

Jean-Luc E Bredas

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559
papers

49,480
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599
ext. papers

54,263
ext. citations

11.2
avg, IF

7.88
L-index

#	Paper	IF	Citations
559	Charge transport in organic semiconductors. <i>Chemical Reviews</i> , 2007 , 107, 926-52	68.1	3363
558	Charge-transfer and energy-transfer processes in pi-conjugated oligomers and polymers: a molecular picture. <i>Chemical Reviews</i> , 2004 , 104, 4971-5004	68.1	2271
557	A universal method to produce low-work function electrodes for organic electronics. <i>Science</i> , 2012 , 336, 327-32	33.3	1642
556	Molecular understanding of organic solar cells: the challenges. <i>Accounts of Chemical Research</i> , 2009 , 42, 1691-9	24.3	1176
555	Introduction to Organic Thin Film Transistors and Design of n-Channel Organic Semiconductors. <i>Chemistry of Materials</i> , 2004 , 16, 4436-4451	9.6	1159
554	Organic photovoltaics. <i>Energy and Environmental Science</i> , 2009 , 2, 251	35.4	1049
553	Structure-Property Relationships for Two-Photon Absorbing Chromophores: Bis-Donor Diphenylpolyene and Bis(styryl)benzene Derivatives. <i>Journal of the American Chemical Society</i> , 2000 , 122, 9500-9510	16.4	768
552	Single-electron transistor of a single organic molecule with access to several redox states. <i>Nature</i> , 2003 , 425, 698-701	50.4	736
551	Mind the gap!. <i>Materials Horizons</i> , 2014 , 1, 17-19	14.4	663
550	Effect of electronic polarization on charge-transport parameters in molecular organic semiconductors. <i>Journal of the American Chemical Society</i> , 2006 , 128, 9882-6	16.4	652
549	Design rules for minimizing voltage losses in high-efficiency organic solar cells. <i>Nature Materials</i> , 2018 , 17, 703-709	27	500
548	Origin of high second- and third-order nonlinear optical response in ammonio/borate diphenylpolyene zwitterions: the remarkable role of polarized aromatic groups. <i>Journal of the American Chemical Society</i> , 2003 , 125, 15651-8	16.4	440
547	Up-Conversion Intersystem Crossing Rates in Organic Emitters for Thermally Activated Delayed Fluorescence: Impact of the Nature of Singlet vs Triplet Excited States. <i>Journal of the American Chemical Society</i> , 2017 , 139, 4042-4051	16.4	438
546	Characterization of the interface dipole at organic/ metal interfaces. <i>Journal of the American Chemical Society</i> , 2002 , 124, 8131-41	16.4	434
545	Charge transport properties in discotic liquid crystals: a quantum-chemical insight into structure-property relationships. <i>Journal of the American Chemical Society</i> , 2004 , 126, 3271-9	16.4	432
544	Quantitative relations between interaction parameter, miscibility and function in organic solar cells. <i>Nature Materials</i> , 2018 , 17, 253-260	27	409
543	Transport Properties in the Rubrene Crystal: Electronic Coupling and Vibrational Reorganization Energy. <i>Advanced Materials</i> , 2005 , 17, 1072-1076	24	384

