Jean-Luc E Bredas

List of Publications by Year
in descending order

578	59,022	863 117	1527 218
papers	citations	h-index	g-index

599	599	599	36840
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Charge Transport in Organic Semiconductors. Chemical Reviews, 2007, 107, 926-952.	23.0	3,853
2	Charge-Transfer and Energy-Transfer Processes in Ï€-Conjugated Oligomers and Polymers:Â A Molecular Picture. Chemical Reviews, 2004, 104, 4971-5004.	23.0	2,539
3	A Universal Method to Produce Lowâ€“Work Function Electrodes for Organic Electronics. Science, 2012, 336, 327-332.	6.0	1,878
4	Molecular Understanding of Organic Solar Cells: The Challenges. Accounts of Chemical Research, 2009, 42, 1691-1699.	7.6	1,291
5	Introduction to Organic Thin Film Transistors and Design of n-Channel Organic Semiconductors. Chemistry of Materials, 2004, 16, 4436-4451.	3.2	1,256
6	Organic photovoltaics. Energy and Environmental Science, 2009, 2, 251.	15.6	1,142
7	Mind the gap!. Materials Horizons, 2014, 1, 17-19.	6.4	850
8	Structureâ^'Property Relationships for Two-Photon Absorbing Chromophores:Â Bis-Donor Diphenylpolyene and Bis(styryl)benzene Derivatives. Journal of the American Chemical Society, 2000, 122, 9500-9510.	6.6	842
9	Single-electron transistor of a single organic molecule with access to several redox states. Nature, 2003, 425, 698-701.	13.7	798
10	Effect of Electronic Polarization on Charge-Transport Parameters in Molecular Organic Semiconductors. Journal of the American Chemical Society, 2006, 128, 9882-9886.	6.6	756
11	Design rules for minimizing voltage losses in high-efficiency organic solar cells. Nature Materials, 2018, 17, 703-709.	13.3	701
12	Up-Conversion Intersystem Crossing Rates in Organic Emitters for Thermally Activated Delayed Fluorescence: Impact of the Nature of Singlet vs Triplet Excited States. Journal of the American Chemical Society, 2017, 139, 4042-4051.	6.6	698
13	Quantitative relations between interaction parameter, miscibility and function in organic solar cells. Nature Materials, 2018, 17, 253-260.	13.3	556
14	Origin of High Second- and Third-Order Nonlinear Optical Response in Ammonio/Borato Diphenylpolyene Zwitterions:â€‰ the Remarkable Role of Polarized Aromatic Groups. Journal of the American Chemical Society, 2003, 125, 15651-15658.	6.6	485
15	Characterization of the Interface Dipole at Organic/ Metal Interfaces. Journal of the American Chemical Society, 2002, 124, 8131-8141.	6.6	471
16	Charge Transport Properties in Discotic Liquid Crystals:â€‰ A Quantum-Chemical Insight into Structureâ^'Property Relationships. Journal of the American Chemical Society, 2004, 126, 3271-3279.	6.6	464
17	Delocalization of exciton and electron wavefunction in non-fullerene acceptor molecules enables efficient organic solar cells. Nature Communications, 2020, 11, 3943.	5.8	458
18	The Vibrational Reorganization Energy in Pentacene:â€‰ Molecular Influences on Charge Transport. Journal of the American Chemical Society, 2002, 124, 7918-7919.	6.6	425

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19	High-efficiency electroluminescence and amplified spontaneous emission from a thermally activated delayed fluorescent near-infrared emitter. Nature Photonics, 2018, 12, 98-104.	15.6	421
20	Transport Properties in the Rubrene Crystal: Electronic Coupling and Vibrational Reorganization Energy. Advanced Materials, 2005, 17, 1072-1076.	11.1	409
21	Organic Thin Film Transistors Based onN-Alkyl Perylene Diimides:Â Charge Transport Kinetics as a Function of Gate Voltage and Temperature. Journal of Physical Chemistry B, 2004, 108, 19281-19292.	1.2	406
22	Thermally Activated Delayed Fluorescence (TADF) Path toward Efficient Electroluminescence in Purely Organic Materials: Molecular Level Insight. Accounts of Chemical Research, 2018, 51, 2215-2224.	7.6	382
23	The Interface Energetics of Self-Assembled Monolayers on Metals. Accounts of Chemical Research, 2008, 41, 721-729.	7.6	371
