

Zhigang Shuai

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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	Efficient degradation of toxic organic pollutants with Ni ₂ O ₃ /TiO _{2-x} B _x under visible irradiation. <i>Journal of the American Chemical Society</i> , 2004 , 126, 4782-3	16.4	1045
404	Electronic structure and carrier mobility in graphdiyne sheet and nanoribbons: theoretical predictions. <i>ACS Nano</i> , 2011 , 5, 2593-600	16.7	697
403	Structures, electronic states, photoluminescence, and carrier transport properties of 1,1-disubstituted 2,3,4,5-tetraphenylsiloles. <i>Journal of the American Chemical Society</i> , 2005 , 127, 6335-46	16.4	458
402	White light emission from a single organic molecule with dual phosphorescence at room temperature. <i>Nature Communications</i> , 2017 , 8, 416	17.4	457
401	Tunable band gap photoluminescence from atomically thin transition-metal dichalcogenide alloys. <i>ACS Nano</i> , 2013 , 7, 4610-6	16.7	442
400	First-principles prediction of charge mobility in carbon and organic nanomaterials. <i>Nanoscale</i> , 2012 , 4, 4348-69	7.7	412
399	Rational Molecular Design for Achieving Persistent and Efficient Pure Organic Room-Temperature Phosphorescence. <i>Chem</i> , 2016 , 1, 592-602	16.2	399
398	Computational methods for design of organic materials with high charge mobility. <i>Chemical Society Reviews</i> , 2010 , 39, 423-34	58.5	360
397	Role of Dimensionality on the Two-Photon Absorption Response of Conjugated Molecules: The Case of Octupolar Compounds. <i>Advanced Functional Materials</i> , 2002 , 12, 631-641	15.6	334
396	Toward quantitative prediction of molecular fluorescence quantum efficiency: role of duschinsky rotation. <i>Journal of the American Chemical Society</i> , 2007 , 129, 9333-9	16.4	324
395	Charge separation in localized and delocalized electronic states in polymeric semiconductors. <i>Nature</i> , 1998 , 392, 903-906	50.4	299
394	Structures, electronic states, and electroluminescent properties of a zinc(II) 2-(2-hydroxyphenyl)benzothiazolate complex. <i>Journal of the American Chemical Society</i> , 2003 , 125, 14816-24	16.4	276
393	Spin-Orbit Coupling and Intersystem Crossing in Conjugated Polymers: A Configuration Interaction Description. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 3899-3907	2.8	269
392	Theory of excited state decays and optical spectra: application to polyatomic molecules. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 7817-31	2.8	267
391	Influences of Crystal Structures and Molecular Sizes on the Charge Mobility of Organic Semiconductors: Oligothiophenes. <i>Chemistry of Materials</i> , 2008 , 20, 3205-3211	9.6	265
390	Excited-State Electronic Structure of Conjugated Oligomers and Polymers: A Quantum-Chemical Approach to Optical Phenomena. <i>Accounts of Chemical Research</i> , 1999 , 32, 267-276	24.3	263
389	Carrier Mobility in Graphyne Should Be Even Larger than That in Graphene: A Theoretical Prediction. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 1443-8	6.4	254

388	Size-tunable emission from 1,3-diphenyl-5-(2-anthryl)-2-pyrazoline nanoparticles. <i>Journal of the American Chemical Society</i> , 2003 , 125, 6740-5	16.4	252
387	Theoretical predictions of size-dependent carrier mobility and polarity in graphene. <i>Journal of the American Chemical Society</i> , 2009 , 131, 17728-9	16.4	247
386	Solution-processed, high-performance nanoribbon transistors based on dithiopyrene. <i>Journal of the American Chemical Society</i> , 2011 , 133, 1-3	16.4	239
385	An Ultra Closely EStacked Organic Semiconductor for High Performance Field-Effect Transistors. <i>Advanced Materials</i> , 2007 , 19, 2613-2617	24	235
384	Efficient and Long-Lived Room-Temperature Organic Phosphorescence: Theoretical Descriptors for Molecular Designs. <i>Journal of the American Chemical Society</i> , 2019 , 141, 1010-1015	16.4	228
383	Singlet and triplet exciton formation rates in conjugated polymer light-emitting diodes. <i>Physical Review Letters</i> , 2000 , 84, 131-4	7.4	223
382	A facile strategy for realizing room temperature phosphorescence and single molecule white light emission. <i>Nature Communications</i> , 2018 , 9, 2963	17.4	216
381	Nuclear tunneling effects of charge transport in rubrene, tetracene, and pentacene. <i>Physical Review B</i> , 2009 , 79,	3.3	215