542	Organic Thin Film Transistors Based on N-Alkyl Perylene Diimides: Charge Transport Kinetics as a Function of Gate Voltage and Temperature. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 19281-19292	3.4	383
541	The vibrational reorganization energy in pentacene: molecular influences on charge transport. <i>Journal of the American Chemical Society</i> , 2002 , 124, 7918-9	16.4	376
540	The interface energetics of self-assembled monolayers on metals. <i>Accounts of Chemical Research</i> , 2008 , 41, 721-9	24.3	340
539	Tuning the charge-transport parameters of perylene diimide single crystals via end and/or core functionalization: a density functional theory investigation. <i>Journal of the American Chemical Society</i> , 2010 , 132, 3375-87	16.4	293
538	High-efficiency electroluminescence and amplified spontaneous emission from a thermally activated delayed fluorescent near-infrared emitter. <i>Nature Photonics</i> , 2018 , 12, 98-104	33.9	287
537	Polarization energies in oligoacene semiconductor crystals. <i>Journal of the American Chemical Society</i> , 2008 , 130, 12377-84	16.4	280
536	Photoinduced charge generation and recombination dynamics in model donor/acceptor pairs for organic solar cell applications: a full quantum-chemical treatment. <i>Journal of the American Chemical Society</i> , 2005 , 127, 6077-86	16.4	277
535	High operational and environmental stability of high-mobility conjugated polymer field-effect transistors through the use of molecular additives. <i>Nature Materials</i> , 2017 , 16, 356-362	27	276
534	Design of polymethine dyes with large third-order optical nonlinearities and loss figures of merit. <i>Science</i> , 2010 , 327, 1485-8	33.3	275
533	The Impact of Molecular Orientation on the Photovoltaic Properties of a Phthalocyanine/Fullerene Heterojunction. <i>Advanced Functional Materials</i> , 2012 , 22, 2987-2995	15.6	268
532	Experimental Demonstration of the Dependence of the First Hyperpolarizability of Donor-Acceptor-Substituted Polyenes on the Ground-State Polarization and Bond Length Alternation. <i>Journal of the American Chemical Society</i> , 1994 , 116, 2619-2620	16.4	265
531	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
530	Reliable Prediction with Tuned Range-Separated Functionals of the Singlet-Triplet Gap in Organic Emitters for Thermally Activated Delayed Fluorescence. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3851-8	6.4	256
529	Organic electronic materials: recent advances in the DFT description of the ground and excited states using tuned range-separated hybrid functionals. <i>Accounts of Chemical Research</i> , 2014 , 47, 3284-9	24.3	253
528	Exciton-dissociation and charge-recombination processes in pentacene/C60 solar cells: theoretical insight into the impact of interface geometry. <i>Journal of the American Chemical Society</i> , 2009 , 131, 15777-83	16.4	252
527	Exciton migration in rigid-rod conjugated polymers: an improved Förster model. <i>Journal of the American Chemical Society</i> , 2005 , 127, 4744-62	16.4	245
526	Toward control of the metal-organic interfacial electronic structure in molecular electronics: a first-principles study on self-assembled monolayers of pi-conjugated molecules on noble metals. <i>Nano Letters</i> , 2007 , 7, 932-40	11.5	244
525	Interface energetics and level alignment at covalent metal-molecule junctions: pi-conjugated thiols on gold. <i>Physical Review Letters</i> , 2006 , 96, 196806	7.4	243