24	Reliable Prediction with Tuned Range-Separated Functionals of the Singletâ€“Triplet Gap in Organic Emitters for Thermally Activated Delayed Fluorescence. Journal of Chemical Theory and Computation, 2015, 11, 3851-3858.	2.3	362
25	High operational and environmental stability of high-mobility conjugated polymer field-effect transistors through the use of molecular additives. Nature Materials, 2017, 16, 356-362.	13.3	345
26	The exciton binding energy in luminescent conjugated polymers. Advanced Materials, 1996, 8, 447-452.	11.1	344
27	Fast spin-flip enables efficient and stable organic electroluminescence from charge-transfer states. Nature Photonics, 2020, 14, 636-642.	15.6	331
28	Organic Electronic Materials: Recent Advances in the DFT Description of the Ground and Excited States Using Tuned Range-Separated Hybrid Functionals. Accounts of Chemical Research, 2014, 47, 3284-3291.	7.6	324
29	Design of Polymethine Dyes with Large Third-Order Optical Nonlinearities and Loss Figures of Merit. Science, 2010, 327, 1485-1488.	6.0	320
30	Tuning the Charge-Transport Parameters of Perylene Diimide Single Crystals via End and/or Core Functionalization: A Density Functional Theory Investigation. Journal of the American Chemical Society, 2010, 132, 3375-3387.	6.6	320
31	Photoinduced Charge Generation and Recombination Dynamics in Model Donor/Acceptor Pairs for Organic Solar Cell Applications:â€‰ A Full Quantum-Chemical Treatment. Journal of the American Chemical Society, 2005, 127, 6077-6086.	6.6	314
32	Polarization Energies in Oligoacene Semiconductor Crystals. Journal of the American Chemical Society, 2008, 130, 12377-12384.	6.6	313
33	Experimental Demonstration of the Dependence of the First Hyperpolarizability of Donor-Acceptor-Substituted Polyenes on the Ground-State Polarization and Bond Length Alternation. Journal of the American Chemical Society, 1994, 116, 2619-2620.	6.6	298
34	The Impact of Molecular Orientation on the Photovoltaic Properties of a Phthalocyanine/Fullerene Heterojunction. Advanced Functional Materials, 2012, 22, 2987-2995.	7.8	298
35	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.	7.6	286
36	Exciton-Dissociation and Charge-Recombination Processes in Pentacene/C₆₀ Solar Cells: Theoretical Insight into the Impact of Interface Geometry. Journal of the American Chemical Society, 2009, 131, 15777-15783.	6.6	275

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37	Critical role of intermediate electronic states for spin-flip processes in charge-transfer-type organic molecules with multiple donors and acceptors. Nature Materials, 2019, 18, 1084-1090.	13.3	271
38	Intersystem Crossing Processes in Nonplanar Aromatic Heterocyclic Molecules. Journal of Physical Chemistry A, 2007, 111, 10490-10499.	1.1	261
39	Interface Energetics and Level Alignment at Covalent Metal-Molecule Junctions: Ï€-Conjugated Thiols on Gold. Physical Review Letters, 2006, 96, 196806.	2.9	258
40	Exciton Migration in Rigid-Rod Conjugated Polymers:Â An Improved FÃ¶rster Model. Journal of the American Chemical Society, 2005, 127, 4744-4762.	6.6	257
41	Toward Control of the Metalâ^'Organic Interfacial Electronic Structure in Molecular Electronics:Â A First-Principles Study on Self-Assembled Monolayers of Ï€-Conjugated Molecules on Noble Metals. Nano Letters, 2007, 7, 932-940.	4.5	257
42	Prediction of Remarkable Ambipolar Charge-Transport Characteristics in Organic Mixed-Stack Charge-Transfer Crystals. Journal of the American Chemical Society, 2012, 134, 2340-2347.	6.6	245
43	Photovoltaic concepts inspired by coherence effects in photosynthetic systems. Nature Materials, 2017, 16, 35-44.	13.3	243
44	Redox States of Long Oligothiophenes: Two Polarons on a Single Chain. Chemistry - A European Journal, 1998, 4, 1509-1522.	1.7	242
