Yoan Olivier

List of Publications by Year in Descending Order

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	Diindolocarbazole - achieving multiresonant thermally activated delayed fluorescence without the need for acceptor units.. *Materials Horizons*, **2022**,	14.4	7
110	Multi-resonant thermally activated delayed fluorescence emitters based on tetracoordinate boron-containing PAHs: colour tuning based on the nature of chelates.. *Chemical Science*, **2022**, 13, 1665-1674	9.4	4
109	Enhancing Thermally Activated Delayed Fluorescence by Fine-Tuning the Dendron Donor Strength.. *Journal of Physical Chemistry B*, **2022**,	3.4	2
108	Violation of Hund's rule in molecules: Predicting the excited-state energy inversion by TD-DFT with double-hybrid methods.. *Journal of Chemical Physics*, **2022**, 156, 034105	3.9	6
107	Spontaneous exciton dissociation enables spin state interconversion in delayed fluorescence organic semiconductors. *Nature Communications*, **2021**, 12, 6640	17.4	5
106	19-2: Invited Paper: Design of Multi-Resonance Thermally Activated Delayed Fluorescence Materials for Organic Light-Emitting Diodes. *Digest of Technical Papers SID International Symposium*, **2021**, 52, 228-231	0.5	0
105	Singlet-Triplet Excited-State Inversion in Heptazine and Related Molecules: Assessment of TD-DFT and ab initio Methods. *ChemPhysChem*, **2021**, 22, 553-560	3.2	13
104	Negative Singlet-Triplet Excitation Energy Gap in Triangle-Shaped Molecular Emitters for Efficient Triplet Harvesting. *Journal of Physical Chemistry A*, **2021**, 125, 513-522	2.8	15
103	Analysis of External and Internal Disorder to Understand Band-Like Transport in n-Type Organic Semiconductors. *Advanced Materials*, **2021**, 33, e2007870	24	8
102	Hypsochromic Shift of Multiple-Resonance-Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. *Angewandte Chemie - International Edition*, **2021**, 60, 17910-17914	16.4	42
101	Hypsochromic Shift of Multiple-Resonance-Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. *Angewandte Chemie*, **2021**, 133, 18054-18058	3.6	10
100	Identification of the Key Parameters for Horizontal Transition Dipole Orientation in Fluorescent and TADF Organic Light-Emitting Diodes. *Advanced Materials*, **2021**, 33, e2100677	24	25
99	Spiro-Based Thermally Activated Delayed Fluorescence Emitters with Reduced Nonradiative Decay for High-Quantum-Efficiency, Low-Roll-Off, Organic Light-Emitting Diodes. *ACS Applied Materials & Interfaces*, **2021**, 13, 44628-44640	9.5	2
98	-Acenoacene molecules: tuning of the singlet and triplet excitation energies by modifying their radical character. *Physical Chemistry Chemical Physics*, **2021**, 23, 24016-24028	3.6	0
97	Carbene–Metal–Amide Polycrystalline Materials Feature Blue Shifted Energy yet Unchanged Kinetics of Emission. *Chemistry of Materials*, **2020**, 32, 4743-4753	9.6	13
96	The design of an extended multiple resonance TADF emitter based on a polycyclic amine/carbonyl system. *Materials Chemistry Frontiers*, **2020**, 4, 2018-2022	7.8	37
95	Multiresonant Thermally Activated Delayed Fluorescence Emitters Based on Heteroatom-Doped Nanographenes: Recent Advances and Prospects for Organic Light-Emitting Diodes. *Advanced Functional Materials*, **2020**, 30, 1908677	15.6	148

