

Yuan-Ping Yi

List of Publications by Year in descending order

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276
papers

20,472
citations

8755

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docs citations

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times ranked

16434
citing authors

#	ARTICLE	IF	CITATIONS
1	Non-fullerene acceptors with branched side chains and improved molecular packing to exceed 18% efficiency in organic solar cells. <i>Nature Energy</i> , 2021, 6, 605-613.	39.5	1,307
2	Anchoring zero valence single atoms of nickel and iron on graphdiyne for hydrogen evolution. <i>Nature Communications</i> , 2018, 9, 1460.	12.8	781
3	A two-dimensional π -conjugated coordination polymer with extremely high electrical conductivity and ambipolar transport behaviour. <i>Nature Communications</i> , 2015, 6, 7408.	12.8	609
4	Novel Thermally Activated Delayed Fluorescence Materials—Thioxanthone Derivatives and Their Applications for Highly Efficient OLEDs. <i>Advanced Materials</i> , 2014, 26, 5198-5204.	21.0	488
5	Toward Quantitative Prediction of Molecular Fluorescence Quantum Efficiency: Role of Duschinsky Rotation. <i>Journal of the American Chemical Society</i> , 2007, 129, 9333-9339.	13.7	414
6	Achieving Highly Efficient Nonfullerene Organic Solar Cells with Improved Intermolecular Interaction and Open-Circuit Voltage. <i>Advanced Materials</i> , 2017, 29, 1700254.	21.0	363
7	Hydrogen substituted graphdiyne as carbon-rich flexible electrode for lithium and sodium ion batteries. <i>Nature Communications</i> , 2017, 8, 1172.	12.8	357
8	Graphdiyne Oxides as Excellent Substrate for Electroless Deposition of Pd Clusters with High Catalytic Activity. <i>Journal of the American Chemical Society</i> , 2015, 137, 5260-5263.	13.7	341
9	Organic Solar Cells with 18% Efficiency Enabled by an Alloy Acceptor: A Two-in-One Strategy. <i>Advanced Materials</i> , 2021, 33, e2100830.	21.0	323
10	The Impact of Molecular Orientation on the Photovoltaic Properties of a Phthalocyanine/Fullerene Heterojunction. <i>Advanced Functional Materials</i> , 2012, 22, 2987-2995.	14.9	298
11	Deep-Red to Near-Infrared Thermally Activated Delayed Fluorescence in Organic Solid Films and Electroluminescent Devices. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 11525-11529.	13.8	293
12	Exciton-Dissociation and Charge-Recombination Processes in Pentacene/C ₆₀ Solar Cells: Theoretical Insight into the Impact of Interface Geometry. <i>Journal of the American Chemical Society</i> , 2009, 131, 15777-15783.	13.7	275
13	Optimized Fibril Network Morphology by Precise Side-Chain Engineering to Achieve High-Performance Bulk-Heterojunction Organic Solar Cells. <i>Advanced Materials</i> , 2018, 30, e1707353.	21.0	271
14	Induction of Strong Long-Lived Room-Temperature Phosphorescence of <i>N</i> -Phenyl-2-naphthylamine Molecules by Confinement in a Crystalline Dibromobiphenyl Matrix. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 15589-15593.	13.8	265
15	High Conductive Two-Dimensional Covalent Organic Framework for Lithium Storage with Large Capacity. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 5366-5375.	8.0	255
16	Ternary Organic Solar Cells Based on Two Compatible Nonfullerene Acceptors with Power Conversion Efficiency >10%. <i>Advanced Materials</i> , 2016, 28, 10008-10015.	21.0	254
17	Prediction of Remarkable Ambipolar Charge-Transport Characteristics in Organic Mixed-Stack Charge-Transfer Crystals. <i>Journal of the American Chemical Society</i> , 2012, 134, 2340-2347.	13.7	245
18	Nitrogen-doped graphdiyne as a metal-free catalyst for high-performance oxygen reduction reactions. <i>Nanoscale</i> , 2014, 6, 11336-11343.	5.6	229