45	A quantum-chemical perspective into low optical-gap polymers for highly-efficient organic solar cells. Chemical Science, 2011, 2, 1200-1218.	3.7	241
46	A unified description of non-radiative voltage losses in organic solar cells. Nature Energy, 2021, 6, 799-806.	19.8	235
47	Long-range corrected hybrid functionals for Ï€-conjugated systems: Dependence of the range-separation parameter on conjugation length. Journal of Chemical Physics, 2011, 135, 204107.	1.2	234
48	Solution-Processed Organic Solar Cells with Power Conversion Efficiencies of 2.5% using Benzothiadiazole/Imide-Based Acceptors. Chemistry of Materials, 2011, 23, 5484-5490.	3.2	232
49	Ultralow Doping in Organic Semiconductors: Evidence of Trap Filling. Physical Review Letters, 2012, 109, 176601.	2.9	231
50	Charge-transfer electronic states inÂorganic solar cells. Nature Reviews Materials, 2019, 4, 689-707.	23.3	229
51	One- and Two-Photon Spectroscopy of Donorâ^'Acceptorâ^'Donor Distyrylbenzene Derivatives:â€‰ Effect of Cyano Substitution and Distortion from Planarity. Journal of Physical Chemistry A, 2002, 106, 11470-11480.	1.1	227
52	Unconventional, Chemically Stable, and Soluble Two-Dimensional Angular Polycyclic Aromatic Hydrocarbons: From Molecular Design to Device Applications. Accounts of Chemical Research, 2015, 48, 500-509.	7.6	227
53	Transition from Tunneling to Hopping Transport in Long, Conjugated Oligo-imine Wires Connected to Metals. Journal of the American Chemical Society, 2010, 132, 4358-4368.	6.6	217
54	Noncovalent Intermolecular Interactions in Organic Electronic Materials: Implications for the Molecular Packing vs Electronic Properties of Acenes. Chemistry of Materials, 2016, 28, 3-16.	3.2	215

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55	A New Design Strategy for Efficient Thermally Activated Delayed Fluorescence Organic Emitters: From Twisted to Planar Structures. Advanced Materials, 2017, 29, 1702767.	11.1	215
56	A Spray-Processable, Low Bandgap, and Ambipolar Donorâ^'Acceptor Conjugated Polymer. Journal of the American Chemical Society, 2009, 131, 2824-2826.	6.6	214
57	Metal-Ion Sensing Fluorophores with Large Two-Photon Absorption Cross Sections:Â Aza-Crown Ether Substituted Donorâ^'Acceptorâ^'Donor Distyrylbenzenes. Journal of the American Chemical Society, 2004, 126, 9291-9306.	6.6	206
58	Impact of Bidirectional Charge Transfer and Molecular Distortions on the Electronic Structure of a Metal-Organic Interface. Physical Review Letters, 2007, 99, 256801.	2.9	206
59	Extended Squaraine Dyes with Large Two-Photon Absorption Cross-Sections. Journal of the American Chemical Society, 2006, 128, 14444-14445.	6.6	205
60	Donorâ€“Acceptor Copolymers of Relevance for Organic Photovoltaics: A Theoretical Investigation of the Impact of Chemical Structure Modifications on the Electronic and Optical Properties. Macromolecules, 2012, 45, 6405-6414.	2.2	203
61	Inside Perovskites: Quantum Luminescence from Bulk Cs₄PbBr₆ Single Crystals. Chemistry of Materials, 2017, 29, 7108-7113.	3.2	200
62	Impact of interfacial molecular orientation on radiative recombination and charge generation efficiency. Nature Communications, 2017, 8, 79.	5.8	198
63	Polaron self-localization in white-light emitting hybrid perovskites. Journal of Materials Chemistry C, 2017, 5, 2771-2780.	2.7	196
64	Alternating Oligo(p-phenylene vinylene)â^'Perylene Bisimide Copolymers:Â Synthesis, Photophysics, and Photovoltaic Properties of a New Class of Donorâ^'Acceptor Materials. Journal of the American Chemical Society, 2003, 125, 8625-8638.	6.6	195
65	Steric Control of the Donor/Acceptor Interface: Implications in Organic Photovoltaic Charge Generation. Journal of the American Chemical Society, 2011, 133, 12106-12114.	6.6	193
66	Green emission from poly(fluorene)s: The role of oxidation. Journal of Chemical Physics, 2002, 117, 6794-6802.	1.2	190