380	A cyclic triphenylamine dimer for organic field-effect transistors with high performance. <i>Journal of the American Chemical Society</i> , 2006 , 128, 15940-1	16.4	212
379	Intersystem crossing processes in nonplanar aromatic heterocyclic molecules. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10490-9	2.8	187
378	1,3-Dithiole-2-thione derivatives featuring an anthracene unit: new selective chemodosimeters for Hg(II) ion. <i>Chemical Communications</i> , 2005 , 2161-3	5.8	187
377	Extended squaraine dyes with large two-photon absorption cross-sections. <i>Journal of the American Chemical Society</i> , 2006 , 128, 14444-5	16.4	181
376	Sulfur-bridged annulene-TCNQ co-crystal: a self-assembled "molecular level heterojunction" with air stable ambipolar charge transport behavior. <i>Advanced Materials</i> , 2012 , 24, 2603-7	24	176
375	Theoretical modelling of carrier transports in molecular semiconductors: molecular design of triphenylamine dimer systems. <i>Nanotechnology</i> , 2007 , 18, 424029	3.4	167
374	Highly Efficient Thermally Activated Delayed Fluorescence via J-Aggregates with Strong Intermolecular Charge Transfer. <i>Advanced Materials</i> , 2019 , 31, e1808242	24	164
373	From charge transport parameters to charge mobility in organic semiconductors through multiscale simulation. <i>Chemical Society Reviews</i> , 2014 , 43, 2662-79	58.5	162
372	Theoretical investigation of the lowest singlet and triplet states in poly(paraphenylene vinylene)oligomers. <i>Journal of Chemical Physics</i> , 1995 , 102, 2042-2049	3.9	161
371	Dynamic Ultralong Organic Phosphorescence by Photoactivation. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 8425-8431	16.4	158

370	Excited state radiationless decay process with Duschinsky rotation effect: formalism and implementation. <i>Journal of Chemical Physics</i> , 2007 , 126, 114302	3.9	157
369	Improving the efficiency of solution processable organic photovoltaic devices by a star-shaped molecular geometry. <i>Journal of Materials Chemistry</i> , 2008 , 18, 4085		155
368	Excited states structure and processes: Understanding organic light-emitting diodes at the molecular level. <i>Physics Reports</i> , 2014 , 537, 123-156	27.7	154
367	Multifunctional bipolar triphenylamine/oxadiazole derivatives: highly efficient blue fluorescence, red phosphorescence host and two-color based white OLEDs. <i>Chemical Communications</i> , 2009 , 77-9	5.8	153
366	Fullerene/sulfur-bridged annulene cocrystals: two-dimensional segregated heterojunctions with ambipolar transport properties and photoresponsivity. <i>Journal of the American Chemical Society</i> , 2013 , 135, 558-61	16.4	150
365	Balanced carrier transports of electrons and holes in silole-based compounds--a theoretical study. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 7138-43	2.8	148
364	Highly sensitive switching of solid-state luminescence by controlling intersystem crossing. <i>Nature Communications</i> , 2018 , 9, 3044	17.4	146
363	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. <i>Advanced Functional Materials</i> , 2007 , 17, 651-661	15.6	140
362	Aggregation induced blue-shifted emission--the molecular picture from a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 5545-52	3.6	138
361	Multiscale study of charge mobility of organic semiconductor with dynamic disorders. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 3309-14	3.6	135
360	Correlation Function Formalism for Triplet Excited State Decay: Combined Spin-Orbit and Nonadiabatic Couplings. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1132-43	6.4	132
359	Polymorphism-Dependent and Switchable Emission of Butterfly-Like Bis(diarylmethylene)dihydroanthracenes. <i>Chemistry of Materials</i> , 2015 , 27, 6601-6607	9.6	131
358	Unravelling Doping Effects on PEDOT at the Molecular Level: From Geometry to Thermoelectric Transport Properties. <i>Journal of the American Chemical Society</i> , 2015 , 137, 12929-38	16.4	129
357	Dynamic Monte Carlo simulation for highly efficient polymer blend photovoltaics. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 36-41	3.4	123