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19	Fine-Tuning of Crystal Packing and Charge Transport Properties of BDOPV Derivatives through Fluorine Substitution. <i>Journal of the American Chemical Society</i> , 2015, 137, 15947-15956.	13.7	224
20	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	222
21	Identification of FeN ₄ as an Efficient Active Site for Electrochemical N ₂ Reduction. <i>ACS Catalysis</i> , 2019, 9, 7311-7317.	11.2	220
22	Excited state radiationless decay process with Duschinsky rotation effect: Formalism and implementation. <i>Journal of Chemical Physics</i> , 2007, 126, 114302.	3.0	213
23	Unusual Aggregation-Induced Emission of a Coumarin Derivative as a Result of the Restriction of an Intramolecular Twisting Motion. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 14492-14497.	13.8	207
24	Flexible n-type High-Performance Thermoelectric Thin Films of Poly(nickel-ethylenetetrathiolate) Prepared by an Electrochemical Method. <i>Advanced Materials</i> , 2016, 28, 3351-3358.	21.0	206
25	Synthesis of Chlorine-Substituted Graphdiyne and Applications for Lithium-Ion Storage. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10740-10745.	13.8	206
26	Extended Squaraine Dyes with Large Two-Photon Absorption Cross-Sections. <i>Journal of the American Chemical Society</i> , 2006, 128, 14444-14445.	13.7	205
27	Terminal π - π stacking determines three-dimensional molecular packing and isotropic charge transport in an A ⁺ A ⁻ electron acceptor for non-fullerene organic solar cells. <i>Journal of Materials Chemistry C</i> , 2017, 5, 4852-4857.	5.5	192
28	Controlled Conjugated Backbone Twisting for an Increased Open-Circuit Voltage while Having a High Short-Circuit Current in Poly(hexylthiophene) Derivatives. <i>Journal of the American Chemical Society</i> , 2012, 134, 5222-5232.	13.7	187
29	N-doped graphdiyne for high-performance electrochemical electrodes. <i>Nano Energy</i> , 2018, 44, 144-154.	16.0	182
30	Solution-Processable Organic Molecule Photovoltaic Materials with Bithienyl-benzodithiophene Central Unit and Indenedione End Groups. <i>Chemistry of Materials</i> , 2013, 25, 2274-2281.	6.7	180
31	Interfacial Passivation for Perovskite Solar Cells: The Effects of the Functional Group in Phenethylammonium Iodide. <i>ACS Energy Letters</i> , 2019, 4, 2913-2921.	17.4	176
32	Nitrogen-Doped Porous Graphdiyne: A Highly Efficient Metal-Free Electrocatalyst for Oxygen Reduction Reaction. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 29744-29752.	8.0	166
33	Synthesis and Electronic Structure of Boron-Graphdiyne with an sp ² -Hybridized Carbon Skeleton and Its Application in Sodium Storage. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3968-3973.	13.8	166
34	Concurrent improvement in <i>J</i> _{SC} and <i>V</i> _{OC} in high-efficiency ternary organic solar cells enabled by a red-absorbing small-molecule acceptor with a high LUMO level. <i>Energy and Environmental Science</i> , 2020, 13, 2115-2123.	30.8	164
35	Rational Tuning of Molecular Interaction and Energy Level Alignment Enables High-Performance Organic Photovoltaics. <i>Advanced Materials</i> , 2019, 31, e1904215.	21.0	162
36	Improving the efficiency of solution processable organic photovoltaic devices by a star-shaped molecular geometry. <i>Journal of Materials Chemistry</i> , 2008, 18, 4085.	6.7	160

