# 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 | A computational scheme for evaluating the phosphorescence quantum efficiency: applied to blue-emitting tetradentate Pt(<scp>ii</scp>) complexes. Materials Horizons, 2022, 9, 334-341. | 12.2 | 15 |
| 2 | Catechol Moiety Integrated Triâ€Aryl Type AIEgen for Visual and Quantitative Boronic Acid Detection. Chemistry - A European Journal, 2022, 28, e202103351. | 3.3 | 3 |
| 3 | Heavyâ€Atomâ€Free Roomâ€Temperature Phosphorescent Rylene Imide for Highâ€Performing Organic Photovoltaics. Advanced Science, 2022, 9, e2103975. | 11.2 | 12 |
| 4 | AIEgens with cyano-modification in different sites: Potential â€˜Meta-site effectâ€™ in mechanochromism behavior. Dyes and Pigments, 2022, 198, 109939. | 3.7 | 3 |
| 5 | Sunlightâ€Coordinated Highâ€Performance Moisture Power in Natural Conditions. Advanced Materials, 2022, 34, e2103897. | 21.0 | 54 |
| 6 | Computational Selection of Thermally Activated Delayed Fluorescence (TADF) Molecules with Promising Electrically Pumped Lasing Property. , 2022, 4, 487-496. | | 20 |
| 7 | A Novel Strategy toward Thermally Activated Delayed Fluorescence from a Locally Excited State. Journal of Physical Chemistry Letters, 2022, 13, 2653-2660. | 4.6 | 25 |
| 8 | Non-Markovian stochastic SchrÃ¶dinger equation: Matrix-product-state approach to the hierarchy of pure states. Physical Review A, 2022, 105, . | 2.5 | 9 |
| 9 | Timeâ€dependent density matrix renormalization group method for quantum dynamics in complex systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, . | 14.6 | 19 |
| 10 | On the fly swapping algorithm for ordering of degrees of freedom in density matrix renormalization group. Journal of Physics Condensed Matter, 2022, 34, 254003. | 1.8 | 7 |
| 11 | An Organizational Structure for the Future. Chemistry International, 2022, 44, 34-37. | 0.3 | 2 |
| 12 | Computational modeling of AIE luminogens. , 2022, , 639-667. | | 0 |
| 13 | The Variance of Photophysical Properties of Tetraphenylethene and Its Derivatives during Their Transitions from Dissolved States to Solid States. Polymers, 2022, 14, 2880. | 4.5 | 1 |
| 14 | Hybrid Quantum-Classical Boson Sampling Algorithm for Molecular Vibrationally Resolved Electronic Spectroscopy with Duschinsky Rotation and Anharmonicity. Journal of Physical Chemistry Letters, 2022, 13, 6391-6399. | 4.6 | 3 |
| 15 | Ferroelectricity in 2D metal phosphorus trichalcogenides and van der Waals heterostructures for photocatalytic water splitting. Journal of Materials Chemistry A, 2021, 9, 2734-2741. | 10.3 | 27 |
| 16 | Simultaneous studies of pressure effect on charge transport and photophysical properties in organic semiconductors: A theoretical investigation. Chinese Chemical Letters, 2021, 32, 1233-1236. | 9.0 | 5 |
| 17 | Theory of Long-Lived Room-Temperature Phosphorescence in Organic Aggregates. Accounts of Chemical Research, 2021, 54, 940-949. | 15.6 | 150 |
| 18 | Influences of dynamic and static disorder on the carrier mobility of BTBT-C12 derivatives: a multiscale computational study. Nanoscale, 2021, 13, 3252-3262. | 5.6 | 3 |

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| 19 | Molecular Design Strategy for Simultaneously Strong Luminescence and High Mobility: Multichannel CH-Ï€ Interaction. Journal of Physical Chemistry Letters, 2021, 12, 938-946. | 4.6 | 17 |
| 20 | Theoretical Characterizations of TADF Materials: Roles of Î”G and the Singletâ€“Triplet Excited States Interconversion. Journal of Physical Chemistry A, 2021, 125, 1468-1475. | 2.5 | 51 |
| 21 | Abnormal Seebeck effect in doped conducting polymers. Applied Physics Letters, 2021, 118, . | 3.3 | 9 |
| 22 | International chemistry for a sustainable society. National Science Review, 2021, 8, nwab038. | 9.5 | 0 |