356	Charge-transfer complex crystal based on extended- π -conjugated acceptor and sulfur-bridged annulene: charge-transfer interaction and remarkable high ambipolar transport characteristics. <i>Advanced Materials</i> , 2014 , 26, 4093-9	24	119
355	Theoretical study of thiophene oligomers: Electronic excitations, relaxation energies, and nonlinear optical properties. <i>Journal of Chemical Physics</i> , 1993 , 98, 8819-8828	3.9	117
354	From Alloy-Like to Cascade Blended Structure: Designing High-Performance All-Small-Molecule Ternary Solar Cells. <i>Journal of the American Chemical Society</i> , 2018 , 140, 1549-1556	16.4	113
353	Evaluation of charge mobility in organic materials: from localized to delocalized descriptions at a first-principles level. <i>Advanced Materials</i> , 2011 , 23, 1145-53	24	113

352	Synthesis and Photovoltaic Properties of a Solution-Processable Organic Molecule Containing Triphenylamine and DCM Moieties. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 8661-8666	3.8	112
351	MOlecular MAterials Property Prediction Package (MOMAP) 1.0: a software package for predicting the luminescent properties and mobility of organic functional materials. <i>Molecular Physics</i> , 2018 , 116, 1078-1090	1.7	110
350	Triplet-Polaron-Interaction-Induced Upconversion from Triplet to Singlet: a Possible Way to Obtain Highly Efficient OLEDs. <i>Advanced Materials</i> , 2016 , 28, 4740-6	24	107
349	Single Crystalline Submicrotubes from Small Organic Molecules. <i>Chemistry of Materials</i> , 2005 , 17, 6430-6435	4.5	106
348	Promoting-mode free formalism for excited state radiationless decay process with Duschinsky rotation effect. <i>Science in China Series B: Chemistry</i> , 2008 , 51, 1153-1158		105
347	Investigation of Exciton Coupling in Oligothiophenes by Circular Dichroism Spectroscopy. <i>Advanced Materials</i> , 1998 , 10, 1343-1348	24	104
346	Effect of length and size of heterojunction on the transport properties of carbon-nanotube devices. <i>Applied Physics Letters</i> , 2007 , 91, 133511	3.4	104
345	Intrinsic and Extrinsic Charge Transport in CH ₃ NH ₃ PbI ₃ Perovskites Predicted from First-Principles. <i>Scientific Reports</i> , 2016 , 7, 19968	4.9	103
344	Multilevel conductance switching of memory device through photoelectric effect. <i>Journal of the American Chemical Society</i> , 2012 , 134, 20053-9	16.4	99
343	Negative differential resistance induced by intermolecular interaction in a bimolecular device. <i>Applied Physics Letters</i> , 2007 , 91, 233512	3.4	97
342	Electrostatic Interaction-Induced Room-Temperature Phosphorescence in Pure Organic Molecules from QM/MM Calculations. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2893-8	6.4	96
341	Toward quantitative prediction of charge mobility in organic semiconductors: tunneling enabled hopping model. <i>Advanced Materials</i> , 2012 , 24, 3568-72	24	96
340	Organic light-emitting diodes: theoretical understanding of highly efficient materials and development of computational methodology. <i>National Science Review</i> , 2017 , 4, 224-239	10.8	94
339	Theoretical investigation of the negative differential resistance in squashed C ₆₀ molecular device. <i>Applied Physics Letters</i> , 2008 , 92, 263304	3.4	94
338	Aggregation effects on the optical emission of 1,1,2,3,4,5-hexaphenylsilole (HPS): a QM/MM study. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 9094-104	2.8	92
337	Static and dynamic third-harmonic generation in long polyacetylene and polyparaphenylene vinylene chains. <i>Physical Review B</i> , 1991 , 44, 5962-5965	3.3	92
336	Theoretical Study of Conversion and Decay Processes of Excited Triplet and Singlet States in a Thermally Activated Delayed Fluorescence Molecule. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 13448-13456	3.8	91
335	Isoidindigo-Based Polymers with Small Effective Masses for High-Mobility Ambipolar Field-Effect Transistors. <i>Advanced Materials</i> , 2017 , 29, 1702115	24	91

- 334 Intramolecular electron transfer within the substituted tetrathiafulvalene-quinone dyads: facilitated by metal ion and photomodulation in the presence of spiropyran. *Journal of the American Chemical Society*, **2007**, 129, 6839-46 16.4 91
- 333 Polyaniline/Fe₃O₄ nanoparticle composite: synthesis and reaction mechanism. *Journal of Physical Chemistry B*, **2009**, 113, 5052-8 3.4 89