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37	Balanced Carrier Transports of Electrons and Holes in Silole-Based Compounds A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 7138-7143.	2.5	159
38	Self-catalyzed growth of Cu@graphdiyne core-shell nanowires array for high efficient hydrogen evolution cathode. <i>Nano Energy</i> , 2016, 30, 858-866.	16.0	149
39	Fluoride graphdiyne as a free-standing electrode displaying ultra-stable and extraordinary high Li storage performance. <i>Energy and Environmental Science</i> , 2018, 11, 2893-2903.	30.8	146
40	Remarkable enhancement of charge carrier mobility of conjugated polymer field-effect transistors upon incorporating an ionic additive. <i>Science Advances</i> , 2016, 2, e1600076.	10.3	139
41	Recovery of Au(III) by radiation synthesized aminomethyl pyridine functionalized adsorbents based on cellulose. <i>Chemical Engineering Journal</i> , 2016, 283, 504-513.	12.7	137
42	Selenium-Substituted Diketopyrrolopyrrole Polymer for High-Performance p-Type Organic Thermoelectric Materials. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 18994-18999.	13.8	136
43	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.	3.1	134
44	Bioinspired Multifunctional Organic Transistors Based on Natural Chlorophyll/Organic Semiconductors. <i>Advanced Materials</i> , 2020, 32, e2001227.	21.0	133
45	Highly Efficient Orange and Red Phosphorescent Organic Light-Emitting Diodes with Low Roll-Off of Efficiency using a Novel Thermally Activated Delayed Fluorescence Material as Host. <i>Advanced Materials</i> , 2015, 27, 4041-4047.	21.0	127
46	Thermal-Driven Phase Separation of Double-Cable Polymers Enables Efficient Single-Component Organic Solar Cells. <i>Joule</i> , 2019, 3, 1765-1781.	24.0	124
47	High-Performance Fluorinated Fused-Ring Electron Acceptor with 3D Stacking and Exciton/Charge Transport. <i>Advanced Materials</i> , 2020, 32, e2000645.	21.0	122
48	Small Exciton Binding Energies Enabling Direct Charge Photogeneration Towards Low-Driving-Force Organic Solar Cells. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15348-15353.	13.8	121
49	Aromatic-Imide-Based Thermally Activated Delayed Fluorescence Materials for Highly Efficient Organic Light-Emitting Diodes. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8818-8822.	13.8	118
50	Bottom-up growth of n-type monolayer molecular crystals on polymeric substrate for optoelectronic device applications. <i>Nature Communications</i> , 2018, 9, 2933.	12.8	118
51	Indigo-Based Polymers with Small Effective Masses for High-Mobility Ambipolar Field-Effect Transistors. <i>Advanced Materials</i> , 2017, 29, 1702115.	21.0	115
52	A comparative theoretical study of exciton-dissociation and charge-recombination processes in oligothiophene/fullerene and oligothiophene/perylene diimide complexes for organic solar cells. <i>Journal of Materials Chemistry</i> , 2011, 21, 1479.	6.7	112
53	Unraveling the influence of non-fullerene acceptor molecular packing on photovoltaic performance of organic solar cells. <i>Nature Communications</i> , 2020, 11, 6005.	12.8	112
54	Charge Mobility Enhancement for Conjugated DPP-Selenophene Polymer by Simply Replacing One Bulky Branching Alkyl Chain with Linear One at Each DPP Unit. <i>Chemistry of Materials</i> , 2018, 30, 3090-3100.	6.7	107

