Jean-Luc E Bredas

List of Publications by Year in Descending Order

559 papers	49,480 citations	108 h-index	201 g-index
599 ext. papers	54,263 ext. citations	11.2 avg, IF	7.88 L-index

#	Paper	IF	Citations
559	Electronic Structure of Zinc-5,10,15,20-tetraethynylporphyrin: Evolution from the Molecule to a One-Dimensional Chain, a Two-Dimensional Covalent Organic Framework, and a Nanotube. *Chemistry of Materials*, **2022**, 34, 1334-1341	9.6	2
558	High-performance ternary perovskite-organic solar cells.. *Advanced Materials*, **2022**, e2109348	24	9
557	Spacer Engineering of Diammonium-Based 2D Perovskites toward Efficient and Stable 2D/3D Heterostructure Perovskite Solar Cells (Adv. Energy Mater. 2/2022). *Advanced Energy Materials*, **2022**, 12, 2270004	21.8	0
556	Electronic structure of confined carbyne from joint wavelength-dependent resonant Raman spectroscopy and density functional theory investigations. *Carbon*, **2022**, 189, 276-283	10.4	0
555	Engineering Surface Orientations for Efficient and Stable Hybrid Perovskite Single-Crystal Solar Cells. *ACS Energy Letters*, **2022**, 7, 1544-1552	20.1	6
554	Asymmetric electron acceptor enables highly luminescent organic solar cells with certified efficiency over 18.. *Nature Communications*, **2022**, 13, 2598	17.4	18
553	Engineering of flat bands and Dirac bands in two-dimensional covalent organic frameworks (COFs): relationships among molecular orbital symmetry, lattice symmetry, and electronic-structure characteristics. *Materials Horizons*, **2021**,	14.4	6
552	Resolving Atomic-Scale Interactions in Non-Fullerene Acceptor Organic Solar Cells with Solid-State NMR Spectroscopy, Crystallographic Modelling, and Molecular Dynamics Simulations. *Advanced Materials*, **2021**, e2105943	24	11
551	Controlled n-Doping of Naphthalene Diimide-Based Two-Dimensional Polymers. *Advanced Materials* , **2021**, e2101932	24	5
550	Impact of Imine Bond Orientations on the Geometric and Electronic Structures of Imine-based Covalent Organic Frameworks. *Chemistry - an Asian Journal*, **2021**, 16, 3781-3789	4.5	3
549	Luminescence and Stability Enhancement of Inorganic Perovskite Nanocrystals via Selective Surface Ligand Binding. *ACS Nano*, **2021**,	16.7	10
548	Thermally Activated Delayed Fluorescence Properties of Trioxoazatriangulene Derivatives Modified with Electron Donating Groups. *Advanced Optical Materials*, **2021**, 9, 2002174	8.1	12
547	Thermally conductive ultra-low-k dielectric layers based on two-dimensional covalent organic frameworks. *Nature Materials*, **2021**, 20, 1142-1148	27	30
546	Quantitative Description of the Lateral Growth of Two-Dimensional Covalent Organic Frameworks Reveals Self-Templation Effects **2021**, 3, 398-405		4
545	Molecular Packing in the Active Layers of Organic Solar Cells Based on Non-Fullerene Acceptors: Impact of Isomerization on Charge Transport, Exciton Dissociation, and Nonradiative Recombination. *ACS Applied Energy Materials*, **2021**, 4, 4002-4011	6.1	2
544	Manipulation of hot carrier cooling dynamics in two-dimensional Dion-Jacobson hybrid perovskites via Rashba band splitting. *Nature Communications*, **2021**, 12, 3995	17.4	11
543	A unified description of non-radiative voltage losses in organic solar cells. *Nature Energy*, **2021**, 6, 799-806	62.3	70

542	Impact of Structural Defects on the Elastic Properties of Two-Dimensional Covalent Organic Frameworks (2D COFs) under Tensile Stress. *Chemistry of Materials*, **2021**, 33, 4529-4540	9.6	6