| 23 | 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. | 4.6 | 35 |
| 24 | Aggregation-Enhanced Thermally Activated Delayed Fluorescence Efficiency for Two-Coordinate Carbeneâ€“Metalâ€“Amide Complexes: A QM/MM Study. Journal of Physical Chemistry Letters, 2021, 12, 2944-2953. | 4.6 | 44 |
| 25 | Intrinsic hydroquinone-functionalized aggregation-induced emission core shows redox and pH sensitivity. Communications Chemistry, 2021, 4, . | 4.5 | 6 |
| 26 | Understanding the Temperature Dependence of the Seebeck Coefficient from First-Principles Band Structure Calculations for Organic Thermoelectric Materials. CCS Chemistry, 2021, 3, 1477-1483. | 7.8 | 16 |
| 27 | Creating Side Transport Pathways in Organic Solar Cells by Introducing Delayed Fluorescence Molecules. Chemistry of Materials, 2021, 33, 4578-4585. | 6.7 | 11 |
| 28 | Supramolecular engineering of charge transfer in wide bandgap organic semiconductors with enhanced visible-to-NIR photoresponse. Nature Communications, 2021, 12, 3667. | 12.8 | 30 |
| 29 | Evaluating the anharmonicity contributions to the molecular excited state internal conversion rates with finite temperature TD-DMRG. Journal of Chemical Physics, 2021, 154, 214109. | 3.0 | 21 |
| 30 | Intermolecular Charge-Transfer-Induced Strong Optical Emission from Herringbone H-Aggregates. Nano Letters, 2021, 21, 5394-5400. | 9.1 | 20 |
| 31 | Molecular mechanism of aggregationâ€induced emission. Aggregate, 2021, 2, e91. | 9.9 | 179 |
| 32 | A general charge transport picture for organic semiconductors with nonlocal electron-phonon couplings. Nature Communications, 2021, 12, 4260. | 12.8 | 38 |
| 33 | Future directions of chemical theory and computation. Pure and Applied Chemistry, 2021, 93, 1423-1433. | 1.9 | 3 |
| 34 | High Mobility Organic Lasing Semiconductor with Crystallizationâ€Enhanced Emission for Lightâ€Emitting Transistors. Angewandte Chemie, 2021, 133, 20436-20441. | 2.0 | 5 |
| 35 | Brightening up Circularly Polarized Luminescence of Monosubstituted Polyacetylene by Conformation Control: Mechanism, Switching, and Sensing. Angewandte Chemie, 2021, 133, 22089-22097. | 2.0 | 20 |
| 36 | Quantum-electrodynamical time-dependent density functional theory within Gaussian atomic basis. Journal of Chemical Physics, 2021, 155, 064107. | 3.0 | 29 |

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| 37 | 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 |
| 38 | High Mobility Organic Lasing Semiconductor with Crystallizationâ€Enhanced Emission for Lightâ€Emitting Transistors. Angewandte Chemie - International Edition, 2021, 60, 20274-20279. | 13.8 | 23 |
| 39 | Intermolecular charge-transfer aggregates enable high-efficiency near-infrared emissions by nonadiabatic coupling suppression. Science China Chemistry, 2021, 64, 1786-1795. | 8.2 | 25 |
| 40 | Chebyshev Matrix Product States with Canonical Orthogonalization for Spectral Functions of Many-Body Systems. Journal of Physical Chemistry Letters, 2021, 12, 9344-9352. | 4.6 | 6 |
| 41 | Enhanced Reverse Intersystem Crossing Promoted by Triplet Excitonâ€“Photon Coupling. Journal of the American Chemical Society, 2021, 143, 17786-17792. | 13.7 | 11 |
| 42 | Front Cover: Molecular mechanism of aggregationâ€induced emission. Aggregate, 2021, 2, e134. | 9.9 | 2 |
| 43 | 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. | 1.3 | 8 |
| 44 | Effect of Strong Intermolecular Interaction in 2D Inorganic Molecular Crystals. Journal of the American Chemical Society, 2021, 143, 20192-20201. | 13.7 | 9 |
| 45 | Emerging technologies for a more sustainable future. Pure and Applied Chemistry, 2021, 93, 1351-1352. | 1.9 | 1 |