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55	Tuning the Crystal Polymorphs of Alkyl Thienoacene via Solution Self-Assembly Toward Air-Stable and High-Performance Organic Field-Effect Transistors. <i>Advanced Materials</i> , 2015, 27, 825-830.	21.0	106
56	Charge Transfer in Molecular Complexes with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F ₄ -TCNQ): A Density Functional Theory Study. <i>Chemistry of Materials</i> , 2011, 23, 5149-5159.	6.7	102
57	Achieving 16.68% efficiency ternary as-cast organic solar cells. <i>Science China Chemistry</i> , 2021, 64, 581-589.	8.2	99
58	A Cofacially Stacked Electron-Deficient Small Molecule with a High Electron Mobility of over 10 cm ² V ⁻¹ s ⁻¹ in Air. <i>Advanced Materials</i> , 2015, 27, 8051-8055.	21.0	97
59	Understanding the Charge Transport and Polarities in Organic Donor-Acceptor Mixed-Stack Crystals: Molecular Insights from the Super-Exchange Couplings. <i>Advanced Materials</i> , 2015, 27, 1443-1449.	21.0	97
60	Highly Conducting Neutral Coordination Polymer with Infinite Two-Dimensional Silver-Sulfur Networks. <i>Journal of the American Chemical Society</i> , 2018, 140, 15153-15156.	13.7	97
61	From Molecular Packing Structures to Electronic Processes: Theoretical Simulations for Organic Solar Cells. <i>Advanced Energy Materials</i> , 2018, 8, 1702743.	19.5	93
62	Exciton Binding Energies of Nonfullerene Small Molecule Acceptors: Implication for Exciton Dissociation Driving Forces in Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018, 122, 22309-22316.	3.1	93
63	Ferrocene as a highly volatile solid additive in non-fullerene organic solar cells with enhanced photovoltaic performance. <i>Energy and Environmental Science</i> , 2020, 13, 5117-5125.	30.8	93
64	Low temperature, atmospheric pressure for synthesis of a new carbon Ene-yne and application in Li storage. <i>Nano Energy</i> , 2017, 33, 343-349.	16.0	92
65	Air-Stable n-Type Thermoelectric Materials Enabled by Organic Diradicaloids. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 4958-4962.	13.8	92
66	Accurate Determination of the Minimum HOMO Offset for Efficient Charge Generation using Organic Semiconducting Alloys. <i>Advanced Energy Materials</i> , 2020, 10, 1903298.	19.5	92
67	Achieving an Efficient and Stable Morphology in Organic Solar Cells Via Fine-Tuning the Side Chains of Small-Molecule Acceptors. <i>Chemistry of Materials</i> , 2020, 32, 2593-2604.	6.7	91
68	Monolayer Two-dimensional Molecular Crystals for an Ultrasensitive OFET-based Chemical Sensor. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4380-4384.	13.8	90
69	Impact of polymorphism on the optoelectronic properties of a low-bandgap semiconducting polymer. <i>Nature Communications</i> , 2019, 10, 2867.	12.8	89
70	Electron-phonon couplings and carrier mobility in graphynes sheet calculated using the Wannier-interpolation approach. <i>Journal of Chemical Physics</i> , 2014, 141, 034704.	3.0	82
71	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.	5.5	82
72	Dicyclohepta[<i>ijkl</i>], [<i>uvw</i>]rubicene with Two Pentagons and Two Heptagons as a Stable and Planar Non-benzenoid Nanographene. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 3529-3533.	13.8	82