67	Humidity Sensing through Reversible Isomerization of a Covalent Organic Framework. Journal of the American Chemical Society, 2020, 142, 783-791.	6.6	190
68	Phosphonic Acids for Interfacial Engineering of Transparent Conductive Oxides. Chemical Reviews, 2016, 116, 7117-7158.	23.0	189
69	Effects of electronegative substitution on the optical and electronic properties of acenes and diazaacenes. Nature Communications, 2010, 1, 91.	5.8	187
70	Controlled Conjugated Backbone Twisting for an Increased Open-Circuit Voltage while Having a High Short-Circuit Current in Poly(hexylthiophene) Derivatives. Journal of the American Chemical Society, 2012, 134, 5222-5232.	6.6	187
71	Molecular behavior of zero-dimensional perovskites. Science Advances, 2017, 3, e1701793.	4.7	187
72	High stability and luminescence efficiency in donorâ€“acceptor neutral radicals not following the Aufbau principle. Nature Materials, 2019, 18, 977-984.	13.3	181

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73	Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals. Journal of the American Chemical Society, 2009, 131, 1502-1512.	6.6	174
74	Optical and Redox Properties of a Series of 3,4-Ethylenedioxythiophene Oligomers. Chemistry - A European Journal, 2002, 8, 2384.	1.7	172
75	Direct-Indirect Nature of the Bandgap in Lead-Free Perovskite Nanocrystals. Journal of Physical Chemistry Letters, 2017, 8, 3173-3177.	2.1	172
76	Conjugated polymers and oligomers: Designing novel materials using a quantum-chemical approach. Advanced Materials, 1995, 7, 263-274.	11.1	162
77	Thermally conductive ultra-low-k dielectric layers based on two-dimensional covalent organic frameworks. Nature Materials, 2021, 20, 1142-1148.	13.3	158
78	Electron Affinities of 1,1-Diaryl-2,3,4,5-tetraphenylsiloles:Â Direct Measurements and Comparison with Experimental and Theoretical Estimates. Journal of the American Chemical Society, 2005, 127, 9021-9029.	6.6	155
79	Dithienopyrrole-based donorâ€“acceptor copolymers: low band-gap materials for charge transport, photovoltaics and electrochromism. Journal of Materials Chemistry, 2010, 20, 123-134.	6.7	154
80	Charge Transport Parameters of the Pentathienoacene Crystal. Journal of the American Chemical Society, 2007, 129, 13072-13081.	6.6	153
81	Modification of the Surface Properties of Indium Tin Oxide with Benzylphosphonic Acids: A Joint Experimental and Theoretical Study. Advanced Materials, 2009, 21, 4496-4501.	11.1	152
82	Multipole expansion in tight-binding Hartree-Fock calculations for infinite model polymers. Physical Review B, 1980, 22, 6254-6267.	1.1	151
83	Two-Photon Absorption at Telecommunications Wavelengths in a Dipolar Chromophore with a Pyrrole Auxiliary Donor and Thiazole Auxiliary Acceptor. Journal of the American Chemical Society, 2005, 127, 7282-7283.	6.6	150
84	Electronic Evolution of Poly(3,4-ethylenedioxythiophene) (PEDOT): From the Isolated Chain to the Pristine and Heavily Doped Crystals. Journal of the American Chemical Society, 2008, 130, 16880-16889.	6.6	150
85	Bistetracene: An Air-Stable, High-Mobility Organic Semiconductor with Extended Conjugation. Journal of the American Chemical Society, 2014, 136, 9248-9251.	6.6	150
86	Evaluating the Performance of DFT Functionals in Assessing the Interaction Energy and Ground-State Charge Transfer of Donor/Acceptor Complexes: Tetrathiafulvaleneâ^'Tetracyanoquinodimethane (TTFâ^'TCNQ) as a Model Case. Journal of Chemical Theory and Computation, 2011, 7, 602-609.	2.3	143
87	Point Defects and Green Emission in Zero-Dimensional Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 5490-5495.	2.1	143
88	Rubrene-Based Single-Crystal Organic Semiconductors: Synthesis, Electronic Structure, and Charge-Transport Properties. Chemistry of Materials, 2013, 25, 2254-2263.	3.2	141
89	Vibronic Coupling in the Ground and Excited States of Oligoacene Cationsâ€. Journal of Physical Chemistry B, 2006, 110, 18904-18911.	1.2	140