| 46 | A general automatic method for optimal construction of matrix product operators using bipartite graph theory. Journal of Chemical Physics, 2020, 153, 084118. | 3.0 | 22 |
| 47 | 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 |
| 48 | Experimentally Observed Reverse Intersystem Crossingâ€Boosted Lasing. Angewandte Chemie, 2020, 132, 21861-21866. | 2.0 | 31 |
| 49 | Experimentally Observed Reverse Intersystem Crossingâ€Boosted Lasing. Angewandte Chemie - International Edition, 2020, 59, 21677-21682. | 13.8 | 46 |
| 50 | Simultaneously and Selectively Imaging a Cytoplasm Membrane and Mitochondria Using a Dual-Colored Aggregation-Induced Emission Probe. Analytical Chemistry, 2020, 92, 14494-14500. | 6.5 | 37 |
| 51 | A novel molecular descriptor for highly efficient (Ï•<sub>TADF</sub> > 90%) transition metal TADF Au(<scp>iii</scp>) complexes. Journal of Materials Chemistry A, 2020, 8, 18721-18725. | 10.3 | 27 |
| 52 | Applying Marcus theory to describe the carrier transports in organic semiconductors: Limitations and beyond. Journal of Chemical Physics, 2020, 153, 080902. | 3.0 | 53 |
| 53 | Computational screen-out strategy for electrically pumped organic laser materials. Nature Communications, 2020, 11, 4485. | 12.8 | 48 |
| 54 | 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 |

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| 55 | Thermal Vibration Correlation Function Formalism for Molecular Excited State Decay Rates. Chinese Journal of Chemistry, 2020, 38, 1223-1232. | 4.9 | 157 |
| 56 | Finite-Temperature TD-DMRG for the Carrier Mobility of Organic Semiconductors. Journal of Physical Chemistry Letters, 2020, 11, 4930-4936. | 4.6 | 27 |
| 57 | Biradicalâ€Featured Stable Organicâ€Smallâ€Molecule Photothermal Materials for Highly Efficient Solarâ€Driven Water Evaporation. Advanced Materials, 2020, 32, e1908537. | 21.0 | 149 |
| 58 | Theoretical and Experimental Investigations on the Aggregationâ€Enhanced Emission from Dark State: Vibronic Coupling Effect. Advanced Electronic Materials, 2020, 6, 2000255. | 5.1 | 25 |
| 59 | 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 |
| 60 | Computational Study on the Charge Transport and Optical Spectra of Anthracene Derivatives in Aggregates. ChemPhysChem, 2020, 21, 952-957. | 2.1 | 19 |
| 61 | Numerical assessment for accuracy and GPU acceleration of TD-DMRG time evolution schemes. Journal of Chemical Physics, 2020, 152, 024127. | 3.0 | 38 |
| 62 | Finite Temperature Dynamical Density Matrix Renormalization Group for Spectroscopy in Frequency Domain. Journal of Physical Chemistry Letters, 2020, 11, 3761-3768. | 4.6 | 18 |
| 63 | Toward Achieving Single-Molecule White Electroluminescence from Dual Emission of Fluorescence and Phosphorescence. Chemistry of Materials, 2020, 32, 4038-4044. | 6.7 | 57 |
| 64 | 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. | 4.6 | 12 |
| 65 | Superexchange Induced Charge Transport in Organic Donorâ€“Acceptor Cocrystals and Copolymers: A Theoretical Perspective. Chemistry of Materials, 2019, 31, 6424-6434. | 6.7 | 39 |
| 66 | 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 |
| 67 | Strong Solid-State Fluorescence Induced by Restriction of the Coordinate Bond Bending in Two-Coordinate Copper(I)â€“Carbene Complexes. Inorganic Chemistry, 2019, 58, 14403-14409. | 4.0 | 35 |
| 68 | Pressure-induced emission enhancement in hexaphenylsilole: a computational study. Journal of Materials Chemistry C, 2019, 7, 1388-1398. | 5.5 | 33 |
| 69 | Highly Efficient Organic Room-Temperature Phosphorescent Luminophores through Tuning Triplet States and Spinâ€“Orbit Coupling with Incorporation of a Secondary Group. Journal of Physical Chemistry Letters, 2019, 10, 7141-7147. | 4.6 | 23 |