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73	Impact of Electron Delocalization on the Nature of the Charge-Transfer States in Model Pentacene/C ₆₀ Interfaces: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27648-27656.	3.1	80
74	Electronic Properties of Mixed-Stack Organic Charge-Transfer Crystals. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14150-14156.	3.1	79
75	Precisely Tailoring the Stoichiometric Stacking of Peryleneâ€”TCNQ Coâ€”Crystals towards Different Nano and Microstructures with Varied Optoelectronic Performances. <i>Small</i> , 2015, 11, 2150-2156.	10.0	79
76	Highâ€”Yield and Damageâ€”Free Exfoliation of Layered Graphdiyne in Aqueous Phase. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 746-750.	13.8	79
77	Bismuth Interfacial Doping of Organic Small Molecules for High Performance nâ€”type Thermoelectric Materials. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10672-10675.	13.8	77
78	Triplet Acceptors with a Dâ€”A Structure and Twisted Conformation for Efficient Organic Solar Cells. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15043-15049.	13.8	77
79	Reducing the Singletâ”Triplet Energy Gap by Endâ€”Group “” Stacking Toward Highâ€”Efficiency Organic Photovoltaics. <i>Advanced Materials</i> , 2020, 32, e2000975.	21.0	77
80	Solvent Effects on the Optical Spectra and Excited-State Decay of Triphenylamine-thiadiazole with Hybridized Local Excitation and Intramolecular Charge Transfer. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5233-5240.	2.5	73
81	A nonfullerene acceptor utilizing a novel asymmetric multifused-ring core unit for highly efficient organic solar cells. <i>Journal of Materials Chemistry C</i> , 2018, 6, 4873-4877.	5.5	73
82	Local Excitation/Charge-Transfer Hybridization Simultaneously Promotes Charge Generation and Reduces Nonradiative Voltage Loss in Nonfullerene Organic Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2911-2918.	4.6	73
83	Controllable Synthesis of Graphdiyne Nanoribbons. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4908-4913.	13.8	71
84	Two-Photon Absorption in Quadrupolar Bis(acceptor)-Terminated Chromophores with Electron-Rich Bis(heterocycle)vinylene Bridges. <i>Chemistry of Materials</i> , 2007, 19, 432-442.	6.7	66
85	Doping mechanisms of N-DMBI-H for organic thermoelectrics: hydrogen removal <i>vs.</i> hydride transfer. <i>Journal of Materials Chemistry A</i> , 2020, 8, 8323-8328.	10.3	66
86	Organic Semiconducting Alloys with Tunable Energy Levels. <i>Journal of the American Chemical Society</i> , 2019, 141, 6561-6568.	13.7	65
87	Airâ€”Stable nâ€”type Thermoelectric Materials Enabled by Organic Diradicaloids. <i>Angewandte Chemie</i> , 2019, 131, 5012-5016.	2.0	64
88	Electron Hopping by Interfacing Semiconducting Graphdiyne Nanosheets and Redox Molecules for Selective Electrocatalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 2074-2082.	13.7	63
89	An improved dynamic Monte Carlo model coupled with Poisson equation to simulate the performance of organic photovoltaic devices. <i>Journal of Chemical Physics</i> , 2011, 134, 124102.	3.0	62
90	Mechanism study on organic ternary photovoltaics with 18.3% certified efficiency: from molecule to device. <i>Energy and Environmental Science</i> , 2022, 15, 855-865.	30.8	62