541	Robust Molecular Dipole-Enabled Defect Passivation and Control of Energy-Level Alignment for High-Efficiency Perovskite Solar Cells. *Angewandte Chemie - International Edition*, **2021**, 60, 17664-17670	16.4	18
540	Developing molecular-level models for organic field-effect transistors.. *National Science Review*, **2021**, 8, nwaa167	10.8	7
539	The Role of Intermolecular Interactions on the Performance of Organic Thermally Activated Delayed Fluorescence (TADF) Materials. *Advanced Optical Materials*, **2021**, 9, 2002135	8.1	8
538	Strong Suppression of Thermal Conductivity in the Presence of Long Terminal Alkyl Chains in Low-Disorder Molecular Semiconductors. *Advanced Materials*, **2021**, 33, e2008708	24	8
537	Molecular packing of non-fullerene acceptors for organic solar cells: Distinctive local morphology in Y6 vs. ITIC derivatives. *Materials Today Advances*, **2021**, 11, 100154	7.4	10
536	Lower limits for non-radiative recombination loss in organic donor/acceptor complexes. *Materials Horizons*, **2021**,	14.4	5
535	Impact of chemical modifications on the luminescence properties of organic neutral radical emitters. *Journal of Materials Chemistry C*, **2021**, 9, 10794-10801	7.1	5
534	Organic Photovoltaics: Understanding the Preaggregation of Polymer Donors in Solution and Its Morphological Impact. *Journal of the American Chemical Society*, **2021**, 143, 1822-1835	16.4	18
533	Mechanism of Formation of Benzotrithiophene-Based Covalent Organic Framework Monolayers on Coinage-Metal Surfaces: C□ Coupling Selectivity and Monomer□Metal Interactions. *Chemistry of Materials*, **2020**, 32, 10688-10696	9.6	3
532	Electronically Coupled 2D Polymer/MoS Heterostructures. *Journal of the American Chemical Society* , **2020**, 142, 21131-21139	16.4	8
531	Modulation of Broadband Emissions in Two-Dimensional <100>-Oriented Ruddlesden□Popper Hybrid Perovskites. *ACS Energy Letters*, **2020**, 5, 2149-2155	20.1	33
530	Bulk Heterojunction Solar Cells: Insight into Ternary Blends from a Characterization of the Intermolecular Packing and Electronic Properties in the Corresponding Binary Blends. *Advanced Theory and Simulations*, **2020**, 3, 2000049	3.5	2
529	Radiative and Nonradiative Recombinations in Organic Radical Emitters: The Effect of Guest□Host Interactions. *Advanced Functional Materials*, **2020**, 30, 2002916	15.6	10
528	Structural and Electronic Impact of an Asymmetric Organic Ligand in Diammonium Lead Iodide Perovskites. *Advanced Energy Materials*, **2020**, 10, 1903900	21.8	8
527	Understanding charge transport in donor/acceptor blends from large-scale device simulations based on experimental film morphologies. *Energy and Environmental Science*, **2020**, 13, 601-615	35.4	8
526	Organic Photovoltaics: Relating Chemical Structure, Local Morphology, and Electronic Properties. *Trends in Chemistry*, **2020**, 2, 535-554	14.8	28
525	Electronic Structure of Multicomponent Organic Molecular Materials: Evaluation of Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2020**, 16, 3712-3719	6.4	11

524	Boosting Self-Trapped Emissions in Zero-Dimensional Perovskite Heterostructures. *Chemistry of Materials*, **2020**, 32, 5036-5043	9.6	24
523	Revealing the Local Electronic Structure of a Single-Layer Covalent Organic Framework through Electronic Decoupling. *Nano Letters*, **2020**, 20, 963-970	11.5	10