524	Thermally Activated Delayed Fluorescence (TADF) Path toward Efficient Electroluminescence in Purely Organic Materials: Molecular Level Insight. <i>Accounts of Chemical Research</i> , 2018 , 51, 2215-2224	24.3	232
523	Redox States of Long Oligothiophenes: Two Polarons on a Single Chain. <i>Chemistry - A European Journal</i> , 1998 , 4, 1509-1522	4.8	228
522	Delocalization of exciton and electron wavefunction in non-fullerene acceptor molecules enables efficient organic solar cells. <i>Nature Communications</i> , 2020 , 11, 3943	17.4	222
521	Solution-Processed Organic Solar Cells with Power Conversion Efficiencies of 2.5% using Benzothiadiazole/Imide-Based Acceptors. <i>Chemistry of Materials</i> , 2011 , 23, 5484-5490	9.6	219
520	A quantum-chemical perspective into low optical-gap polymers for highly-efficient organic solar cells. <i>Chemical Science</i> , 2011 , 2, 1200-1218	9.4	218
519	One- and Two-Photon Spectroscopy of Donor-Acceptor Donor Distyrylbenzene Derivatives: Effect of Cyano Substitution and Distortion from Planarity. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 11470-11480	2.8	215
518	Prediction of remarkable ambipolar charge-transport characteristics in organic mixed-stack charge-transfer crystals. <i>Journal of the American Chemical Society</i> , 2012 , 134, 2340-7	16.4	211
517	Long-range corrected hybrid functionals for π -conjugated systems: dependence of the range-separation parameter on conjugation length. <i>Journal of Chemical Physics</i> , 2011 , 135, 204107	3.9	210
516	A spray-processable, low bandgap, and ambipolar donor-acceptor conjugated polymer. <i>Journal of the American Chemical Society</i> , 2009 , 131, 2824-6	16.4	208
515	Transition from tunneling to hopping transport in long, conjugated oligo-imine wires connected to metals. <i>Journal of the American Chemical Society</i> , 2010 , 132, 4358-68	16.4	200
514	Metal-ion sensing fluorophores with large two-photon absorption cross sections: aza-crown ether substituted donor-acceptor-donor distyrylbenzenes. <i>Journal of the American Chemical Society</i> , 2004 , 126, 9291-306	16.4	193
513	Ultralow doping in organic semiconductors: evidence of trap filling. <i>Physical Review Letters</i> , 2012 , 109, 176601	7.4	192
512	Photovoltaic concepts inspired by coherence effects in photosynthetic systems. <i>Nature Materials</i> , 2016 , 16, 35-44	27	191
511	Intersystem crossing processes in nonplanar aromatic heterocyclic molecules. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 10490-9	2.8	187
510	Impact of bidirectional charge transfer and molecular distortions on the electronic structure of a metal-organic interface. <i>Physical Review Letters</i> , 2007 , 99, 256801	7.4	186
509	Steric control of the donor/acceptor interface: implications in organic photovoltaic charge generation. <i>Journal of the American Chemical Society</i> , 2011 , 133, 12106-14	16.4	184
508	Alternating oligo(p-phenylene vinylene)-perylene bisimide copolymers: synthesis, photophysics, and photovoltaic properties of a new class of donor-acceptor materials. <i>Journal of the American Chemical Society</i> , 2003 , 125, 8625-38	16.4	184
507	Green emission from poly(fluorene)s: The role of oxidation. <i>Journal of Chemical Physics</i> , 2002 , 117, 6794-6802	16.4	183

506	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
505	Unconventional, chemically stable, and soluble two-dimensional angular polycyclic aromatic hydrocarbons: from molecular design to device applications. <i>Accounts of Chemical Research</i> , 2015 , 48, 500-9	24.3	180
504	Noncovalent Intermolecular Interactions in Organic Electronic Materials: Implications for the Molecular Packing vs Electronic Properties of Acenes. <i>Chemistry of Materials</i> , 2016 , 28, 3-16	9.6	179
503	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, 5222-32	16.4	177
502	Donor-Acceptor Copolymers of Relevance for Organic Photovoltaics: A Theoretical Investigation of the Impact of Chemical Structure Modifications on the Electronic and Optical Properties. <i>Macromolecules</i> , 2012 , 45, 6405-6414	5.5	169
501	Effects of electronegative substitution on the optical and electronic properties of acenes and diazaacenes. <i>Nature Communications</i> , 2010 , 1, 91	17.4	166
500	Impact of perfluorination on the charge-transport parameters of oligoacene crystals. <i>Journal of the American Chemical Society</i> , 2009 , 131, 1502-12	16.4	165
499	Impact of interfacial molecular orientation on radiative recombination and charge generation efficiency. <i>Nature Communications</i> , 2017 , 8, 79	17.4	160
498	Inside Perovskites: Quantum Luminescence from Bulk Cs ₄ PbBr ₆ Single Crystals. <i>Chemistry of Materials</i> , 2017 , 29, 7108-7113	9.6	160
497	Optical and redox properties of a series of 3,4-ethylenedioxythiophene oligomers. <i>Chemistry - A European Journal</i> , 2002 , 8, 2384-96	4.8	156
496	Polaron self-localization in white-light emitting hybrid perovskites. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 2771-2780	7.1	155
495	Fast spin-flip enables efficient and stable organic electroluminescence from charge-transfer states. <i>Nature Photonics</i> , 2020 , 14, 636-642	33.9	154
494	A New Design Strategy for Efficient Thermally Activated Delayed Fluorescence Organic Emitters: From Twisted to Planar Structures. <i>Advanced Materials</i> , 2017 , 29, 1702767	24	151
493	Electron affinities of 1,1-diaryl-2,3,4,5-tetraphenylsiloles: direct measurements and comparison with experimental and theoretical estimates. <i>Journal of the American Chemical Society</i> , 2005 , 127, 9021-9	16.4	148
492	Conjugated polymers and oligomers: Designing novel materials using a quantum-chemical approach. <i>Advanced Materials</i> , 1995 , 7, 263-274	24	148
491	Critical role of intermediate electronic states for spin-flip processes in charge-transfer-type organic molecules with multiple donors and acceptors. <i>Nature Materials</i> , 2019 , 18, 1084-1090	27	146
490	Multipole expansion in tight-binding Hartree-Fock calculations for infinite model polymers. <i>Physical Review B</i> , 1980 , 22, 6254-6267	3.3	145
489	Charge transport parameters of the pentathienoacene crystal. <i>Journal of the American Chemical Society</i> , 2007 , 129, 13072-81	16.4	142