94	A Deep Blue B,N-Doped Heptacene Emitter That Shows Both Thermally Activated Delayed Fluorescence and Delayed Fluorescence by Triplet-Triplet Annihilation. *Journal of the American Chemical Society*, **2020**, 142, 6588-6599	16.4	71
93	Computational Studies of Molecular Materials for Unconventional Energy Conversion: The Challenge of Light Emission by Thermally Activated Delayed Fluorescence. *Molecules*, **2020**, 25,	4.8	10
92	Exciton efficiency beyond the spin statistical limit in organic light emitting diodes based on anthracene derivatives. *Journal of Materials Chemistry C*, **2020**, 8, 3773-3783	7.1	13
91	Intramolecular Borylation via Sequential B-Mes Bond Cleavage for the Divergent Synthesis of B,N,B-Doped Benzo[4]helicenes. *Angewandte Chemie - International Edition*, **2020**, 59, 3156-3160	16.4	42
90	Divergente Synthese von B,N,B-Benzo[4]helicenen durch intramolekulare Borylierung unter sequenzieller B-Mes-Bindungsspaltung. *Angewandte Chemie*, **2020**, 132, 3181-3185	3.6	12
89	Improving Processability and Efficiency of Resonant TADF Emitters: A Design Strategy. *Advanced Optical Materials*, **2020**, 8, 1901627	8.1	85
88	White-light electroluminescence from a layer incorporating a single fully-organic spiro compound with phosphine oxide substituents. *Journal of Materials Chemistry C*, **2020**, 8, 14462-14468	7.1	4
87	Luminescent Dinuclear Copper(I) Complexes Bearing an Imidazolylpyrimidine Bridging Ligand. *Inorganic Chemistry*, **2020**, 59, 14772-14784	5.1	9
86	Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules. *Nature Communications*, **2019**, 10, 597	17.4	113
85	Multiple Charge Transfer States in Donor–Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. *Chemistry of Materials*, **2019**, 31, 6808-6817	9.6	13
84	Polaron spin dynamics in high-mobility polymeric semiconductors. *Nature Physics*, **2019**, 15, 814-822	16.2	27
83	Short contacts between chains enhancing luminescence quantum yields and carrier mobilities in conjugated copolymers. *Nature Communications*, **2019**, 10, 2614	17.4	29
82	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. *Journal of Materials Chemistry C*, **2019**, 7, 4382-4391	7.1	8
81	Photoluminescence Quenching Probes Spin Conversion and Exciton Dynamics in Thermally Activated Delayed Fluorescence Materials. *Advanced Materials*, **2019**, 31, e1804490	24	25
80	Tuning conformation, assembly, and charge transport properties of conjugated polymers by printing flow. *Science Advances*, **2019**, 5, eaaw7757	14.3	63
79	Crossed 2D versus Slipped 1D π-Stacking in Polymorphs of Crystalline Organic Thin Films: Impact on the Electronic and Optical Response. *Advanced Optical Materials*, **2019**, 7, 1900749	8.1	9
78	Resilience to Conformational Fluctuations Controls Energetic Disorder in Conjugated Polymer Materials: Insights from Atomistic Simulations. *Chemistry of Materials*, **2019**, 31, 6889-6899	9.6	14
77	Comprehensive modelling study of singlet exciton diffusion in donor-acceptor dyads: when small changes in chemical structure matter. *Physical Chemistry Chemical Physics*, **2019**, 21, 25023-25034	3.6	9

76	Robust singlet fission in pentacene thin films with tuned charge transfer interactions. *Nature Communications*, **2018**, 9, 954	17.4	50
75	Carbene-Metal-Amide Bond Deformation, Rather Than Ligand Rotation, Drives Delayed Fluorescence. *Journal of Physical Chemistry Letters*, **2018**, 9, 1620-1626	6.4	46
74	Unusual electromechanical response in rubrene single crystals. *Materials Horizons*, **2018**, 5, 41-50	14.4	24
73	Collective molecular switching in hybrid superlattices for light-modulated two-dimensional electronics. *Nature Communications*, **2018**, 9, 2661	17.4	42
72	N-doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. *International Journal of Quantum Chemistry*, **2018**, 118, e25562	2.1	7
71	Application of Rubrene Air-Gap Transistors as Sensitive MEMS Physical Sensors. *ACS Applied Materials & Interfaces*, **2018**, 10, 41570-41577	9.5	9
70	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. *Journal of Physical Chemistry Letters*, **2018**, 9, 6149-6163	6.4	76
69	Deep-Blue Oxadiazole-Containing Thermally Activated Delayed Fluorescence Emitters for Organic Light-Emitting Diodes. *ACS Applied Materials & Interfaces*, **2018**, 10, 33360-33372	9.5	58
68	20-1: Invited Paper: Towards Deep-Blue Materials with Efficient Triplet Harvesting. *Digest of Technical Papers SID International Symposium*, **2018**, 49, 239-242	0.5	1
67	Vibrationally Assisted Intersystem Crossing in Benchmark Thermally Activated Delayed Fluorescence Molecules. *Journal of Physical Chemistry Letters*, **2018**, 9, 4053-4058	6.4	47
66	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. *Chemical Science*, **2017**, 8, 3126-3136	9.4	50
65	Ultrafast Exciton-to-Polaron Conversion in Densely Packed Small Organic Semiconducting Molecules. *Advanced Optical Materials*, **2017**, 5, 1700024	8.1	13
64	Estimation of Electronic Couplings from Current Measurements. *Nano Letters*, **2017**, 17, 3215-3224	11.5	23
63	Periodic potentials in hybrid van der Waals heterostructures formed by supramolecular lattices on graphene. *Nature Communications*, **2017**, 8, 14767	17.4	56
62	Dynamic nature of excited states of donor–acceptor TADF materials for OLEDs: how theory can reveal structure–property relationships. *Journal of Materials Chemistry C*, **2017**, 5, 5718-5729	7.1	71
61	Measurements of Ambipolar Seebeck Coefficients in High-Mobility Diketopyrrolopyrrole Donor–Acceptor Copolymers. *Advanced Electronic Materials*, **2017**, 3, 1700225	6.4	19
60	Pressure sensor based on organic single crystal air-gap transistor **2017**,		1
59	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. *Physical Review Materials*, **2017**, 1,	3.2	65

