

Yoan Olivier

List of Publications by Year in descending order

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117
papers

11,685
citations

38742

50
h-index

27406

106
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123
all docs

123
docs citations

123
times ranked

11917
citing authors

#	ARTICLE	IF	CITATIONS
1	Charge Transport in Organic Semiconductors. <i>Chemical Reviews</i> , 2007, 107, 926-952.	47.7	3,853
2	Approaching disorder-free transport in high-mobility conjugated polymers. <i>Nature</i> , 2014, 515, 384-388.	27.8	844
3	Multiresonant Thermally Activated Delayed Fluorescence Emitters Based on Heteroatom-Doped Nanographenes: Recent Advances and Prospects for Organic Light-Emitting Diodes. <i>Advanced Functional Materials</i> , 2020, 30, 1908677.	14.9	385
4	Charge-Transfer Excitations Steer the Davydov Splitting and Mediate Singlet Exciton Fission in Pentacene. <i>Physical Review Letters</i> , 2013, 110, 226402.	7.8	253
5	Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules. <i>Nature Communications</i> , 2019, 10, 597.	12.8	253
6	The nature of singlet excitons in oligoacene molecular crystals. <i>Journal of Chemical Physics</i> , 2011, 134, 204703.	3.0	233
7	Free Radical Scavenging by Natural Polyphenols: Atom versus Electron Transfer. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2082-2092.	2.5	224
8	25th Anniversary Article: High-Mobility Hole and Electron Transport Conjugated Polymers: How Structure Defines Function. <i>Advanced Materials</i> , 2014, 26, 2119-2136.	21.0	199
9	A Deep Blue B,N-Doped Heptacene Emitter That Shows Both Thermally Activated Delayed Fluorescence and Delayed Fluorescence by Triplet-Triplet Annihilation. <i>Journal of the American Chemical Society</i> , 2020, 142, 6588-6599.	13.7	189
10	Improving Processability and Efficiency of Resonant TADF Emitters: A Design Strategy. <i>Advanced Optical Materials</i> , 2020, 8, 1901627.	7.3	182
11	Charge Hopping in Organic Semiconductors: Influence of Molecular Parameters on Macroscopic Mobilities in Model One-Dimensional Stacks. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6356-6364.	2.5	155
12	Bulky End-Capped [1]Benzothieno[3,2- <i>b</i>]benzothiophenes: Reaching High-Mobility Organic Semiconductors by Fine Tuning of the Crystalline Solid-State Order. <i>Advanced Materials</i> , 2015, 27, 3066-3072.	21.0	155
13	Hypsochromic Shift of Multiple-Resonance-Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 17910-17914.	13.8	152
14	Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl[1]benzothieno[3,2- <i>b</i>]benzothiophene. <i>Advanced Materials</i> , 2016, 28, 7106-7114.	21.0	138
15	First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular Stacking. <i>Physical Review Letters</i> , 2015, 115, 107401.	7.8	137
16	Maximizing Singlet Fission by Intermolecular Packing. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3345-3353.	4.6	135
17	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6149-6163.	4.6	121
18	Unraveling the Mechanism of Molecular Doping in Organic Semiconductors. <i>Advanced Materials</i> , 2012, 24, 1535-1539.	21.0	114