488	Two-photon absorption at telecommunications wavelengths in a dipolar chromophore with a pyrrole auxiliary donor and thiazole auxiliary acceptor. <i>Journal of the American Chemical Society</i> , 2005 , 127, 7282-3	16.4	142
487	Charge-transfer electronic states in organic solar cells. <i>Nature Reviews Materials</i> , 2019 , 4, 689-707	73.3	140
486	Bistetracene: an air-stable, high-mobility organic semiconductor with extended conjugation. <i>Journal of the American Chemical Society</i> , 2014 , 136, 9248-51	16.4	140
485	Dithienopyrrole-based donor-acceptor copolymers: low band-gap materials for charge transport, photovoltaics and electrochromism. <i>Journal of Materials Chemistry</i> , 2010 , 20, 123-134		140
484	Direct-Indirect Nature of the Bandgap in Lead-Free Perovskite Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 3173-3177	6.4	139
483	Molecular behavior of zero-dimensional perovskites. <i>Science Advances</i> , 2017 , 3, e1701793	14.3	137
482	Quantum Chemistry Aided Design of Organic Polymers. <i>World Scientific Lecture and Course Notes in Chemistry</i> , 1991 ,		136
481	Modification of the Surface Properties of Indium Tin Oxide with Benzylphosphonic Acids: A Joint Experimental and Theoretical Study. <i>Advanced Materials</i> , 2009 , 21, 4496-4501	24	135
480	Phosphonic Acids for Interfacial Engineering of Transparent Conductive Oxides. <i>Chemical Reviews</i> , 2016 , 116, 7117-58	68.1	135
479	Correlation between the Microscopic Morphology and the Solid-State Photoluminescence Properties in Fluorene-Based Polymers and Copolymers. <i>Chemistry of Materials</i> , 2004 , 16, 994-1001	9.6	133
478	Evaluating the Performance of DFT Functionals in Assessing the Interaction Energy and Ground-State Charge Transfer of Donor/Acceptor Complexes: Tetrathiafulvalene-Tetracyanoquinodimethane (TTF-TCNQ) as a Model Case. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 602-9	6.4	132
477	Electronic delocalization in discotic liquid crystals: a joint experimental and theoretical study. <i>Journal of the American Chemical Society</i> , 2004 , 126, 11889-99	16.4	132
476	Shallow trap states in pentacene thin films from molecular sliding. <i>Applied Physics Letters</i> , 2005 , 86, 1521-15	11.5	128
475	Vibronic coupling in the ground and excited states of oligoacene cations. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 18904-11	3.4	128
474	Intervalence transitions in the mixed-valence monocations of bis(triarylaminines) linked with vinylene and phenylene-vinylene bridges. <i>Journal of the American Chemical Society</i> , 2005 , 127, 16900-11	16.4	126
473	Organic/metal interfaces in self-assembled monolayers of conjugated thiols: A first-principles benchmark study. <i>Surface Science</i> , 2006 , 600, 4548-4562	1.8	122
472	On the Interface Dipole at the Pentacene-Bullerene Heterojunction: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 3215-3224	3.8	121
471	Rubrene-Based Single-Crystal Organic Semiconductors: Synthesis, Electronic Structure, and Charge-Transport Properties. <i>Chemistry of Materials</i> , 2013 , 25, 2254-2263	9.6	120