- 332 Triplet formation and decay in conjugated polymer devices. *Chemical Physics Letters*, **2002**, 360, 195-201 2.5 89
- 331 Side Chain Engineering of Copolymers Based on Bithiazole and Benzodithiophene for Enhanced Photovoltaic Performance. *Macromolecules*, **2011**, 44, 4230-4240 5.5 87
- 330 Charge transfer rates in organic semiconductors beyond first-order perturbation: from weak to strong coupling regimes. *Journal of Chemical Physics*, **2009**, 130, 024704 3.9 86
- 329 Solution-processed solid solution of a novel carbazole derivative for high-performance blue phosphorescent organic light-emitting diodes. *Advanced Materials*, **2010**, 22, 4167-71 2.4 86
- 328 First synthesis of 2,3,6,7-tetrabromonaphthalene diimide. *Organic Letters*, **2007**, 9, 3917-20 6.2 86
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- 326 A Densely and Uniformly Packed Organic Semiconductor Based on Annelated Bithiophenes for High-Performance Thin Film Transistors. *Advanced Functional Materials*, **2009**, 19, 272-276 15.6 84
- 325 Vibration correlation function formalism of radiative and non-radiative rates for complex molecules. *Chemical Physics*, **2010**, 370, 215-222 2.3 83
- 324 Theoretical insights into the aggregation-induced emission by hydrogen bonding: a QM/MM study. *Journal of Physical Chemistry A*, **2012**, 116, 3881-8 2.8 82
- 323 Nonlinear optical processes in short polyenes: Configuration interaction description of two-photon absorption and third-harmonic generation. *Journal of Chemical Physics*, **1992**, 97, 1132-1137 3.9 82
- 322 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 2.4 79
- 321 Thin film field-effect transistors of 2,6-diphenyl anthracene (DPA). *Chemical Communications*, **2015**, 51, 11777-9 5.8 78
- 320 Low-dimensional aggregates from stilbazolium-like dyes. *Angewandte Chemie - International Edition*, **2004**, 43, 4060-3 16.4 78
- 319 Unraveling the aggregation effect on amorphous phase AIE luminogens: a computational study. *Nanoscale*, **2016**, 8, 15173-80 7.7 77
- 318 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
- 317 Nature of photoexcitations in poly (paraphenylene vinylene) and its oligomers. *Chemical Physics Letters*, **1994**, 228, 301-306 2.5 77

316	Modeling thermoelectric transport in organic materials. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 16505-20	3.6	75
315	Theoretical comparative studies of charge mobilities for molecular materials: P ₆₆ versus bnp ₆₆ . <i>Organic Electronics</i> , 2008 , 9, 635-640	3.5	75
314	From Molecular Packing Structures to Electronic Processes: Theoretical Simulations for Organic Solar Cells. <i>Advanced Energy Materials</i> , 2018 , 8, 1702743	21.8	73
313	Negative differential resistance behaviors in porphyrin molecular junctions modulated with side groups. <i>Applied Physics Letters</i> , 2008 , 92, 243303	3.4	71
312	Electronic structure of π -conjugated oligomers and polymers: a quantum-chemical approach to transport properties. <i>Synthetic Metals</i> , 2001 , 125, 107-116	3.6	71
311	Energy Level Alignment and Charge Carrier Mobility in Noncovalently Functionalized Graphene. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 2158-2165	6.4	70
310	Symmetrized density-matrix renormalization-group method for excited states of Hubbard models. <i>Physical Review B</i> , 1996 , 54, 7598-7601	3.3	70
309	Electronic structure and nonlinear optical properties of the fullerenes C ₆₀ and C ₇₀ : A valence-effective-Hamiltonian study. <i>Physical Review B</i> , 1992 , 46, 16135-16141	3.3	69
308	Photoactive gate dielectrics. <i>Advanced Materials</i> , 2010 , 22, 3282-7	24	67
307	Understanding the efficiency drooping of the deep blue organometallic phosphors: a computational study of radiative and non-radiative decay rates for triplets. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 6829-6838	7.1	66
306	Search for Organic Thermoelectric Materials with High Mobility: The Case of 2,7-Dialkyl[1]benzothieno[3,2-b][1]benzothiophene Derivatives. <i>Chemistry of Materials</i> , 2014 , 26, 2669-2677	2.6	66
305	Quantum chemical insights into the aggregation induced emission phenomena: a QM/MM study for pyrazine derivatives. <i>Journal of Computational Chemistry</i> , 2012 , 33, 1862-9	3.5	66
304	Organic thin-film transistors of phthalocyanines. <i>Pure and Applied Chemistry</i> , 2008 , 80, 2231-2240	2.1	66