522	Humidity Sensing through Reversible Isomerization of a Covalent Organic Framework. *Journal of the American Chemical Society*, **2020**, 142, 783-791	16.4	90
521	Nucleation-Elongation Dynamics of Two-Dimensional Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2020**, 142, 1367-1374	16.4	36
520	Suppression of Concentration Quenching in Ortho-Substituted Thermally Activated Delayed Fluorescence Emitters. *Advanced Theory and Simulations*, **2020**, 3, 1900185	3.5	8
519	Organic Solar Cells Based on Non-fullerene Small-Molecule Acceptors: Impact of Substituent Position. *Matter*, **2020**, 2, 119-135	12.7	20
518	Organic Neutral Radical Emitters: Impact of Chemical Substitution and Electronic-State Hybridization on the Luminescence Properties. *Journal of the American Chemical Society*, **2020**, 142, 17782-17786	16.4	12
517	Impact of secondary donor units on the excited-state properties and thermally activated delayed fluorescence (TADF) efficiency of pentacarbazole-benzonitrile emitters. *Journal of Chemical Physics*, **2020**, 153, 144708	3.9	7
516	Hyperfluorescence-Based Emission in Purely Organic Materials: Suppression of Energy-Loss Mechanisms via Alignment of Triplet Excited States **2020**, 2, 1412-1418		12
515	Delocalization of exciton and electron wavefunction in non-fullerene acceptor molecules enables efficient organic solar cells. *Nature Communications*, **2020**, 11, 3943	17.4	222
514	Electronic, vibrational, and charge-transport properties of benzothienobenzothiophene–TCNQ co-crystals. *Materials Chemistry Frontiers*, **2020**, 4, 3623-3631	7.8	6
513	Fast spin-flip enables efficient and stable organic electroluminescence from charge-transfer states. *Nature Photonics*, **2020**, 14, 636-642	33.9	154
512	A Novel Mitigation Mechanism for Photo-Induced Trapping in an Anthradithiophene Derivative Using Additives. *Advanced Electronic Materials*, **2020**, 6, 2000250	6.4	2
511	Doping Modulation of the Charge Injection Barrier between a Covalent Organic Framework Monolayer and Graphene. *Chemistry of Materials*, **2020**, 32, 9228-9237	9.6	5
510	Thermally Activated Delayed Fluorescence Sensitization for Highly Efficient Blue Fluorescent Emitters. *Advanced Functional Materials*, **2020**, 30, 2005898	15.6	11
509	Short Excited-State Lifetimes Enable Photo-Oxidatively Stable Rubrene Derivatives. *Journal of Physical Chemistry A*, **2019**, 123, 7558-7566	2.8	6
508	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	27	146
507	Charge-transfer electronic states in organic solar cells. *Nature Reviews Materials*, **2019**, 4, 689-707	73.3	140

506	Dynamically Switching the Electronic and Electrostatic Properties of Indium Tin Oxide Electrodes with Photochromic Monolayers: Toward Photoswitchable Optoelectronic Devices. *ACS Applied Nano Materials*, **2019**, 2, 1102-1110	5.6	15
505	Quantum Well Energetics of an n = 2 Ruddlesden Popper Phase Perovskite. *Advanced Energy Materials*, **2019**, 9, 1901005	21.8	17
504	Intramolecular Noncovalent Interactions Facilitate Thermally Activated Delayed Fluorescence (TADF). *Journal of Physical Chemistry Letters*, **2019**, 10, 3260-3268	6.4	41
503	Design and synthesis of two-dimensional covalent organic frameworks with four-arm cores: prediction of remarkable ambipolar charge-transport properties. *Materials Horizons*, **2019**, 6, 1868-1876	14.4	41