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91	Insertion of double bond π -bridges of "D" A acceptors for high performance near-infrared polymer solar cells. <i>Journal of Materials Chemistry A</i> , 2017, 5, 22588-22597.	10.3	61
92	Achieving Small Exciton Binding Energies in Small Molecule Acceptors for Organic Solar Cells: Effect of Molecular Packing. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4888-4894.	4.6	60
93	Direct Synthesis of Crystalline Graphdiyne Analogue Based on Supramolecular Interactions. <i>Journal of the American Chemical Society</i> , 2019, 141, 48-52.	13.7	60
94	From Dark TICT State to Emissive <i>quasi</i> -TICT State: The AIE Mechanism of <i>N</i> -(3-(benzo[d]oxazol-2-yl)phenyl)-4- <i>tert</i> -butylbenzamide. <i>Journal of Physical Chemistry C</i> , 2015, 119, 2133-2141.	3.1	58
95	Highly efficient blue organic light-emitting diodes from pyrimidine-based thermally activated delayed fluorescence emitters. <i>Journal of Materials Chemistry C</i> , 2018, 6, 2351-2359.	5.5	58
96	Electrical Loss Management by Molecularly Manipulating Dopant-free Poly(3-hexylthiophene) towards 16.93% CsPbI ₂ Br Solar Cells. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 16388-16393.	13.8	57
97	Helical Molecular Duplex Strands: Multiple Hydrogen-Bond-Mediated Assembly of Self-Complementary Oligomeric Hydrazide Derivatives. <i>Journal of Organic Chemistry</i> , 2007, 72, 4936-4946.	3.2	56
98	Experimental Evidence for "Hot Exciton" Thermally Activated Delayed Fluorescence Emitters. <i>Advanced Optical Materials</i> , 2019, 7, 1801190.	7.3	56
99	Increasing donor-acceptor spacing for reduced voltage loss in organic solar cells. <i>Nature Communications</i> , 2021, 12, 6679.	12.8	56
100	Thermally populated "bright" states for wide-range and high temperature sensing in air. <i>Chemical Communications</i> , 2017, 53, 5702-5705.	4.1	54
101	Intrinsic charge transport in single crystals of organic molecular semiconductors: A theoretical perspective. <i>MRS Bulletin</i> , 2013, 38, 57-64.	3.5	53
102	Tuning transport performance in two-dimensional metal-organic framework semiconductors: Role of the metal <i>d</i> band. <i>Applied Physics Letters</i> , 2018, 112, .	3.3	53
103	High two-photon cross-sections in bis(diarylaminostyryl) chromophores with electron-rich heterocycle and bis(heterocycle)vinylene bridges. <i>Chemical Communications</i> , 2007, , 1372-1374.	4.1	52
104	Synthesis of Chlorine-Substituted Graphdiyne and Applications for Lithium-Ion Storage. <i>Angewandte Chemie</i> , 2017, 129, 10880-10885.	2.0	52
105	Preparation and structure study of phosphorus-doped porous graphdiyne and its efficient lithium storage application. <i>2D Materials</i> , 2019, 6, 035020.	4.4	52
106	The Impact of Interlayer Electronic Coupling on Charge Transport in Organic Semiconductors: A Case Study on Titanylphthalocyanine Single Crystals. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5206-5209.	13.8	51
107	Isomery-Dependent Miscibility Enables High-Performance All-Small-Molecule Solar Cells. <i>Small</i> , 2019, 15, 1804271.	10.0	50
108	Longer and Stronger: Improving Persistent Luminescence in Size-Tuned Zinc Gallate Nanoparticles by Alcohol-Mediated Chromium Doping. <i>ACS Nano</i> , 2020, 14, 12113-12124.	14.6	50