| 70 | Festschrift in Honor of Prof. Jean-Luc BrÃ©das on His 65th Birthday. Chemistry of Materials, 2019, 31, 6307-6308. | 6.7 | 2 |
| 71 | Highâ€Performance Organic Thermoelectric Materials: Theoretical Insights and Computational Design. Advanced Electronic Materials, 2019, 5, 1800882. | 5.1 | 39 |
| 72 | Highly Efficient Thermally Activated Delayed Fluorescence via Jâ€Aggregates with Strong Intermolecular Charge Transfer. Advanced Materials, 2019, 31, e1808242. | 21.0 | 278 |

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| 73 | Reducing Lattice Thermal Conductivity of the Thermoelectric SnSe Monolayer: Role of Phononâ€“Electron Coupling. Journal of Physical Chemistry C, 2019, 123, 12001-12006. | 3.1 | 32 |
| 74 | Boosting the Seebeck Coefficient for Organic Coordination Polymers: Role of Doping-Induced Polaron Band Formation. Journal of Physical Chemistry Letters, 2019, 10, 2493-2499. | 4.6 | 16 |
| 75 | 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 |
| 76 | 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. | 5.3 | 33 |
| 77 | 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. | 1.4 | 2 |
| 78 | General Approach To Compute Phosphorescent OLED Efficiency. Journal of Physical Chemistry C, 2018, 122, 6340-6347. | 3.1 | 70 |
| 79 | From Molecular Packing Structures to Electronic Processes: Theoretical Simulations for Organic Solar Cells. Advanced Energy Materials, 2018, 8, 1702743. | 19.5 | 93 |
| 80 | 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 |
| 81 | 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 |
| 82 | Lattice thermal conductivity of monolayer AsP from first-principles molecular dynamics. Physical Chemistry Chemical Physics, 2018, 20, 14024-14030. | 2.8 | 34 |
| 83 | Asymmetric photon transport in organic semiconductor nanowires through electrically controlled exciton diffusion. Science Advances, 2018, 4, eaap9861. | 10.3 | 56 |
| 84 | Janus monolayer of WSeTe, a new structural phase transition material driven by electrostatic gating. Nanoscale, 2018, 10, 21629-21633. | 5.6 | 68 |
| 85 | High performance thermoelectric materials based on metal organic coordination polymers through firstâ€principles band engineering. Journal of Computational Chemistry, 2018, 39, 2582-2588. | 3.3 | 12 |
| 86 | Suppressing charge recombination in small-molecule ternary organic solar cells by modulating donorâ€“acceptor interfacial arrangements. Physical Chemistry Chemical Physics, 2018, 20, 24570-24576. | 2.8 | 13 |
| 87 | Effect of donor length on electronic structures and charge transport polarity for DTDPP-based Dâ€“A copolymers: a computational study based on a super-exchange model. Journal of Materials Chemistry A, 2018, 6, 11985-11993. | 10.3 | 19 |
| 88 | Dynamic Ultralong Organic Phosphorescence by Photoactivation. Angewandte Chemie - International Edition, 2018, 57, 8425-8431. | 13.8 | 241 |
| 89 | Dynamic Ultralong Organic Phosphorescence by Photoactivation. Angewandte Chemie, 2018, 130, 8561-8567. | 2.0 | 47 |
| 90 | Highly sensitive switching of solid-state luminescence by controlling intersystem crossing. Nature Communications, 2018, 9, 3044. | 12.8 | 203 |

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| 91 | 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. | 3.1 | 14 |
| 92 | A facile strategy for realizing room temperature phosphorescence and single molecule white light emission. Nature Communications, 2018, 9, 2963. | 12.8 | 339 |
| 93 | 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 |
| 94 | 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. | 1.3 | 1 |
| 95 | 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. | 4.9 | 21 |
