

Yoan Olivier

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111
papers

8,840
citations

44
h-index

93
g-index

123
ext. papers

10,257
ext. citations

9.9
avg, IF

6.05
L-index

#	Paper	IF	Citations
111	Charge transport in organic semiconductors. <i>Chemical Reviews</i> , 2007 , 107, 926-52	68.1	3363
110	Approaching disorder-free transport in high-mobility conjugated polymers. <i>Nature</i> , 2014 , 515, 384-8	50.4	692
109	Charge-transfer excitations steer the Davydov splitting and mediate singlet exciton fission in pentacene. <i>Physical Review Letters</i> , 2013 , 110, 226402	7.4	217
108	The nature of singlet excitons in oligoacene molecular crystals. <i>Journal of Chemical Physics</i> , 2011 , 134, 204703	3.9	208
107	25th anniversary article: high-mobility hole and electron transport conjugated polymers: how structure defines function. <i>Advanced Materials</i> , 2014 , 26, 2119-36	24	182
106	Free radical scavenging by natural polyphenols: atom versus electron transfer. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 2082-92	2.8	172
105	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	15.6	148
104	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, 6356-64	2.8	139
103	Bulky end-capped [1]benzothieno[3,2-b]benzothiophenes: reaching high-mobility organic semiconductors by fine tuning of the crystalline solid-state order. <i>Advanced Materials</i> , 2015 , 27, 3066-72 ²⁴		133
102	First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular π -Stacking. <i>Physical Review Letters</i> , 2015 , 115, 107401	7.4	122
101	Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl[1]benzothieno[3,2-b][1]benzothiophene. <i>Advanced Materials</i> , 2016 , 28, 7106-14 ²⁴		117
100	Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules. <i>Nature Communications</i> , 2019 , 10, 597	17.4	113
99	Maximizing Singlet Fission by Intermolecular Packing. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3345-53 ²⁴		113
98	Unraveling the mechanism of molecular doping in organic semiconductors. <i>Advanced Materials</i> , 2012 , 24, 1535-9	24	101
97	Depolarization Effects in Self-Assembled Monolayers: A Quantum-Chemical Insight. <i>Advanced Functional Materials</i> , 2007 , 17, 1143-1148	15.6	96
96	Hall-effect measurements probing the degree of charge-carrier delocalization in solution-processed crystalline molecular semiconductors. <i>Physical Review Letters</i> , 2011 , 107, 066601	7.4	94
95	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, 168-77	6.4	86

94	Improving Processability and Efficiency of Resonant TADF Emitters: A Design Strategy. <i>Advanced Optical Materials</i> , 2020 , 8, 1901627	8.1	85
93	Theoretical characterization of the structural and hole transport dynamics in liquid-crystalline phthalocyanine stacks. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 14102-11	3.4	82
92	Charge Separation and Recombination at Polymer-Fullerene Heterojunctions: Delocalization and Hybridization Effects. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 536-40	6.4	81
91	What Currently Limits Charge Carrier Mobility in Crystals of Molecular Semiconductors?. <i>Israel Journal of Chemistry</i> , 2014 , 54, 595-620	3.4	81
90	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	24	80
89	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 6149-6163	6.4	76
88	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	15.6	72
87	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	7.1	71
86	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	16.4	71
85	Influence of intermolecular vibrations on the electronic coupling in organic semiconductors: the case of anthracene and perfluoropentacene. <i>ChemPhysChem</i> , 2009 , 10, 2265-73	3.2	69
84	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. <i>Physical Review Materials</i> , 2017 , 1,	3.2	65
83	Liquid-Phase Exfoliation of Graphite into Single- and Few-Layer Graphene with π -Functionalized Alkanes. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2714-21	6.4	64
82	Tuning conformation, assembly, and charge transport properties of conjugated polymers by printing flow. <i>Science Advances</i> , 2019 , 5, eaaw7757	14.3	63
81	Exploring the energy landscape of the charge transport levels in organic semiconductors at the molecular scale. <i>Accounts of Chemical Research</i> , 2013 , 46, 434-43	24.3	59
80	Asymmetric electron and hole transport in a high-mobility n-type conjugated polymer. <i>Physical Review B</i> , 2012 , 86,	3.3	58
79	Deep-Blue Oxadiazole-Containing Thermally Activated Delayed Fluorescence Emitters for Organic Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 33360-33372	9.5	58
78	Periodic potentials in hybrid van der Waals heterostructures formed by supramolecular lattices on graphene. <i>Nature Communications</i> , 2017 , 8, 14767	17.4	56
77	Molecular packing and charge transport parameters in crystalline organic semiconductors from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 9381-8	3.6	56