90	Excitonic and Polaronic Properties of 2D Hybrid Organicâ€“Inorganic Perovskites. ACS Energy Letters, 2017, 2, 417-423.	8.8	140

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91	Shallow trap states in pentacene thin films from molecular sliding. Applied Physics Letters, 2005, 86, 152115.	1.5	139
92	Correlation between the Microscopic Morphology and the Solid-State Photoluminescence Properties in Fluorene-Based Polymers and Copolymers. Chemistry of Materials, 2004, 16, 994-1001.	3.2	138
93	Theoretical Characterization of the Indium Tin Oxide Surface and of Its Binding Sites for Adsorption of Phosphonic Acid Monolayers. Chemistry of Materials, 2008, 20, 5131-5133.	3.2	138
94	Electronic Delocalization in Discotic Liquid Crystals:Â A Joint Experimental and Theoretical Study. Journal of the American Chemical Society, 2004, 126, 11889-11899.	6.6	136
95	Intervalence Transitions in the Mixed-Valence Monocations of Bis(triarylamines) Linked with Vinylene and Phenyleneâ^'Vinylene Bridges. Journal of the American Chemical Society, 2005, 127, 16900-16911.	6.6	135
96	Aromatic Amines:â€‰ A Comparison of Electron-Donor Strengths. Journal of Physical Chemistry A, 2005, 109, 9346-9352.	1.1	134
97	Organic Photovoltaics. Accounts of Chemical Research, 2009, 42, 1689-1690.	7.6	134
98	Intrinsic Lead Ion Emissions in Zero-Dimensional Cs₄PbBr₆ Nanocrystals. ACS Energy Letters, 2017, 2, 2805-2811.	8.8	133
99	Fused electron deficient semiconducting polymers for air stable electron transport. Nature Communications, 2018, 9, 416.	5.8	133
100	The metal-on-polymer interface in polymer light emitting diodes. Advanced Materials, 1996, 8, 48-52.	11.1	129
101	Thieno[3,4â€c]pyroleâ€4,6â€dioneâ€3,4â€difluorothiophene Polymer Acceptors for Efficient Allâ€Polymer Bulk Heterojunction Solar Cells. Angewandte Chemie - International Edition, 2016, 55, 12996-13000.	7.2	129
102	Organic/metal interfaces in self-assembled monolayers of conjugated thiols: A first-principles benchmark study. Surface Science, 2006, 600, 4548-4562.	0.8	128
103	Interaction of Charge Carriers with Lattice Vibrations in Oligoacene Crystals from Naphthalene to Pentacene. Journal of the American Chemical Society, 2010, 132, 14437-14446.	6.6	128
104	Highly Dipolar, Optically Nonlinear Adducts of Tetracyano-p-quinodimethane:Â Synthesis, Physical Characterization, and Theoretical Aspects. Journal of the American Chemical Society, 1997, 119, 3144-3154.	6.6	126
105	Use of Xâ€Ray Diffraction, Molecular Simulations, and Spectroscopy to Determine the Molecular Packing in a Polymerâ€Fullerene Bimolecular Crystal. Advanced Materials, 2012, 24, 6071-6079.	11.1	126
106	Assessing the nature of the charge-transfer electronic states in organic solar cells. Nature Communications, 2018, 9, 5295.	5.8	126
107	Preparation and Characterization of Ï€-Stacking Quinodimethane Oligothiophenes. Predicting Semiconductor Behavior and Bandwidths from Crystal Structures and Molecular Orbital Calculations. Journal of the American Chemical Society, 2004, 126, 15295-15308.	6.6	124
108	Photoelectron Spectroscopic Study of the Electronic Band Structure of Polyfluorene and Fluorene-Arylamine Copolymers at Interfaces. Journal of Physical Chemistry C, 2007, 111, 1378-1384.	1.5	124

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109	Synthetic Principles Directing Charge Transport in Low-Band-Gap Dithienosiloleâ€“Benzothiadiazole Copolymers. Journal of the American Chemical Society, 2012, 134, 8944-8957.	6.6	124
110	Ionization Energies, Electron Affinities, and Polarization Energies of Organic Molecular Crystals: Quantitative Estimations from a Polarizable Continuum Model (PCM)-Tuned Range-Separated Density Functional Approach. Journal of Chemical Theory and Computation, 2016, 12, 2906-2916.	2.3	124
111	Design of Organic Chromophores for All-Optical Signal Processing Applications. Chemistry of Materials, 2014, 26, 549-560.	3.2	123