303	Binaphthalene molecules with tetrathiafulvalene units: CD spectrum modulation and new chiral molecular switches by reversible oxidation and reduction of tetrathiafulvalene units. <i>Journal of Organic Chemistry</i> , 2006 , 71, 2123-30	4.2	66
302	Indirect-to-Direct Band Gap Crossover in Few-Layer Transition Metal Dichalcogenides: A Theoretical Prediction. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 21866-21870	3.8	66
301	General model for the description of the third-order optical nonlinearities in conjugated systems: Application to the all-trans β -carotene molecule. <i>Physical Review B</i> , 1997 , 55, 1505-1516	3.3	64
300	Influence of alkyl side-chain length on the carrier mobility in organic semiconductors: herringbone vs. π - π stacking. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 4546-4555	7.1	64
299	Making silole photovoltaically active by attaching carbazolyl donor groups to the silolyl acceptor core. <i>Chemical Communications</i> , 2005 , 3583-5	5.8	63

- 298 Two-Photon Absorption in Quadrupolar Bis(acceptor)-Terminated Chromophores with Electron-Rich Bis(heterocycle)vinylene Bridges. *Chemistry of Materials*, **2007**, 19, 432-442 9.6 62
- 297 Water transport and purification in nanochannels controlled by asymmetric wettability. *Small*, **2011**, 7, 2225-31 11 61
- 296 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
- 295 Correction vector method for exact dynamic NLO coefficients in restricted configuration space. *Chemical Physics Letters*, **1995**, 245, 224-229 2.5 59
- 294 An Acetylene-Containing Perylene Diimide Copolymer for High Mobility n-Channel Transistor in Air. *Macromolecules*, **2013**, 46, 2152-2158 5.5 58
- 293 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 3.9 58
- 292 First-principles investigation of organic semiconductors for thermoelectric applications. *Journal of Chemical Physics*, **2009**, 131, 224704 3.9 58
- 291 General Approach To Compute Phosphorescent OLED Efficiency. *Journal of Physical Chemistry C*, **2018**, 122, 6340-6347 3.8 57
- 290 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
- 289 Coordination complexes of 2-(4-quinoly)nitronyl nitroxide with M(hfac)₂ [M = Mn(II), Co(II), and Cu(II)]: syntheses, crystal structures, and magnetic characterization. *Inorganic Chemistry*, **2004**, 43, 4091-8¹ 5.1 57
- 288 Absorption and Emission in Quaterthienyl Thin Films. *Advanced Materials*, **2003**, 15, 818-822 24 57
- 287 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 3.9 57
- 286 A-ED-EA Electron-Donating Small Molecules for Solution-Processed Organic Solar Cells: A Review. *Macromolecular Rapid Communications*, **2017**, 38, 1700470 4.8 55
- 285 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
- 284 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
- 283 Geometric and electronic structures of the boron-doped photocatalyst TiO₂. *Journal of Physics Condensed Matter*, **2006**, 18, 87-96 1.8 55
- 282 Computational evaluation of optoelectronic properties for organic/carbon materials. *Accounts of Chemical Research*, **2014**, 47, 3301-9 24.3 54
- 281 Theoretical study of radiative and non-radiative decay processes in pyrazine derivatives. *Journal of Chemical Physics*, **2011**, 135, 014304 3.9 54

280	Biradical-Featured Stable Organic-Small-Molecule Photothermal Materials for Highly Efficient Solar-Driven Water Evaporation. <i>Advanced Materials</i> , 2020 , 32, e1908537	24	53
279	Organic Laser Molecule with High Mobility, High Photoluminescence Quantum Yield, and Deep-Blue Lasing Characteristics. <i>Journal of the American Chemical Society</i> , 2020 , 142, 6332-6339	16.4	53
278	The role of acoustic phonon scattering in charge transport in organic semiconductors: a first-principles deformation-potential study. <i>Science in China Series B: Chemistry</i> , 2009 , 52, 1646-1652		53
277	Molecular Design of Negative Differential Resistance Device through Intermolecular Interaction. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 19098-19102	3.8	53
276	Time-Dependent Density Matrix Renormalization Group Algorithms for Nearly Exact Absorption and Fluorescence Spectra of Molecular Aggregates at Both Zero and Finite Temperature. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5027-5039	6.4	52