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19	Highly Luminescent 2D-Type Slab Crystals Based on a Molecular Charge-Transfer Complex as Promising Organic Light-Emitting Transistor Materials. <i>Advanced Materials</i> , 2017, 29, 1701346.	21.0	111
20	Theoretical Rationalization of the Singlet-Triplet Gap in OLEDs Materials: Impact of Charge-Transfer Character. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 168-177.	5.3	108
21	Tuning conformation, assembly, and charge transport properties of conjugated polymers by printing flow. <i>Science Advances</i> , 2019, 5, eaaw7757.	10.3	105
22	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. <i>Physical Review Materials</i> , 2017, 1, .	2.4	102
23	Hall-Effect Measurements Probing the Degree of Charge-Carrier Delocalization in Solution-Processed Crystalline Molecular Semiconductors. <i>Physical Review Letters</i> , 2011, 107, 066601.	7.8	101
24	Identification of the Key Parameters for Horizontal Transition Dipole Orientation in Fluorescent and TADF Organic Light-Emitting Diodes. <i>Advanced Materials</i> , 2021, 33, e2100677.	21.0	99
25	Depolarization Effects in Self-Assembled Monolayers: A Quantum-Chemical Insight. <i>Advanced Functional Materials</i> , 2007, 17, 1143-1148.	14.9	97
26	What Currently Limits Charge Carrier Mobility in Crystals of Molecular Semiconductors?. <i>Israel Journal of Chemistry</i> , 2014, 54, 595-620.	2.3	97
27	Dynamic nature of excited states of donor-acceptor TADF materials for OLEDs: how theory can reveal structure-property relationships. <i>Journal of Materials Chemistry C</i> , 2017, 5, 5718-5729.	5.5	97
28	Charge Separation and Recombination at Polymer-Fullerene Heterojunctions: Delocalization and Hybridization Effects. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 536-540.	4.6	93
29	Intramolecular Borylation via Sequential B-Mes Bond Cleavage for the Divergent Synthesis of B,N-Doped Benzo[4]helicenes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 3156-3160.	13.8	90
30	Theoretical Characterization of the Structural and Hole Transport Dynamics in Liquid-Crystalline Phthalocyanine Stacks. <i>Journal of Physical Chemistry B</i> , 2009, 113, 14102-14111.	2.6	83
31	Modeling Polymer Dielectric/Pentacene Interfaces: On the Role of Electrostatic Energy Disorder on Charge Carrier Mobility. <i>Advanced Functional Materials</i> , 2009, 19, 3254-3261.	14.9	81
32	The design of an extended multiple resonance TADF emitter based on a polycyclic amine/carbonyl system. <i>Materials Chemistry Frontiers</i> , 2020, 4, 2018-2022.	5.9	81
33	Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene. <i>ChemPhysChem</i> , 2009, 10, 2265-2273.	2.1	77
34	Robust singlet fission in pentacene thin films with tuned charge transfer interactions. <i>Nature Communications</i> , 2018, 9, 954.	12.8	76
35	Liquid-Phase Exfoliation of Graphite into Single- and Few-Layer Graphene with \pm -Functionalized Alkanes. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2714-2721.	4.6	73
36	Vibrationally Assisted Intersystem Crossing in Benchmark Thermally Activated Delayed Fluorescence Molecules. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4053-4058.	4.6	69

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37	Periodic potentials in hybrid van der Waals heterostructures formed by supramolecular lattices on graphene. <i>Nature Communications</i> , 2017, 8, 14767.	12.8	68
38	Deep-Blue Oxadiazole-Containing Thermally Activated Delayed Fluorescence Emitters for Organic Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 33360-33372.	8.0	67
39	Exploring the Energy Landscape of the Charge Transport Levels in Organic Semiconductors at the Molecular Scale. <i>Accounts of Chemical Research</i> , 2013, 46, 434-443.	15.6	64
40	Donor-acceptor stacking arrangements in bulk and thin-film high-mobility conjugated polymers characterized using molecular modelling and MAS and surface-enhanced solid-state NMR spectroscopy. <i>Chemical Science</i> , 2017, 8, 3126-3136.	7.4	64
41	Asymmetric electron and hole transport in a high-mobility n -type conjugated polymer. <i>Physical Review B</i> , 2012, 86,	3.2	63
42	Thienoacene dimers based on the thieno[3,2-b]thiophene moiety: synthesis, characterization and electronic properties. <i>Journal of Materials Chemistry C</i> , 2015, 3, 674-685.	5.5	62
43	Short contacts between chains enhancing luminescence quantum yields and carrier mobilities in conjugated copolymers. <i>Nature Communications</i> , 2019, 10, 2614.	12.8	60
44	Molecular packing and charge transport parameters in crystalline organic semiconductors from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9381.	2.8	57
45	Carbene-Metal Amide Bond Deformation, Rather Than Ligand Rotation, Drives Delayed Fluorescence. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1620-1626.	4.6	57
46	Deposition of Functional Organic Thin Films by Pulsed Plasma Polymerization: A Joint Theoretical and Experimental Study. <i>Plasma Processes and Polymers</i> , 2010, 7, 172-181.	3.0	55
47	Charge Dissociation at Interfaces between Discotic Liquid Crystals: The Surprising Role of Column Mismatch. <i>Journal of the American Chemical Society</i> , 2014, 136, 2911-2920.	13.7	55
48	Supramolecular Organization and Charge Transport Properties of Self-Assembled π -Stacks of Perylene Diimide Dyes. <i>Journal of Physical Chemistry B</i> , 2011, 115, 5593-5603.	2.6	54
49	Collective molecular switching in hybrid superlattices for light-modulated two-dimensional electronics. <i>Nature Communications</i> , 2018, 9, 2661.	12.8	53
50	Structure Influence on Charge Transport in Naphthalenediimide-Thiophene Copolymers. <i>Chemistry of Materials</i> , 2014, 26, 6796-6804.	6.7	51
51	Polarizability and Internal Charge Transfer in Thiophene-Triphenylamine Hybrid π -Conjugated Systems. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9379-9386.	2.6	50
52	Diindolocarbazole achieving multiresonant thermally activated delayed fluorescence without the need for acceptor units. <i>Materials Horizons</i> , 2022, 9, 1068-1080.	12.2	48
53	Excited-State Modulation in Donor-Substituted Multiresonant Thermally Activated Delayed Fluorescence Emitters. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 22341-22352.	8.0	47
54	Singlet-Triplet Excited-State Inversion in Heptazine and Related Molecules: Assessment of TD-DFT and <i>ab initio</i> Methods. <i>ChemPhysChem</i> , 2021, 22, 553-560.	2.1	45