76	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	7.1	52
75	Charge dissociation at interfaces between discotic liquid crystals: the surprising role of column mismatch. <i>Journal of the American Chemical Society</i> , 2014 , 136, 2911-20	16.4	51
74	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	9.4	50
73	Robust singlet fission in pentacene thin films with tuned charge transfer interactions. <i>Nature Communications</i> , 2018 , 9, 954	17.4	50
72	Polarizability and internal charge transfer in thiophene-triphenylamine hybrid π -conjugated systems. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 9379-86	3.4	48
71	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	3.4	47
70	Vibrationally Assisted Intersystem Crossing in Benchmark Thermally Activated Delayed Fluorescence Molecules. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4053-4058	6.4	47
69	Carbene-Metal-Amide Bond Deformation, Rather Than Ligand Rotation, Drives Delayed Fluorescence. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 1620-1626	6.4	46
68	Structure Influence on Charge Transport in Naphthalenediimide π -thiophene Copolymers. <i>Chemistry of Materials</i> , 2014 , 26, 6796-6804	9.6	44
67	Supramolecular organization and charge transport properties of self-assembled π -stacks of perylene diimide dyes. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 5593-603	3.4	43
66	Collective molecular switching in hybrid superlattices for light-modulated two-dimensional electronics. <i>Nature Communications</i> , 2018 , 9, 2661	17.4	42
65	Intramolecular Borylation via Sequential B-Mes Bond Cleavage for the Divergent Synthesis of B,N,B-Doped Benzo[4]helicenes. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 3156-3160	16.4	42
64	Hypsochromic Shift of Multiple-Resonance-Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 17910-17914	16.4	42
63	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	7.8	37
62	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	5.5	37
61	Conjugated poly(azomethine)s via simple one-step polycondensation chemistry: synthesis, thermal and optoelectronic properties. <i>Polymer Chemistry</i> , 2013 , 4, 4182	4.9	37
60	Do charges delocalize over multiple molecules in fullerene derivatives?. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 3747-3756	7.1	36
59	Theoretical characterization of charge transport in one-dimensional collinear arrays of organic conjugated molecules. <i>ChemPhysChem</i> , 2010 , 11, 1062-8	3.2	34

58	Short contacts between chains enhancing luminescence quantum yields and carrier mobilities in conjugated copolymers. <i>Nature Communications</i> , 2019 , 10, 2614	17.4	29
57	Electron-Withdrawing Substituted Tetrathiafulvalenes as Ambipolar Semiconductors \square <i>Chemistry of Materials</i> , 2011 , 23, 851-861	9.6	29
56	Polaron spin dynamics in high-mobility polymeric semiconductors. <i>Nature Physics</i> , 2019 , 15, 814-822	16.2	27
55	Quinquephenyl: the simplest rigid-rod-like nematic liquid crystal, or is it? An atomistic simulation. <i>ChemPhysChem</i> , 2014 , 15, 1345-55	3.2	27
54	Ultrafast Charge Generation Pathways in Photovoltaic Blends Based on Novel Star-Shaped Conjugated Molecules. <i>Advanced Energy Materials</i> , 2015 , 5, 1401657	21.8	26
53	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	3.8	26
52	Photoluminescence Quenching Probes Spin Conversion and Exciton Dynamics in Thermally Activated Delayed Fluorescence Materials. <i>Advanced Materials</i> , 2019 , 31, e1804490	24	25
51	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	15.6	25
50	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	24	25
49	Unusual electromechanical response in rubrene single crystals. <i>Materials Horizons</i> , 2018 , 5, 41-50	14.4	24
48	Estimation of \square Electronic Couplings from Current Measurements. <i>Nano Letters</i> , 2017 , 17, 3215-3224	11.5	23
47	Measurements of Ambipolar Seebeck Coefficients in High-Mobility Diketopyrrolopyrrole Donor \square Acceptor Copolymers. <i>Advanced Electronic Materials</i> , 2017 , 3, 1700225	6.4	19
46	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. <i>Journal of Chemical Physics</i> , 2013 , 138, 204304	3.9	17
45	Structural and Charge-Transport Properties of a Liquid-Crystalline \square Disubstituted Thiophene Derivative: A Joint Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 4617-4627	3.8	17
44	Bis(arylene-ethynylene)-s-tetrazines: A Promising Family of n-Type Organic Semiconductors?. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 18945-18955	3.8	16
43	Cost-Effective Force Field Tailored for Solid-Phase Simulations of OLED Materials. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3383-92	6.4	16
42	Roles of local and nonlocal electron-phonon couplings in triplet exciton diffusion in the anthracene crystal. <i>Physical Review B</i> , 2013 , 88,	3.3	16
41	Electronic and structural characterisation of a tetrathiafulvalene compound as a potential candidate for ambipolar transport properties. <i>CrystEngComm</i> , 2011 , 13, 6597	3.3	16