502	Synergistic Use of Bithiazole and Pyridinyl Substitution for Effective Electron Transport Polymer Materials. *Chemistry of Materials*, **2019**, 31, 3957-3966	9.6	17
501	Emergence of an Antiferromagnetic Mott Insulating Phase in Hexagonal Conjugated Covalent Organic Frameworks. *Advanced Materials*, **2019**, 31, e1900355	24	26
500	Nanoscrolls Formed from Two-Dimensional Covalent Organic Frameworks. *Chemistry of Materials*, **2019**, 31, 3265-3273	9.6	7
499	Unlocking the Effect of Trivalent Metal Doping in All-Inorganic CsPbBr3 Perovskite. *ACS Energy Letters*, **2019**, 4, 789-795	20.1	77
498	Low Energetic Disorder in Small-Molecule Non-Fullerene Electron Acceptors **2019**, 1, 350-353		17
497	Pathway Complexity in the Stacking of Imine-Linked Macrocycles Related to Two-Dimensional Covalent Organic Frameworks. *Chemistry of Materials*, **2019**, 31, 7104-7111	9.6	9
496	High stability and luminescence efficiency in donor-acceptor neutral radicals not following the Aufbau principle. *Nature Materials*, **2019**, 18, 977-984	27	80
495	All-Polymer Solar Cells: Impact of the Length of the Branched Alkyl Side Chains on the Polymer Acceptors on the Interchain Packing and Electronic Properties in Amorphous Blends. *Chemistry of Materials*, **2019**, 31, 6239-6248	9.6	19
494	Tuning Hot Carrier Cooling Dynamics by Dielectric Confinement in Two-Dimensional Hybrid Perovskite Crystals. *ACS Nano*, **2019**, 13, 12621-12629	16.7	55
493	Charge-Transport Properties of F6TNAP-Based Charge-Transfer Cocrystals. *Advanced Functional Materials*, **2019**, 29, 1904858	15.6	23
492	Quantum-Chemical Evaluation of Impact of Chlorination versus Fluorination on the Electronic Properties of Donors and Acceptors for Organic Solar Cells. *Advanced Theory and Simulations*, **2019**, 2, 1900136	3.5	8
491	Chemical Control over Nucleation and Anisotropic Growth of Two-Dimensional Covalent Organic Frameworks. *ACS Central Science*, **2019**, 5, 1892-1899	16.8	26
490	Electronic Structure of Two-Dimensional Conjugated Covalent Organic Frameworks. *Chemistry of Materials*, **2019**, 31, 3051-3065	9.6	60
489	Charge-Transfer States at Organic Organic Interfaces: Impact of Static and Dynamic Disorders. *Advanced Energy Materials*, **2019**, 9, 1803926	21.8	40

488	Chemical Stabilities of the Lowest Triplet State in Aryl Sulfones and Aryl Phosphine Oxides Relevant to OLED Applications. *Chemistry of Materials*, **2019**, 31, 1507-1519	9.6	19
487	Acceptor Gradient Polymer Donors for Non-Fullerene Organic Solar Cells. *Chemistry of Materials*, **2019**, 31, 9729-9741	9.6	10
486	Local Electronic Structure of Molecular Heterojunctions in a Single-Layer 2D Covalent Organic Framework. *Advanced Materials*, **2019**, 31, e1805941	24	35
485	Impact of Organic Spacers on the Carrier Dynamics in 2D Hybrid Lead-Halide Perovskites. *ACS Energy Letters*, **2019**, 4, 17-25	20.1	36
484	Nonfullerene Small-Molecule Acceptors for Organic Photovoltaics: Understanding the Impact of Methoxy Substitution Position on Molecular Packing and Electron-Transfer Properties. *Advanced Functional Materials*, **2019**, 29, 1806845	15.6	15
483	Bond Ellipticity Alternation: An Accurate Descriptor of the Nonlinear Optical Properties of π-Conjugated Chromophores. *Journal of Physical Chemistry Letters*, **2018**, 9, 1377-1383	6.4	14
482	Every Atom Counts: Elucidating the Fundamental Impact of Structural Change in Conjugated Polymers for Organic Photovoltaics. *Chemistry of Materials*, **2018**, 30, 2995-3009	9.6	33