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55	On the Supramolecular Packing of High Electron Mobility Naphthalene Diimide Copolymers: The Perfect Registry of Asymmetric Branched Alkyl Side Chains. <i>Macromolecules</i> , 2013, 46, 8171-8178.	4.8	44
56	Do charges delocalize over multiple molecules in fullerene derivatives?. <i>Journal of Materials Chemistry C</i> , 2016, 4, 3747-3756.	5.5	44
57	Conjugated poly(azomethine)s via simple one-step polycondensation chemistry: synthesis, thermal and optoelectronic properties. <i>Polymer Chemistry</i> , 2013, 4, 4182.	3.9	41
58	Negative Singlet-Triplet Excitation Energy Gap in Triangle-Shaped Molecular Emitters for Efficient Triplet Harvesting. <i>Journal of Physical Chemistry A</i> , 2021, 125, 513-522.	2.5	41
59	Polaron spin dynamics in high-mobility polymeric semiconductors. <i>Nature Physics</i> , 2019, 15, 814-822.	16.7	40
60	Hypsochromic Shift of Multiple-Resonance-Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. <i>Angewandte Chemie</i> , 2021, 133, 18054-18058.	2.0	39
61	Theoretical Characterization of Charge Transport in One-Dimensional Collinear Arrays of Organic Conjugated Molecules. <i>ChemPhysChem</i> , 2010, 11, 1062-1068.	2.1	37
62	Ultrafast Charge Generation Pathways in Photovoltaic Blends Based on Novel Star-Shaped Conjugated Molecules. <i>Advanced Energy Materials</i> , 2015, 5, 1401657.	19.5	35
63	Estimation of π - π Electronic Couplings from Current Measurements. <i>Nano Letters</i> , 2017, 17, 3215-3224.	9.1	35
64	Electron-Withdrawing Substituted Tetrathiafulvalenes as Ambipolar Semiconductors. <i>Chemistry of Materials</i> , 2011, 23, 851-861.	6.7	32
65	Modeling of Multiresonant Thermally Activated Delayed Fluorescence Emitters—Properly Accounting for Electron Correlation Is Key!. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4903-4918.	5.3	32
66	Photoluminescence Quenching Probes Spin Conversion and Exciton Dynamics in Thermally Activated Delayed Fluorescence Materials. <i>Advanced Materials</i> , 2019, 31, e1804490.	21.0	31
67	Quinquephenyl: The Simplest Rigid-Rod-Like Nematic Liquid Crystal, or is it? An Atomistic Simulation. <i>ChemPhysChem</i> , 2014, 15, 1345-1355.	2.1	30
68	Resilience to Conformational Fluctuations Controls Energetic Disorder in Conjugated Polymer Materials: Insights from Atomistic Simulations. <i>Chemistry of Materials</i> , 2019, 31, 6889-6899.	6.7	30
69	Divergente Synthese von B,N-Benzo[4]helicenen durch intramolekulare Borylierung unter sequenzieller B-Mes-Bindungsspaltung. <i>Angewandte Chemie</i> , 2020, 132, 3181-3185.	2.0	30
70	Multi-resonant thermally activated delayed fluorescence emitters based on tetracoordinate boron-containing PAHs: colour tuning based on the nature of chelates. <i>Chemical Science</i> , 2022, 13, 1665-1674.	7.4	30
71	Temperature Dependence of Charge Localization in High-Mobility, Solution-Crystallized Small Molecule Semiconductors Studied by Charge Modulation Spectroscopy. <i>Advanced Functional Materials</i> , 2016, 26, 2326-2333.	14.9	29
72	Unusual electromechanical response in rubrene single crystals. <i>Materials Horizons</i> , 2018, 5, 41-50.	12.2	28