112	Heteroannulated acceptors based on benzothiadiazole. Materials Horizons, 2015, 2, 22-36.	6.4	123
113	Design of Emission Ratiometric Metal-Ion Sensors with Enhanced Two-Photon Cross Section and Brightness. Journal of the American Chemical Society, 2007, 129, 11888-11889.	6.6	122
114	On the Interface Dipole at the Pentaceneâˆ'Fullerene Heterojunction: A Theoretical Study. Journal of Physical Chemistry C, 2010, 114, 3215-3224.	1.5	122
115	Spiro-OMeTAD single crystals: Remarkably enhanced charge-carrier transport via mesoscale ordering. Science Advances, 2016, 2, e1501491.	4.7	122
116	Delocalization in Platinumâˆ'Alkynyl Systems:Â A Metal-Bridged Organic Mixed-Valence Compound. Journal of the American Chemical Society, 2004, 126, 11782-11783.	6.6	121
117	Triplet Excimer Formation in Platinum-Based Phosphors: A Theoretical Study of the Roles of Ptâˆ'Pt Bimetallic Interactions and Interligand Ï€âˆ'Ï€ Interactions. Journal of the American Chemical Society, 2009, 131, 11371-11380.	6.6	121
118	Nucleation and Growth of Covalent Organic Frameworks from Solution: The Example of COF-5. Journal of the American Chemical Society, 2017, 139, 16310-16318.	6.6	121
119	Investigation of Exciton Coupling in Oligothiophenes by Circular Dichroism Spectroscopy. Advanced Materials, 1998, 10, 1343-1348.	11.1	119
120	Ring Substituents Mediate the Morphology of PBDTTPD-PCBM Bulk-Heterojunction Solar Cells. Chemistry of Materials, 2014, 26, 2299-2306.	3.2	119
121	Halogen Migration in Hybrid Perovskites: The Organic Cation Matters. Journal of Physical Chemistry Letters, 2018, 9, 5474-5480.	2.1	119
122	Near-Infrared Electroluminescence and Low Threshold Amplified Spontaneous Emission above 800 nm from a Thermally Activated Delayed Fluorescent Emitter. Chemistry of Materials, 2018, 30, 6702-6710.	3.2	119
123	Impact of Dielectric Constant on the Singletâ€“Triplet Gap in Thermally Activated Delayed Fluorescence Materials. Journal of Physical Chemistry Letters, 2017, 8, 2393-2398.	2.1	118
124	Breakdown of the mirror image symmetry in the optical absorption/emission spectra of oligo(para-phenylene)s. Journal of Chemical Physics, 2005, 122, 054501.	1.2	117
125	Communication: Orbital instabilities and triplet states from time-dependent density functional theory and long-range corrected functionals. Journal of Chemical Physics, 2011, 135, 151103.	1.2	117
126	Design of Efficient Ambipolar Host Materials for Organic Blue Electrophosphorescence: Theoretical Characterization of Hosts Based on Carbazole Derivatives. Journal of the American Chemical Society, 2011, 133, 17895-17900.	6.6	116

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127	Unlocking the Effect of Trivalent Metal Doping in All-Inorganic CsPbBr₃ Perovskite. ACS Energy Letters, 2019, 4, 789-795.	8.8	116
128	Photophysical Properties of Ruthenium(II) Polyazaaromatic Compounds:Â A Theoretical Insight. Journal of the American Chemical Society, 2004, 126, 683-692.	6.6	114
129	Pyrroline Chromophores for Electro-Optics. Chemistry of Materials, 2006, 18, 2982-2988.	3.2	114
130	Impact of Molecular Packing on Electronic Polarization in Organic Crystals: The Case of Pentacene vs TIPS-Pentacene. Journal of the American Chemical Society, 2014, 136, 6421-6427.	6.6	113
131	Asymmetric electron acceptor enables highly luminescent organic solar cells with certified efficiency over 18%. Nature Communications, 2022, 13, 2598.	5.8	113
132	A comparative theoretical study of exciton-dissociation and charge-recombination processes in oligothiophene/fullerene and oligothiophene/perylenediimide complexes for organic solar cells. Journal of Materials Chemistry, 2011, 21, 1479.	6.7	112
133	Zinc Oxide as a Model Transparent Conducting Oxide: A Theoretical and Experimental Study of the Impact of Hydroxylation, Vacancies, Interstitials, and Extrinsic Doping on the Electronic Properties of the Polar ZnO (0002) Surface. Chemistry of Materials, 2012, 24, 3044-3055.	3.2	110