481	Quantitative relations between interaction parameter, miscibility and function in organic solar cells. *Nature Materials*, **2018**, 17, 253-260	27	409
480	High-efficiency electroluminescence and amplified spontaneous emission from a thermally activated delayed fluorescent near-infrared emitter. *Nature Photonics*, **2018**, 12, 98-104	33.9	287
479	Fused electron deficient semiconducting polymers for air stable electron transport. *Nature Communications*, **2018**, 9, 416	17.4	91
478	Hydrolytic Stability of Boronate Ester-Linked Covalent Organic Frameworks. *Advanced Theory and Simulations*, **2018**, 1, 1700015	3.5	31
477	Characterization of the Valence and Conduction Band Levels of n = 1 2D Perovskites: A Combined Experimental and Theoretical Investigation. *Advanced Energy Materials*, **2018**, 8, 1703468	21.8	48
476	Bulk Heterojunction Solar Cells: Impact of Minor Structural Modifications to the Polymer Backbone on the Polymer–Fullerene Mixing and Packing and on the Fullerene–Fullerene Connecting Network. *Advanced Functional Materials*, **2018**, 28, 1705868	15.6	28
475	Electrode Work Function Engineering with Phosphonic Acid Monolayers and Molecular Acceptors: Charge Redistribution Mechanisms. *Advanced Functional Materials*, **2018**, 28, 1704438	15.6	18
474	Voltage Losses in Organic Solar Cells: Understanding the Contributions of Intramolecular Vibrations to Nonradiative Recombinations. *Advanced Energy Materials*, **2018**, 8, 1702227	21.8	33
473	Local Electronic Structure of a Single-Layer Porphyrin-Containing Covalent Organic Framework. *ACS Nano*, **2018**, 12, 385-391	16.7	41
472	Discovery of Non-linear Optical Materials by Function-Based Screening of Multi-component Solids. *CheM*, **2018**, 4, 150-161	16.2	20
471	Langmuir-Blodgett Thin Films of Diketopyrrolopyrrole-Based Amphiphiles. *ACS Applied Materials & Interfaces*, **2018**, 10, 11995-12004	9.5	13

470	Characterization of the structural, mechanical, and electronic properties of fullerene mixtures: a molecular simulations description. *Journal of Materials Chemistry C*, **2018**, 6, 3642-3650	7.1	8
469	Assessment of the Factors Influencing Charge-Carrier Mobility Measurements in Organic Field-Effect Transistors. *Advanced Functional Materials*, **2018**, 28, 1803096	15.6	16
468	Large Out-of-Plane Deformations of Two-Dimensional Covalent Organic Framework (COF) Sheets. *Journal of Physical Chemistry Letters*, **2018**, 9, 4215-4220	6.4	7
467	Design rules for minimizing voltage losses in high-efficiency organic solar cells. *Nature Materials*, **2018**, 17, 703-709	27	500
466	Impact of Hydroxylation and Hydration on the Reactivity of □Fe2O3 (0001) and (102) Surfaces under Environmental and Electrochemical Conditions. *Advanced Energy Materials*, **2018**, 8, 1800545	21.8	7
465	Thermally Activated Delayed Fluorescence (TADF) Path toward Efficient Electroluminescence in Purely Organic Materials: Molecular Level Insight. *Accounts of Chemical Research*, **2018**, 51, 2215-2224	24.3	232
464	Increased Exciton Delocalization of Polymer upon Blending with Fullerene. *Advanced Materials*, **2018**, 30, e1801392	24	14
463	Impact of Phonon Dispersion on Nonlocal Electron□Phonon Couplings in Organic Semiconductors: The Naphthalene Crystal as a Case Study. *Journal of Physical Chemistry C*, **2018**, 122, 44-49	3.8	10