275	Electron-phonon couplings and carrier mobility in graphynes sheet calculated using the Wannier-interpolation approach. <i>Journal of Chemical Physics</i> , 2014 , 141, 034704	3.9	52
274	Helical molecular duplex strands: multiple hydrogen-bond-mediated assembly of self-complementary oligomeric hydrazide derivatives. <i>Journal of Organic Chemistry</i> , 2007 , 72, 4936-46	4.2	52
273	Efficient ambipolar transport properties in alternate stacking donor-acceptor complexes: from experiment to theory. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14094-103	3.6	52
272	Theory of Charge Transport in Carbon Electronic Materials. <i>Springer Briefs in Molecular Science</i> , 2012 ,	0.6	51
271	High two-photon cross-sections in bis(diarylamino)styryl chromophores with electron-rich heterocycle and bis(heterocycle)vinylene bridges. <i>Chemical Communications</i> , 2007 , 1372-4	5.8	51
270	Dibenzotetrathiafulvalene Bisimides: New Building Blocks for Organic Electronic Materials**. <i>Advanced Materials</i> , 2007 , 19, 3037-3042	24	51
269	Size-dependent exciton chirality in (R)-(+)-1,1'-bi-2-naphthol dimethyl ether nanoparticles. <i>Journal of the American Chemical Society</i> , 2004 , 126, 15439-44	16.4	50
268	Theoretical insight into the aggregation induced emission phenomena of diphenyldibenzofulvene: a nonadiabatic molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 14207-16	3.6	49
267	Side Chain Engineering of Polythiophene Derivatives with a ThienyleneVinylene Conjugated Side Chain for Application in Polymer Solar Cells. <i>Macromolecules</i> , 2012 , 45, 2312-2320	5.5	49
266	Phenyl-substituted fluorene-dimer cored anthracene derivatives: highly fluorescent and stable materials for high performance organic blue- and white-light-emitting diodes. <i>Journal of Materials Chemistry</i> , 2010 , 20, 3186		49
265	Low-lying electronic excitations and nonlinear optic properties of polymers via symmetrized density matrix renormalization group method. <i>Synthetic Metals</i> , 1997 , 85, 1019-1022	3.6	49
264	Coupled-cluster approach for studying the electronic and nonlinear optical properties of conjugated molecules. <i>Physical Review B</i> , 2000 , 62, 15452-15460	3.3	49
263	Using the isotope effect to probe an aggregation induced emission mechanism: theoretical prediction and experimental validation. <i>Chemical Science</i> , 2016 , 7, 5573-5580	9.4	49

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260	Tuning the fluorescence of 1-imino nitroxide pyrene with two chemical inputs: mimicking the performance of an "AND" gate. <i>Chemical Communications</i> , 2004 , 670-1	5.8	48
259	Real-time monitoring of hydrophobic aggregation reveals a critical role of cooperativity in hydrophobic effect. <i>Nature Communications</i> , 2017 , 8, 15639	17.4	47
258	Effects of intermolecular interaction and molecule-electrode couplings on molecular electronic conductance. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 12304-8	3.4	47
257	Theory of Long-Lived Room-Temperature Phosphorescence in Organic Aggregates. <i>Accounts of Chemical Research</i> , 2021 , 54, 940-949	24.3	46
256	Hydrogen Bonding-Induced Morphology Dependence of Long-Lived Organic Room-Temperature Phosphorescence: A Computational Study. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 6948-6954	6.4	45
255	Layer-by-layer removal of insulating few-layer mica flakes for asymmetric ultra-thin nanopore fabrication. <i>Nano Research</i> , 2012 , 5, 99-108	10	45
254	Theoretical study of substitution effects on molecular reorganization energy in organic semiconductors. <i>Journal of Chemical Physics</i> , 2011 , 135, 104703	3.9	45
253	Naphtho[1,2-b:5,6-b']dithiophene-Based Small Molecules for Thick-Film Organic Solar Cells with High Fill Factors. <i>Chemistry of Materials</i> , 2016 , 28, 943-950	9.6	44
252	The effects of pyridine derivative additives on interface processes at nanocrystalline TiO ₂ thin film in dye-sensitized solar cells. <i>Surface and Interface Analysis</i> , 2007 , 39, 809-816	1.5	44
251	Dynamical nonlinear optical coefficients from the symmetrized density-matrix renormalization-group method. <i>Physical Review B</i> , 1999 , 59, 14827-14830	3.3	44
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