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73	Emission and Absorption Tuning in TADF B,N-Doped Heptacenes: Toward Ideal Blue Hyperfluorescent OLEDs. <i>Advanced Optical Materials</i> , 2022, 10, .	7.3	28
74	Exciton efficiency beyond the spin statistical limit in organic light emitting diodes based on anthracene derivatives. <i>Journal of Materials Chemistry C</i> , 2020, 8, 3773-3783.	5.5	27
75	Polymorphism in Bulk and Thin Films: The Curious Case of Dithiophene-DPP(Boc)-Dithiophene. <i>Journal of Physical Chemistry C</i> , 2014, 118, 657-669.	3.1	26
76	Measurements of Ambipolar Seebeck Coefficients in High-Mobility Diketopyrrolopyrrole Donor-Acceptor Copolymers. <i>Advanced Electronic Materials</i> , 2017, 3, 1700225.	5.1	26
77	Luminescent Dinuclear Copper(I) Complexes Bearing an Imidazolopyrimidine Bridging Ligand. <i>Inorganic Chemistry</i> , 2020, 59, 14772-14784.	4.0	26
78	Violation of Hund's rule in molecules: Predicting the excited-state energy inversion by TD-DFT with double-hybrid methods. <i>Journal of Chemical Physics</i> , 2022, 156, 034105.	3.0	26
79	Carbene-Metal-Amide Polycrystalline Materials Feature Blue Shifted Energy yet Unchanged Kinetics of Emission. <i>Chemistry of Materials</i> , 2020, 32, 4743-4753.	6.7	25
80	Analysis of External and Internal Disorder to Understand Band-Like Transport in n-Type Organic Semiconductors. <i>Advanced Materials</i> , 2021, 33, 2007870.	21.0	24
81	An S-shaped double helicene showing both multi-resonance thermally activated delayed fluorescence and circularly polarized luminescence. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4861-4870.	5.5	23
82	Roles of local and nonlocal electron-phonon couplings in triplet exciton diffusion in the anthracene crystal. <i>Physical Review B</i> , 2013, 88, .	3.2	22
83	Tuning of the Photovoltaic Parameters of Molecular Donors by Covalent Bridging. <i>Advanced Functional Materials</i> , 2013, 23, 4854-4861.	14.9	20
84	Multiple Charge Transfer States in Donor-Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. <i>Chemistry of Materials</i> , 2019, 31, 6808-6817.	6.7	20
85	Photoluminescence and electrochemiluminescence of thermally activated delayed fluorescence (TADF) emitters containing diphenylphosphine chalcogenide-substituted carbazole donors. <i>Journal of Materials Chemistry C</i> , 2022, 10, 4646-4667.	5.5	20
86	Electronic and structural characterisation of a tetrathiafulvalene compound as a potential candidate for ambipolar transport properties. <i>CrystEngComm</i> , 2011, 13, 6597.	2.6	19
87	Benzodicarbomethoxytetrathiafulvalene Derivatives as Soluble Organic Semiconductors. <i>Journal of Organic Chemistry</i> , 2011, 76, 154-163.	3.2	19
88	Structural and Charge-Transport Properties of a Liquid-Crystalline 1,3-Disubstituted Thiophene Derivative: A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4617-4627.	3.1	18
89	Bis(arylene-ethynylene)-tetrazines: A Promising Family of n-Type Organic Semiconductors?. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18945-18955.	3.1	18
90	Computational Studies of Molecular Materials for Unconventional Energy Conversion: The Challenge of Light Emission by Thermally Activated Delayed Fluorescence. <i>Molecules</i> , 2020, 25, 1006.	3.8	18