470	Theoretical Characterization of the Indium Tin Oxide Surface and of Its Binding Sites for Adsorption of Phosphonic Acid Monolayers. <i>Chemistry of Materials</i> , 2008 , 20, 5131-5133	9.6	120
469	Preparation and characterization of pi-stacking quinodimethane oligothiophenes. Predicting semiconductor behavior and bandwidths from crystal structures and molecular orbital calculations. <i>Journal of the American Chemical Society</i> , 2004 , 126, 15295-308	16.4	120
468	Aromatic amines: a comparison of electron-donor strengths. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 9346-52	2.8	118
467	The metal-on-polymer interface in polymer light emitting diodes. <i>Advanced Materials</i> , 1996 , 8, 48-52	24	117
466	Synthetic principles directing charge transport in low-band-gap dithienosilole-benzothiadiazole copolymers. <i>Journal of the American Chemical Society</i> , 2012 , 134, 8944-57	16.4	116
465	Electronic evolution of poly(3,4-ethylenedioxythiophene) (PEDOT): from the isolated chain to the pristine and heavily doped crystals. <i>Journal of the American Chemical Society</i> , 2008 , 130, 16880-9	16.4	116
464	Highly Dipolar, Optically Nonlinear Adducts of Tetracyano-p-quinodimethane: Synthesis, Physical Characterization, and Theoretical Aspects. <i>Journal of the American Chemical Society</i> , 1997 , 119, 3144-3154	16.4	114
463	Design of emission ratiometric metal-ion sensors with enhanced two-photon cross section and brightness. <i>Journal of the American Chemical Society</i> , 2007 , 129, 11888-9	16.4	114
462	Photophysical properties of ruthenium(II) polycyclic aromatic compounds: a theoretical insight. <i>Journal of the American Chemical Society</i> , 2004 , 126, 683-92	16.4	114
461	Delocalization in platinum-alkynyl systems: a metal-bridged organic mixed-valence compound. <i>Journal of the American Chemical Society</i> , 2004 , 126, 11782-3	16.4	114
460	Thieno[3,4-c]pyrrole-4,6-dione-3,4-difluorothiophene Polymer Acceptors for Efficient All-Polymer Bulk Heterojunction Solar Cells. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 12996-13000	16.4	113
459	Ring Substituents Mediate the Morphology of PBDTPD-PCBM Bulk-Heterojunction Solar Cells. <i>Chemistry of Materials</i> , 2014 , 26, 2299-2306	9.6	113
458	Use of X-ray diffraction, molecular simulations, and spectroscopy to determine the molecular packing in a polymer-fullerene bimolecular crystal. <i>Advanced Materials</i> , 2012 , 24, 6071-9	24	113
457	Interaction of charge carriers with lattice vibrations in oligoacene crystals from naphthalene to pentacene. <i>Journal of the American Chemical Society</i> , 2010 , 132, 14437-46	16.4	113
456	Design of efficient ambipolar host materials for organic blue electrophosphorescence: theoretical characterization of hosts based on carbazole derivatives. <i>Journal of the American Chemical Society</i> , 2011 , 133, 17895-900	16.4	111
455	Photoelectron Spectroscopic Study of the Electronic Band Structure of Polyfluorene and Fluorene-Arylamine Copolymers at Interfaces. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 1378-1384	3.8	110
454	Intrinsic Lead Ion Emissions in Zero-Dimensional Cs ₄ PbBr ₆ Nanocrystals. <i>ACS Energy Letters</i> , 2017 , 2, 2805-2811	20.1	109
453	Triplet excimer formation in platinum-based phosphors: a theoretical study of the roles of Pt-Pt bimetallic interactions and interligand pi-pi interactions. <i>Journal of the American Chemical Society</i> , 2009 , 131, 11371-80	16.4	106