| 96 | Theoretical investigations on the electron-vibration couplings and description of opto-electronic properties of materials. Scientia Sinica Chimica, 2018, 48, 154-163. | 0.4 | 1 |
| 97 | 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 |
| 98 | Doping optimization of organic-inorganic hybrid perovskite CH 3 NH 3 PbI 3 for high thermoelectric efficiency. Synthetic Metals, 2017, 225, 108-114. | 3.9 | 34 |
| 99 | 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. | 6.7 | 19 |
| 100 | Super-exchange-induced high performance charge transport in donorâ€“acceptor copolymers. Journal of Materials Chemistry C, 2017, 5, 3247-3253. | 5.5 | 42 |
| 101 | Role of the Dark 2A<sub>g</sub> State in Donorâ€“Acceptor Copolymers as a Pathway for Singlet Fission: A DMRG Study. Journal of Physical Chemistry Letters, 2017, 8, 2175-2181. | 4.6 | 30 |
| 102 | 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 |
| 103 | Real-time monitoring of hydrophobic aggregation reveals a critical role of cooperativity in hydrophobic effect. Nature Communications, 2017, 8, 15639. | 12.8 | 67 |
| 104 | Excitonic coupling effect on the nonradiative decay rate in molecular aggregates: Formalism and application. Chemical Physics Letters, 2017, 683, 507-514. | 2.6 | 24 |
| 105 | Thermoelectrics: Tuning Thermal Transport in Chainâ€Oriented Conducting Polymers for Enhanced Thermoelectric Efficiency: A Computational Study (Adv. Funct. Mater. 40/2017). Advanced Functional Materials, 2017, 27, . | 14.9 | 0 |
| 106 | Aâ€“Ïâ€“Dâ€“Ïâ€“A Electronâ€Donating Small Molecules for Solutionâ€Processed Organic Solar Cells: A Review. Macromolecular Rapid Communications, 2017, 38, 1700470. | 3.9 | 70 |
| 107 | Intrinsic Charge Transport in Stanene: Roles of Bucklings and Electronâ€“Phonon Couplings. Advanced Electronic Materials, 2017, 3, 1700143. | 5.1 | 47 |
| 108 | Tuning Thermal Transport in Chainâ€Oriented Conducting Polymers for Enhanced Thermoelectric Efficiency: A Computational Study. Advanced Functional Materials, 2017, 27, 1702847. | 14.9 | 62 |

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| 109 | Isoindigoâ€Based Polymers with Small Effective Masses for Highâ€Mobility Ambipolar Fieldâ€Effect Transistors. Advanced Materials, 2017, 29, 1702115. | 21.0 | 115 |
| 110 | Puckered Arsenene: A Promising Room-Temperature Thermoelectric Material from First-Principles Prediction. Journal of Physical Chemistry C, 2017, 121, 19080-19086. | 3.1 | 56 |
| 111 | GeAs<sub>2</sub>: 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 |
| 112 | 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. | 8.2 | 4 |
| 113 | White light emission from a single organic molecule with dual phosphorescence at room temperature. Nature Communications, 2017, 8, 416. | 12.8 | 621 |
| 114 | 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. | 2.0 | 7 |
| 115 | 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 |
| 116 | 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 |
| 117 | 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 |
| 118 | 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 |
| 119 | Inner Space Perturbation Theory in Matrix Product States: Replacing Expensive Iterative Diagonalization. Journal of Chemical Theory and Computation, 2016, 12, 4871-4878. | 5.3 | 18 |
| 120 | Rational Molecular Design for Achieving Persistent and Efficient Pure Organic Room-Temperature Phosphorescence. CheM, 2016, 1, 592-602. | 11.7 | 610 |
| 121 | Theoretical Insights into the Mechanism of AIE. ACS Symposium Series, 2016, , 35-59. | 0.5 | 3 |
| 122 | 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 |
| 123 | Intrinsic and Extrinsic Charge Transport in CH3NH3PbI3 Perovskites Predicted from First-Principles. Scientific Reports, 2016, 6, 19968. | 3.3 | 119 |
