physics, 2020, 153, 080902.	3.0	53
158	High two-photon cross-sections in bis(diarylaminostyryl) chromophores with electron-rich heterocycle and bis(heterocycle)vinylene bridges. Chemical Communications, 2007, , 1372-1374.	4.1	52
159	Phenyl-substituted fluorene-dimer cored anthracene derivatives: highly fluorescent and stable materials for high performance organic blue- and white-light-emitting diodes. Journal of Materials Chemistry, 2010, 20, 3186.	6.7	52
160	Theoretical study of substitution effects on molecular reorganization energy in organic semiconductors. Journal of Chemical Physics, 2011, 135, 104703.	3.0	52
161	Tuning the fluorescence of 1-imino nitroxide pyrene with two chemical inputs: mimicking the performance of an â€œANDâ€•gate. Chemical Communications, 2004, , 670-671.	4.1	51
162	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, 5206-5209.	13.8	51

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