452	Excitonic and Polaronic Properties of 2D Hybrid Organic-Inorganic Perovskites. <i>ACS Energy Letters</i> , 2017 , 2, 417-423	20.1	105
451	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		105
450	Breakdown of the mirror image symmetry in the optical absorption/emission spectra of oligo(para-phenylene)s. <i>Journal of Chemical Physics</i> , 2005 , 122, 54501	3.9	105
449	Investigation of Exciton Coupling in Oligothiophenes by Circular Dichroism Spectroscopy. <i>Advanced Materials</i> , 1998 , 10, 1343-1348	24	104
448	Modeling Electron and Hole Transport in Fluoroarene-Oligothiophene Semiconductors: Investigation of Geometric and Electronic Structure Properties. <i>Advanced Functional Materials</i> , 2008 , 18, 332-340	15.6	104
447	Pyrroline Chromophores for Electro-Optics. <i>Chemistry of Materials</i> , 2006 , 18, 2982-2988	9.6	103
446	Point Defects and Green Emission in Zero-Dimensional Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5490-5495	6.4	103
445	Design of Organic Chromophores for All-Optical Signal Processing Applications. <i>Chemistry of Materials</i> , 2014 , 26, 549-560	9.6	102
444	Electronic coupling in tetraanisylarylenediamine mixed-valence systems: the interplay between bridge energy and geometric factors. <i>Journal of the American Chemical Society</i> , 2005 , 127, 8508-16	16.4	102
443	Impact of molecular packing on electronic polarization in organic crystals: the case of pentacene vs TIPS-pentacene. <i>Journal of the American Chemical Society</i> , 2014 , 136, 6421-7	16.4	100
442	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. <i>Chemistry of Materials</i> , 2012 , 24, 3044-3055	9.6	100
441	Communication: orbital instabilities and triplet states from time-dependent density functional theory and long-range corrected functionals. <i>Journal of Chemical Physics</i> , 2011 , 135, 151103	3.9	100
440	Synthesis of Acenaphthyl and Phenanthrene Based Fused-Aromatic Thienopyrazine Co-Polymers for Photovoltaic and Thin Film Transistor Applications. <i>Chemistry of Materials</i> , 2009 , 21, 3618-3628	9.6	98
439	Interaction of Charge Carriers with Lattice Vibrations in Organic Molecular Semiconductors: Naphthalene as a Case Study. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 4679-4686	3.8	97
438	Spiro-OMeTAD single crystals: Remarkably enhanced charge-carrier transport via mesoscale ordering. <i>Science Advances</i> , 2016 , 2, e1501491	14.3	96
437	Heteroannulated acceptors based on benzothiadiazole. <i>Materials Horizons</i> , 2015 , 2, 22-36	14.4	94
436	Three-dimensional packing structure and electronic properties of biaxially oriented poly(2,5-bis(3-alkylthiophene-2-yl)thieno[3,2-b]thiophene) films. <i>Journal of the American Chemical Society</i> , 2012 , 134, 6177-90	16.4	93
435	Fused electron deficient semiconducting polymers for air stable electron transport. <i>Nature Communications</i> , 2018 , 9, 416	17.4	91