40	Benzodicarbomethoxytetrathiafulvalene derivatives as soluble organic semiconductors. <i>Journal of Organic Chemistry</i> , 2011 , 76, 154-63	4.2	15
39	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	2.8	15
38	Resilience to Conformational Fluctuations Controls Energetic Disorder in Conjugated Polymer Materials: Insights from Atomistic Simulations. <i>Chemistry of Materials</i> , 2019 , 31, 6889-6899	9.6	14
37	Ultrafast Exciton-to-Polaron Conversion in Densely Packed Small Organic Semiconducting Molecules. <i>Advanced Optical Materials</i> , 2017 , 5, 1700024	8.1	13
36	Multiple Charge Transfer States in Donor-Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. <i>Chemistry of Materials</i> , 2019 , 31, 6808-6817	9.6	13
35	Carbene-Metal-Amide Polycrystalline Materials Feature Blue Shifted Energy yet Unchanged Kinetics of Emission. <i>Chemistry of Materials</i> , 2020 , 32, 4743-4753	9.6	13
34	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	7.1	13
33	Singlet-Triplet Excited-State Inversion in Heptazine and Related Molecules: Assessment of TD-DFT and ab initio Methods. <i>ChemPhysChem</i> , 2021 , 22, 553-560	3.2	13
32	Reliable DFT-based estimates of cohesive energies of organic solids: the anthracene crystal. <i>Journal of Chemical Physics</i> , 2012 , 137, 194311	3.9	12
31	Divergente Synthese von B,N,B-Benzo[4]helicenen durch intramolekulare Borylierung unter sequenzieller B-Mes-Bindungsspaltung. <i>Angewandte Chemie</i> , 2020 , 132, 3181-3185	3.6	12
30	Computational Studies of Molecular Materials for Unconventional Energy Conversion: The Challenge of Light Emission by Thermally Activated Delayed Fluorescence. <i>Molecules</i> , 2020 , 25,	4.8	10
29	Hypsochromic Shift of Multiple-Resonance-Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. <i>Angewandte Chemie</i> , 2021 , 133, 18054-18058	3.6	10
28	Crossed 2D versus Slipped 1D π -Stacking in Polymorphs of Crystalline Organic Thin Films: Impact on the Electronic and Optical Response. <i>Advanced Optical Materials</i> , 2019 , 7, 1900749	8.1	9
27	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	3.9	9
26	Luminescent Dinuclear Copper(I) Complexes Bearing an Imidazolylpyrimidine Bridging Ligand. <i>Inorganic Chemistry</i> , 2020 , 59, 14772-14784	5.1	9
25	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	3.6	9
24	Application of Rubrene Air-Gap Transistors as Sensitive MEMS Physical Sensors. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 41570-41577	9.5	9
23	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 4382-4391	7.1	8

22	Analysis of External and Internal Disorder to Understand Band-Like Transport in n-Type Organic Semiconductors. <i>Advanced Materials</i> , 2021 , 33, e2007870	24	8
21	Electronic Structure and Charge Transport in Nanostripped Graphene. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 20024-20032	3.8	7
20	Diindolocarbazole - achieving multiresonant thermally activated delayed fluorescence without the need for acceptor units.. <i>Materials Horizons</i> , 2022 ,	14.4	7
19	N-doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25562	2.1	7
18	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	3.9	6
17	Tuning of the Photovoltaic Parameters of Molecular Donors by Covalent Bridging. <i>Advanced Functional Materials</i> , 2013 , 23, n/a-n/a	15.6	5
16	Spontaneous exciton dissociation enables spin state interconversion in delayed fluorescence organic semiconductors. <i>Nature Communications</i> , 2021 , 12, 6640	17.4	5
15	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	9.4	4
14	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	7.1	4
13	Photoluminescence and Electrochemiluminescence of Thermally Activated Delayed Fluorescence (TADF) Emitters Containing Diphenylphosphine Chalcogenide-Substituted Carbazole Donors. <i>Journal of Materials Chemistry C</i> ,	7.1	3
12	Charge Transport in Conjugated Materials: From Theoretical Models to Experimental Systems. <i>AIP Conference Proceedings</i> , 2008 ,	0	2
11	Enhancing Thermally Activated Delayed Fluorescence by Fine-Tuning the Dendron Donor Strength.. <i>Journal of Physical Chemistry B</i> , 2022 ,	3.4	2
10	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	9.5	2
9	Pressure sensor based on organic single crystal air-gap transistor 2017 ,		1
8	20-1: Invited Paper: Towards Deep-Blue Materials with Efficient Triplet Harvesting. <i>Digest of Technical Papers SID International Symposium</i> , 2018 , 49, 239-242	0.5	1
7	19-2: Invited Paper: Design of Multi-Resonance Thermally Activated Delayed Fluorescence Materials for Organic Light-Emitting Diodes. <i>Digest of Technical Papers SID International Symposium</i> , 2021 , 52, 228-231	0.5	0
6	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> , 2100846	8.1	0
5	-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	3.6	0

- 4 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. Mater. 33/2016). *Advanced Materials*, **2016**, 28, 7291-7291 24
- 3 Charge Transport in Organic Semiconductors: A Multiscale Modeling **2014**, 1-38
- 2 Inside Cover: Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene (ChemPhysChem 13/2009). *ChemPhysChem*, **2009**, 10, 2158-2158 3.2
- 1 Ultrafast Electron and Hole Dynamics in Novel Conjugated Star-Shaped Molecules. *Springer Proceedings in Physics*, **2015**, 564-567 0.2