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91	Spontaneous exciton dissociation enables spin state interconversion in delayed fluorescence organic semiconductors. <i>Nature Communications</i> , 2021, 12, 6640.	12.8	18
92	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. <i>Journal of Chemical Physics</i> , 2013, 138, 204304.	3.0	17
93	Cost-Effective Force Field Tailored for Solid-Phase Simulations of OLED Materials. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3383-3392.	5.3	17
94	Ultrafast Exciton-to-Polaron Conversion in Densely Packed Small Organic Semiconducting Molecules. <i>Advanced Optical Materials</i> , 2017, 5, 1700024.	7.3	16
95	White-light electroluminescence from a layer incorporating a single fully-organic spiro compound with phosphine oxide substituents. <i>Journal of Materials Chemistry C</i> , 2020, 8, 14462-14468.	5.5	15
96	Spiro-Based Thermally Activated Delayed Fluorescence Emitters with Reduced Nonradiative Decay for High-Quantum-Efficiency, Low-Roll-Off, Organic Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 44628-44640.	8.0	15
97	Comprehensive modelling study of singlet exciton diffusion in donor-acceptor dyads: when small changes in chemical structure matter. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25023-25034.	2.8	14
98	Dynamic self-stabilization in the electronic and nanomechanical properties of an organic polymer semiconductor. <i>Nature Communications</i> , 2022, 13, .	12.8	14
99	Crossed 2D versus Slipped 1D π - π Stacking in Polymorphs of Crystalline Organic Thin Films: Impact on the Electronic and Optical Response. <i>Advanced Optical Materials</i> , 2019, 7, 1900749.	7.3	13
100	Reliable DFT-based estimates of cohesive energies of organic solids: The anthracene crystal. <i>Journal of Chemical Physics</i> , 2012, 137, 194311.	3.0	12
101	Determining the cohesive energy of coronene by dispersion-corrected DFT methods: Periodic boundary conditions vs. molecular pairs. <i>Journal of Chemical Physics</i> , 2015, 142, 054702.	3.0	10
102	Electronic Structure and Charge Transport in Nanostripped Graphene. <i>Journal of Physical Chemistry C</i> , 2016, 120, 20024-20032.	3.1	10
103	Application of Rubrene Air-Gap Transistors as Sensitive MEMS Physical Sensors. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 41570-41577.	8.0	10
104	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4382-4391.	5.5	10
105	N-doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25562.	2.0	9
106	Tuning Short Contacts between Polymer Chains To Enhance Charge Transport in Amorphous Donor-Acceptor Polymers. <i>Journal of Physical Chemistry C</i> , 2022, 126, 3118-3126.	3.1	8
107	Enhancing Thermally Activated Delayed Fluorescence by Fine-Tuning the Dendron Donor Strength. <i>Journal of Physical Chemistry B</i> , 2022, 126, 552-562.	2.6	7
108	Substitution Effects on a New Pyridylbenzimidazole Acceptor for Thermally Activated Delayed Fluorescence and Their Use in Organic Light-Emitting Diodes. <i>Advanced Optical Materials</i> , 2021, 9, 2100846.	7.3	6

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109	<i>peri</i> -Acenoacene molecules: tuning of the singlet and triplet excitation energies by modifying their radical character. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24016-24028.	2.8	5
110	Multi-Edge Resonant Tender X-ray Diffraction for Probing the Crystalline Packing of Conjugated Polymers. <i>Macromolecules</i> , 2022, 55, 4733-4741.	4.8	4
111	Charge Transport in Conjugated Materials: From Theoretical Models to Experimental Systems. AIP Conference Proceedings, 2008, , .	0.4	2
112	Pressure sensor based on organic single crystal air-gap transistor. , 2017, , .		1
113	20â€1: <i>Invited Paper:</i> Towards Deepâ€Blue Materials with Efficient Triplet Harvesting. Digest of Technical Papers SID International Symposium, 2018, 49, 239-242.	0.3	1
114	19â€2: <i>Invited Paper:</i> Design of Multiâ€Resonance Thermally Activated Delayed Fluorescence Materials for Organic Lightâ€Emitting Diodes. Digest of Technical Papers SID International Symposium, 2021, 52, 228-231.	0.3	1
115	Inside Cover: Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene (<i>ChemPhysChem</i> 13/2009). <i>ChemPhysChem</i> , 2009, 10, 2158-2158.	2.1	0
116	Charge Carrier Mobility: Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl[1]benzothieno[3,2-b][1]benzothiophene (Adv.) Tj ETQq0 0 0 rgB0/Overlock 10 Tf 5		
117	Ultrafast Charge Dynamics in Novel Star-Shaped Small Molecules: the Effect of Donor and Acceptor Groups. , 2016, , .		0