134	Modeling Electron and Hole Transport in Fluoroareneâ€Oligothiopene Semiconductors: Investigation of Geometric and Electronic Structure Properties. Advanced Functional Materials, 2008, 18, 332-340.	7.8	109
135	Synthesis of Acenaphthyl and Phenanthrene Based Fused-Aromatic Thienopyrazine Co-Polymers for Photovoltaic and Thin Film Transistor Applications. Chemistry of Materials, 2009, 21, 3618-3628.	3.2	109
136	Three-Dimensional Packing Structure and Electronic Properties of Biaxially Oriented Poly(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2-b]thiophene) Films. Journal of the American Chemical Society, 2012, 134, 6177-6190.	6.6	108
137	Electronic Coupling in Tetraanisylarylenediamine Mixed-Valence Systems:Â The Interplay between Bridge Energy and Geometric Factors. Journal of the American Chemical Society, 2005, 127, 8508-8516.	6.6	107
138	Electronic Structure of Two-Dimensional Ï€-Conjugated Covalent Organic Frameworks. Chemistry of Materials, 2019, 31, 3051-3065.	3.2	105
139	Effect of Molecular Packing and Charge Delocalization on the Nonradiative Recombination of Chargeâ€Transfer States in Organic Solar Cells. Advanced Energy Materials, 2016, 6, 1601325.	10.2	103
140	Interaction of Charge Carriers with Lattice Vibrations in Organic Molecular Semiconductors: Naphthalene as a Case Study. Journal of Physical Chemistry C, 2009, 113, 4679-4686.	1.5	102
141	Charge Transfer in Molecular Complexes with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F₄-TCNQ): A Density Functional Theory Study. Chemistry of Materials, 2011, 23, 5149-5159.	3.2	102
142	Lowest excited states and optical absorption spectra of donorâ€“acceptor copolymers for organic photovoltaics: a new picture emerging from tuned long-range corrected density functionals. Physical Chemistry Chemical Physics, 2012, 14, 14243.	1.3	101
143	Static and Dynamic Energetic Disorders in the C₆₀, PC₆₁BM, C₇₀, and PC₇₁BM Fullerenes. Journal of Physical Chemistry Letters, 2015, 6, 3657-3662.	2.1	101
144	Pyridine-Induced Dimensionality Change in Hybrid Perovskite Nanocrystals. Chemistry of Materials, 2017, 29, 4393-4400.	3.2	100

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145	Geometric Structure and Torsional Potential of Biisothianaphthene. A Comparative DFT and ab Initio Study. Journal of the American Chemical Society, 1997, 119, 1360-1369.	6.6	99
146	Electronic and vibrational properties of nickel sulfides from first principles. Journal of Chemical Physics, 2007, 127, 214705.	1.2	98
147	Factors Governing Intercalation of Fullerenes and Other Small Molecules Between the Side Chains of Semiconducting Polymers Used in Solar Cells. Advanced Energy Materials, 2012, 2, 1208-1217.	10.2	97
148	25th Anniversary Article: Design of Polymethine Dyes for Allâ€Optical Switching Applications: Guidance from Theoretical and Computational Studies. Advanced Materials, 2014, 26, 68-84.	11.1	97
149	Closely Stacked Oligo(phenylene ethynylene)s: Effect of Ï€-Stacking on the Electronic Properties of Conjugated Chromophores. Journal of the American Chemical Society, 2012, 134, 7176-7185.	6.6	96
150	Tuning Hot Carrier Cooling Dynamics by Dielectric Confinement in Two-Dimensional Hybrid Perovskite Crystals. ACS Nano, 2019, 13, 12621-12629.	7.3	96
151	High Charge-Carrier Mobility in an Amorphous Hexaazatrinaphthylene Derivative. Journal of the American Chemical Society, 2005, 127, 16358-16359.	6.6	95
152	Phosphine Oxide Derivatives as Hosts for Blue Phosphors: A Joint Theoretical and Experimental Study of Their Electronic Structure. Chemistry of Materials, 2010, 22, 247-254.	3.2	95
153	Magnetite Fe₃O₄ (111) Surfaces: Impact of Defects on Structure, Stability, and Electronic Properties. Chemistry of Materials, 2015, 27, 5856-5867.	3.2	93
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