434	Impact of Dielectric Constant on the Singlet-Triplet Gap in Thermally Activated Delayed Fluorescence Materials. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2393-2398	6.4	90
433	Factors Governing Intercalation of Fullerenes and Other Small Molecules Between the Side Chains of Semiconducting Polymers Used in Solar Cells. <i>Advanced Energy Materials</i> , 2012 , 2, 1208-1217	21.8	90
432	Humidity Sensing through Reversible Isomerization of a Covalent Organic Framework. <i>Journal of the American Chemical Society</i> , 2020 , 142, 783-791	16.4	90
431	Static and Dynamic Energetic Disorders in the C60, PC61BM, C70, and PC71BM Fullerenes. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 3657-62	6.4	89
430	Phosphine Oxide Derivatives as Hosts for Blue Phosphors: A Joint Theoretical and Experimental Study of Their Electronic Structure. <i>Chemistry of Materials</i> , 2010 , 22, 247-254	9.6	89
429	Geometric Structure and Torsional Potential of Biisothianaphthene. A Comparative DFT and ab Initio Study. <i>Journal of the American Chemical Society</i> , 1997 , 119, 1360-1369	16.4	89
428	Closely stacked oligo(phenylene ethynylene)s: effect of π -stacking on the electronic properties of conjugated chromophores. <i>Journal of the American Chemical Society</i> , 2012 , 134, 7176-85	16.4	88
427	Theoretical characterization of titanyl phthalocyanine as a p-type organic semiconductor: short intermolecular pi-pi interactions yield large electronic couplings and hole transport bandwidths. <i>Journal of Chemical Physics</i> , 2008 , 128, 034701	3.9	88
426	Effect of Molecular Packing and Charge Delocalization on the Nonradiative Recombination of Charge-Transfer States in Organic Solar Cells. <i>Advanced Energy Materials</i> , 2016 , 6, 1601325	21.8	88
425	Charge Transfer in Molecular Complexes with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ): A Density Functional Theory Study. <i>Chemistry of Materials</i> , 2011 , 23, 5149-5159	9.6	87
424	High charge-carrier mobility in an amorphous hexaazatrinaphthylene derivative. <i>Journal of the American Chemical Society</i> , 2005 , 127, 16358-9	16.4	87
423	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. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2906-16	6.4	87
422	Charge-Transfer Localization in Molecularly Doped Thiophene-Based Donor Polymers. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 2037-2041	6.4	86
421	Benzothiadiazole-Dithienopyrrole Donor-Acceptor-Donor and Acceptor-Donor-Acceptor Triads: Synthesis and Optical, Electrochemical, and Charge-Transport Properties. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 23149-23163	3.8	85
420	Chain-Length Dependence of Singlet and Triplet Exciton Formation Rates in Organic Light-Emitting Diodes. <i>Advanced Functional Materials</i> , 2004 , 14, 684-692	15.6	85
419	25th anniversary article: Design of polymethine dyes for all-optical switching applications: guidance from theoretical and computational studies. <i>Advanced Materials</i> , 2014 , 26, 68-83	24	84
418	Intermixing at the pentacene-fullerene bilayer interface: a molecular dynamics study. <i>Advanced Materials</i> , 2013 , 25, 878-82	24	84
417	Nucleation and Growth of Covalent Organic Frameworks from Solution: The Example of COF-5. <i>Journal of the American Chemical Society</i> , 2017 , 139, 16310-16318	16.4	83

4 ¹⁶	Influence of Structural Dynamics on Polarization Energies in Anthracene Single Crystals. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 20678-20685	3.8	83
4 ¹⁵	Tuning the Optoelectronic Properties of Vinylene-Linked Donor-Acceptor Copolymers for Organic Photovoltaics. <i>Macromolecules</i> , 2010 , 43, 6685-6698	5.5	83
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