462	Effects of meso-M(PPh3)2Cl (M = Pd, Ni) substituents on the linear and third-order nonlinear optical properties of chalcogenopyrylium-terminated heptamethines in solution and solid states. *Journal of Materials Chemistry C*, **2018**, 6, 3613-3620	7.1	11
461	Isoindigo-3,4-Difluorothiophene Polymer Acceptors Yield "All-Polymer" Bulk-Heterojunction Solar Cells with over 7 % Efficiency. *Angewandte Chemie - International Edition*, **2018**, 57, 531-535	16.4	51
460	Isoindigo-3,4-Difluorothiophene Polymer Acceptors Yield □All-Polymer□Bulk-Heterojunction Solar Cells with over 7 % Efficiency. *Angewandte Chemie*, **2018**, 130, 540-544	3.6	11
459	Impact of solution temperature-dependent aggregation on the solid-state packing and electronic properties of polymers for organic photovoltaics. *Journal of Materials Chemistry C*, **2018**, 6, 13162-13170	7.1	14
458	Assessing the nature of the charge-transfer electronic states in organic solar cells. *Nature Communications*, **2018**, 9, 5295	17.4	83
457	Donor Conjugated Polymers with Polar Side Chain Groups: The Role of Dielectric Constant and Energetic Disorder on Photovoltaic Performance. *Advanced Functional Materials*, **2018**, 28, 1803418	15.6	26
456	Layer-Dependent Rashba Band Splitting in 2D Hybrid Perovskites. *Chemistry of Materials*, **2018**, 30, 8538-8545	9.6	66
455	Crystal Engineering of Dibenzothiophenothieno[3,2-b]thiophene (DBTTT) Isomers for Organic Field-Effect Transistors. *Chemistry of Materials*, **2018**, 30, 7587-7592	9.6	15
454	Quasi-One-Dimensional Charge Transport Can Lead to Nonlinear Current Characteristics in Organic Field-Effect Transistors. *Journal of Physical Chemistry Letters*, **2018**, 9, 6550-6555	6.4	12
453	Efficient Electron Mobility in an All-Acceptor Napthalenediimide-Bithiazole Polymer Semiconductor with Large Backbone Torsion. *ACS Applied Materials & Interfaces*, **2018**, 10, 40070-40077	9.5	12

452	Halogen Migration in Hybrid Perovskites: The Organic Cation Matters. *Journal of Physical Chemistry Letters*, **2018**, 9, 5474-5480	6.4	77
451	Synthesis and properties of isoindigo and benzo[1,2-b:4,5-b']bis[b]benzothiophene oligomers. *Chemical Communications*, **2018**, 54, 11152-11155	5.8	8
450	A Thiazole□Naphthalene Diimide Based n-Channel Donor□Acceptor Conjugated Polymer. *Macromolecules*, **2018**, 51, 7320-7328	5.5	22
449	Point Defects and Green Emission in Zero-Dimensional Perovskites. *Journal of Physical Chemistry Letters*, **2018**, 9, 5490-5495	6.4	103
448	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	9.6	72
447	Why Can High Charge-Carrier Mobilities be Achieved Along □Conjugated Polymer Chains with Alternating Donor□Acceptor Moieties?. *Advanced Theory and Simulations*, **2018**, 1, 1800016	3.5	9
446	Modeling of Actual-Size Organic Electronic Devices from Efficient Molecular-Scale Simulations. *Advanced Functional Materials*, **2018**, 28, 1801460	15.6	6
445	Excitonic and Polaronic Properties of 2D Hybrid Organic□Inorganic Perovskites. *ACS Energy Letters*, **2017**, 2, 417-423	20.1	105
444	Organic Field-Effect Transistors: A 3D Kinetic Monte Carlo Simulation of the Current Characteristics in Micrometer-Sized Devices. *Advanced Functional Materials*, **2017**, 27, 1605715	15.6	20
443	Open-Circuit Voltage in Organic Solar Cells: The Impacts of Donor Semicrystallinity and Coexistence of Multiple Interfacial Charge-Transfer Bands. *Advanced Energy Materials*, **2017**, 7, 1601995	21.8	30