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109	Tunable Electron Donating and Accepting Properties Achieved by Modulating the Steric Hindrance of Side Chains in A-D-A Small-Molecule Photovoltaic Materials. <i>Chemistry of Materials</i> , 2018, 30, 619-628.	6.7	49
110	Symmetry effects on nonlocal electron-phonon coupling in organic semiconductors. <i>Physical Review B</i> , 2012, 85, .	3.2	48
111	Nonlocal electron-phonon coupling in the pentacene crystal: Beyond the Γ -point approximation. <i>Journal of Chemical Physics</i> , 2012, 137, 164303.	3.0	48
112	Diaceno[<i>a</i>] <i>e</i>]pentalenes from Homoannulations of <i>o</i> -Alkynylaryliodides Utilizing a Unique Pd(OAc) ₂ / <i>n</i> -Bu ₄ NOAc Catalytic Combination. <i>Organic Letters</i> , 2014, 16, 4924-4927.	4.6	48
113	Triplet decay-induced negative temperature dependence of the transient photoluminescence decay of thermally activated delayed fluorescence emitter. <i>Journal of Materials Chemistry C</i> , 2017, 5, 12077-12084.	5.5	48
114	Origin of High Efficiencies for Thermally Activated Delayed Fluorescence Organic Light-Emitting Diodes: Atomistic Insight into Molecular Orientation and Torsional Disorder. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27191-27197.	3.1	48
115	Developing Quinoidal Fluorophores with Unusually Strong Red/Near-Infrared Emission. <i>Journal of the American Chemical Society</i> , 2015, 137, 11294-11302.	13.7	47
116	Deep-Red to Near-Infrared Thermally Activated Delayed Fluorescence in Organic Solid Films and Electroluminescent Devices. <i>Angewandte Chemie</i> , 2017, 129, 11683-11687.	2.0	47
117	Synthesis and Electronic Structure of Boron-Graphdiyne with an <i>sp</i> ² -Hybridized Carbon Skeleton and Its Application in Sodium Storage. <i>Angewandte Chemie</i> , 2018, 130, 4032-4037.	2.0	47
118	Atomistic Insight Into Donor/Acceptor Interfaces in High-Efficiency Nonfullerene Organic Solar Cells. <i>Solar Rrl</i> , 2018, 2, 1800190.	5.8	47
119	Barrier-Free Charge Separation Enabled by Electronic Polarization in High-Efficiency Non-fullerene Organic Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2585-2591.	4.6	47
120	Hot Charge-Transfer States Determine Exciton Dissociation in the DTDCTB/C ₆₀ Complex for Organic Solar Cells: A Theoretical Insight. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11320-11326.	3.1	46
121	Origin of Photocurrent and Voltage Losses in Organic Solar Cells. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900067.	2.8	46
122	Nature of the Lowest Singlet and Triplet Excited States of Organic Thermally Activated Delayed Fluorescence Emitters: A Self-Consistent Quantum Mechanics/Embedded Charge Study. <i>Chemistry of Materials</i> , 2019, 31, 6665-6671.	6.7	46
123	Molecular Insight into Efficient Charge Generation in Low-Driving-Force Nonfullerene Organic Solar Cells. <i>Accounts of Chemical Research</i> , 2022, 55, 869-877.	15.6	46
124	Heteroatom substitution-induced asymmetric A ² D ² A type non-fullerene acceptor for efficient organic solar cells. <i>Journal of Energy Chemistry</i> , 2020, 40, 144-150.	12.9	45
125	Two-Photon Absorption Properties of Iron(II) and Ruthenium(II) Trischelate Complexes of 2,2â€²:4,4â€²-â€²:4â€²-Quaterpyridinium Ligands. <i>Journal of Physical Chemistry A</i> , 2007, 111, 472-478. ⁴⁴	2.5	44
126	Organic Cocrystal Photovoltaic Behavior: A Model System to Study Charge Recombination of C ₆₀ and C ₇₀ at the Molecular Level. <i>Advanced Electronic Materials</i> , 2016, 2, 1500423.	5.1	42

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127	Charge transport in organic donor-acceptor mixed-stack crystals: the role of nonlocal electron-phonon couplings. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 4418-4425.	2.8	42
128	Super-exchange-induced high performance charge transport in donor-acceptor copolymers. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3247-3253.	5.5	42
129	Influences of Conjugation Extent on the Aggregation-Induced Emission Quantum Efficiency in Silole Derivatives: A Computational Study. <i>Chemistry - an Asian Journal</i> , 2015, 10, 2154-2161.	3.3	40
130	An Amidine-Type Dopant for Solution-Processed Field-Effect Transistors and Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2017, 27, 1703254.	14.9	40
131	Y6 and its derivatives: molecular design and physical mechanism. <i>National Science Review</i> , 2021, 8, nwab121.	9.5	40
132	Superexchange Induced Charge Transport in Organic Donor-Acceptor Cocrystals and Copolymers: A Theoretical Perspective. <i>Chemistry of Materials</i> , 2019, 31, 6424-6434.	6.7	39
133	Clustering-Triggered Efficient Room-Temperature Phosphorescence from Nonconventional Luminophores. <i>ChemPhysChem</i> , 2020, 21, 36-42.	2.1	39
134	Sub-5 nm single crystalline organic p-n heterojunctions. <i>Nature Communications</i> , 2021, 12, 2774.	12.8	39
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