| 124 | 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 |
| 125 | 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 |
| 126 | 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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| 127 | Unraveling the aggregation effect on amorphous phase AIE luminogens: a computational study. Nanoscale, 2016, 8, 15173-15180. | 5.6 | 112 |
| 128 | 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 |
| 129 | Naphtho[1,2-b:5,6-bâ€²]dithiophene-Based Small Molecules for Thick-Film Organic Solar Cells with High Fill Factors. Chemistry of Materials, 2016, 28, 943-950. | 6.7 | 50 |
| 130 | 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. | 8.0 | 49 |
| 131 | Effect of Intermolecular Excited-state Interaction on Vibrationally Resolved Optical Spectra in Organic Molecular Aggregates. Acta Chimica Sinica, 2016, 74, 902. | 1.4 | 27 |
| 132 | Mechanism of charge transport in organic semiconductors and carbon nanomaterials. Materials Research Society Symposia Proceedings, 2015, 1733, 1. | 0.1 | 0 |
| 133 | Influences of Conjugation Extent on the Aggregationâ€Induced Emission Quantum Efficiency in Silole Derivatives: A Computational Study. Chemistry - an Asian Journal, 2015, 10, 2154-2161. | 3.3 | 40 |
| 134 | Synergistic Photomodulation of Capacitive Coupling and Charge Separation Toward Functional Organic Fieldâ€Effect Transistors with High Responsivity. Advanced Electronic Materials, 2015, 1, 1500159. | 5.1 | 28 |
| 135 | Thin film field-effect transistors of 2,6-diphenyl anthracene (DPA). Chemical Communications, 2015, 51, 11777-11779. | 4.1 | 107 |
| 136 | Negative isotope effect for charge transport in acenes and derivatives â€“ a theoretical conclusion. Physical Chemistry Chemical Physics, 2015, 17, 3273-3280. | 2.8 | 19 |
| 137 | Electronic properties and charge carrier mobilities of graphynes and graphdiynes from first principles. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 215-227. | 14.6 | 42 |
| 138 | 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 |
| 139 | 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 |
| 140 | Theoretical Modeling of the Optical and Electrical Processes in Polymeric Solar Cells. Topics in Applied Physics, 2015, , 101-142. | 0.8 | 6 |
| 141 | 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 |
| 142 | Polymorphism-Dependent and Switchable Emission of Butterfly-Like Bis(diarylmethylene)dihydroanthracenes. Chemistry of Materials, 2015, 27, 6601-6607. | 6.7 | 144 |
| 143 | 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 |
| 144 | Comparative study on the methodologies for calculating the excited state in DMRG. Scientia Sinica Chimica, 2015, 45, 1316-1324. | 0.4 | 2 |

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|---|---|---|---|
| 145 | Naphtho[1,2-b:5,6-bâ€²]dithiophene Based Two-Dimensional Conjugated Polymers for Highly Efficient Thick-Film Inverted Polymer Solar Cells. Chemistry of Materials, 2014, 26, 6947-6954. | 6.7 | 45 |
| 146 | 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. | 14.9 | 0 |
| 147 | Chemical Sciences: Contributions to Building a Sustainable Society and Sharing of International Responsibilities. ACS Symposium Series, 2014, , 101-139. | 0.5 | 1 |
| 148 | Rubrene analogues with the aggregation-induced emission enhancement behaviour. Journal of Materials Chemistry C, 2014, 2, 884-890. | 5.5 | 22 |
| 149 | Excited states structure and processes: Understanding organic light-emitting diodes at the molecular level. Physics Reports, 2014, 537, 123-156. | 25.6 | 264 |
| 150 | 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 |
| 151 | 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 |
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