442	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	16.4	438
441	Polaron self-localization in white-light emitting hybrid perovskites. *Journal of Materials Chemistry C*, **2017**, 5, 2771-2780	7.1	155
440	Reduction of the Work Function of Gold by N-Heterocyclic Carbenes. *Chemistry of Materials*, **2017**, 29, 3403-3411	9.6	50
439	Thieno[3,4-c]Pyrrole-4,6-Dione-Based Polymer Acceptors for High Open-Circuit Voltage All-Polymer Solar Cells. *Advanced Energy Materials*, **2017**, 7, 1602574	21.8	65
438	Suppressing Energy Loss due to Triplet Exciton Formation in Organic Solar Cells: The Role of Chemical Structures and Molecular Packing. *Advanced Energy Materials*, **2017**, 7, 1602713	21.8	21
437	Charge-Transfer States in Organic Solar Cells: Understanding the Impact of Polarization, Delocalization, and Disorder. *ACS Applied Materials & Interfaces*, **2017**, 9, 18095-18102	9.5	68
436	Pyridine-Induced Dimensionality Change in Hybrid Perovskite Nanocrystals. *Chemistry of Materials*, **2017**, 29, 4393-4400	9.6	68
435	Impact of Dielectric Constant on the Singlet-Triplet Gap in Thermally Activated Delayed Fluorescence Materials. *Journal of Physical Chemistry Letters*, **2017**, 8, 2393-2398	6.4	90

434	Understanding the effects of electronic polarization and delocalization on charge-transport levels in oligoacene systems. *Journal of Chemical Physics*, **2017**, 146, 224705	3.9	12
433	Kinetic Monte Carlo Modeling of Charge Carriers in Organic Electronic Devices: Suppression of the Self-Interaction Error. *Journal of Physical Chemistry Letters*, **2017**, 8, 2507-2512	6.4	15
432	Time dependent □ density functional theory characterization of organic dyes for dye-sensitized solar cells. *Molecular Simulation*, **2017**, 43, 1523-1531	2	13
431	Topological Transformation of □ Conjugated Molecules Reduces Resistance to Crystallization. *Angewandte Chemie*, **2017**, 129, 9446-9449	3.6	6
430	Topological Transformation of □ Conjugated Molecules Reduces Resistance to Crystallization. *Angewandte Chemie - International Edition*, **2017**, 56, 9318-9321	16.4	10
429	Assessment of Front-Substituted Zwitterionic Cyanine Polymethines for All-Optical Switching Applications. *Journal of Physical Chemistry C*, **2017**, 121, 14166-14175	3.8	8
428	Singlet Fission in Rubrene Derivatives: Impact of Molecular Packing. *Chemistry of Materials*, **2017**, 29, 2777-2787	9.6	39
427	Computational Design of Functional Materials. *Chemistry of Materials*, **2017**, 29, 2399-2401	9.6	8
426	Impact of morphology on polaron delocalization in a semicrystalline conjugated polymer. *Physical Chemistry Chemical Physics*, **2017**, 19, 3627-3639	3.6	30
425	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	27	276
424	Charge-Transfer Dynamics in the Lowest Excited State of a Pentacene-Fullerene Complex: Implications for Organic Solar Cells. *Journal of Physical Chemistry Letters*, **2017**, 8, 5171-5176	6.4	24
423	Energetic fluctuations in amorphous semiconducting polymers: Impact on charge-carrier mobility. *Journal of Chemical Physics*, **2017**, 147, 134904	3.9	18
422	Electronic Properties of 1,5-Diaminonaphthalene:Tetrahalo-1,4-benzoquinone Donor□Acceptor Cocrystals. *Journal of Physical Chemistry C*, **2017**, 121, 23633-23641	3.8	20
421	Characterization of intrinsic hole transport in single-crystal spiro-OMeTAD. *Npj Flexible Electronics*, **2017**, 1,	10.7	30
420	A New Design Strategy for Efficient Thermally Activated Delayed Fluorescence Organic Emitters: From Twisted to Planar Structures. *Advanced Materials*, **2017**, 29, 1702767	24	151
419	Impact of Active Layer Morphology on Bimolecular Recombination Dynamics in Organic Solar Cells. *Journal of Physical Chemistry C*, **2017**, 121, 24954-24961	3.8	23
418	Nucleation and Growth of Covalent Organic Frameworks from Solution: The Example of COF-5. *Journal of the American Chemical Society*, **2017**, 139, 16310-16318	16.4	83
417	Noncovalent Interactions in Organic Electronic Materials **2017**, 277-302		4

416	Impact of interfacial molecular orientation on radiative recombination and charge generation efficiency. *Nature Communications*, **2017**, 8, 79	17.4	160
415	Inside Perovskites: Quantum Luminescence from Bulk Cs4PbBr6 Single Crystals. *Chemistry of Materials*, **2017**, 29, 7108-7113	9.6	160
414	Structural variations to a donor polymer with low energy losses. *Journal of Materials Chemistry A*, **2017**, 5, 18618-18626	13	11
413	Impact of position of electron withdrawing cyano groups on nonlinear optical properties of centrosymmetric donor-acceptor system. *International Journal of Quantum Chemistry*, **2017**, 117, e25441	2.1	2
412	Molecular behavior of zero-dimensional perovskites. *Science Advances*, **2017**, 3, e1701793	14.3	137
411	Intrinsic Lead Ion Emissions in Zero-Dimensional Cs4PbBr6 Nanocrystals. *ACS Energy Letters*, **2017**, 2, 2805-2811	20.1	109
410	Direct-Indirect Nature of the Bandgap in Lead-Free Perovskite Nanocrystals. *Journal of Physical Chemistry Letters*, **2017**, 8, 3173-3177	6.4	139
409	Effect of Solid-State Polarization on Charge-Transfer Excitations and Transport Levels at Organic Interfaces from a Screened Range-Separated Hybrid Functional. *Journal of Physical Chemistry Letters*, **2017**, 8, 3277-3283	6.4	55
408	Computational Methodologies for Developing Structure–Morphology–Performance Relationships in Organic Solar Cells: A Protocol Review. *Chemistry of Materials*, **2017**, 29, 346-354	9.6	47
407	Molecular Understanding of Fullerene–Electron Donor Interactions in Organic Solar Cells. *Advanced Energy Materials*, **2017**, 7, 1601370	21.8	58
406	Tetraaryl pyrenes: photophysical properties, computational studies, crystal structures, and application in OLEDs. *Journal of Materials Chemistry C*, **2016**, 4, 3041-3058	7.1	28
405	Photovoltaic concepts inspired by coherence effects in photosynthetic systems. *Nature Materials*, **2016**, 16, 35-44	27	191
404	Surface Polarization Drives Photoinduced Charge Separation at the P3HT/Water Interface. *ACS Energy Letters*, **2016**, 1, 454-463	20.1	39
403	Unipolar Electron Transport Polymers: A Thiazole Based All-Electron Acceptor Approach. *Chemistry of Materials*, **2016**, 28, 6045-6049	9.6	64
402	Thieno[3,4-c]pyrrole-4,6-dione-3,4-difluorothiophene Polymer Acceptors for Efficient All-Polymer Bulk Heterojunction Solar Cells. *Angewandte Chemie - International Edition*, **2016**, 55, 12996-13000	16.4	113
401	Thieno[3,4-c]pyrrole-4,6-dione-3,4-difluorothiophene Polymer Acceptors for Efficient All-Polymer Bulk Heterojunction Solar Cells. *Angewandte Chemie*, **2016**, 128, 13190-13194	3.6	26
400	Impact of Fluorine Substituents on Conjugated Polymer Main-Chain Conformations, Packing, and Electronic Couplings. *Advanced Materials*, **2016**, 28, 8197-8205	24	65
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