58	Highly Luminescent 2D-Type Slab Crystals Based on a Molecular Charge-Transfer Complex as Promising Organic Light-Emitting Transistor Materials. *Advanced Materials*, **2017**, 29, 1701346	24	80
57	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	
56	Electronic Structure and Charge Transport in Nanostripped Graphene. *Journal of Physical Chemistry C*, **2016**, 120, 20024-20032	3.8	7
55	Liquid-Phase Exfoliation of Graphite into Single- and Few-Layer Graphene with Functionalized Alkanes. *Journal of Physical Chemistry Letters*, **2016**, 7, 2714-21	6.4	64
54	Charge Separation and Recombination at Polymer-Fullerene Heterojunctions: Delocalization and Hybridization Effects. *Journal of Physical Chemistry Letters*, **2016**, 7, 536-40	6.4	81
53	Do charges delocalize over multiple molecules in fullerene derivatives?. *Journal of Materials Chemistry C*, **2016**, 4, 3747-3756	7.1	36
52	Temperature Dependence of Charge Localization in High-Mobility, Solution-Crystallized Small Molecule Semiconductors Studied by Charge Modulation Spectroscopy. *Advanced Functional Materials*, **2016**, 26, 2326-2333	15.6	25
51	Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl[1]benzothieno[3,2-b][1]benzothiophene. *Advanced Materials*, **2016**, 28, 7106-14	24	117
50	Bis(arylene-ethynylene)-s-tetrazines: A Promising Family of n-Type Organic Semiconductors?. *Journal of Physical Chemistry C*, **2015**, 119, 18945-18955	3.8	16
49	Cost-Effective Force Field Tailored for Solid-Phase Simulations of OLED Materials. *Journal of Chemical Theory and Computation*, **2015**, 11, 3383-92	6.4	16
48	Bulky end-capped [1]benzothieno[3,2-b]benzothiophenes: reaching high-mobility organic semiconductors by fine tuning of the crystalline solid-state order. *Advanced Materials*, **2015**, 27, 3066-72	24	133
47	Ultrafast Charge Generation Pathways in Photovoltaic Blends Based on Novel Star-Shaped Conjugated Molecules. *Advanced Energy Materials*, **2015**, 5, 1401657	21.8	26
46	Thienoacene dimers based on the thieno[3,2-b]thiophene moiety: synthesis, characterization and electronic properties. *Journal of Materials Chemistry C*, **2015**, 3, 674-685	7.1	52
45	First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular Stacking. *Physical Review Letters*, **2015**, 115, 107401	7.4	122
44	Theoretical rationalization of the singlet-triplet gap in OLEDs materials: impact of charge-transfer character. *Journal of Chemical Theory and Computation*, **2015**, 11, 168-77	6.4	86
43	Determining the cohesive energy of coronene by dispersion-corrected DFT methods: periodic boundary conditions vs. molecular pairs. *Journal of Chemical Physics*, **2015**, 142, 054702	3.9	9
42	Ultrafast Electron and Hole Dynamics in Novel Conjugated Star-Shaped Molecules. *Springer Proceedings in Physics*, **2015**, 564-567	0.2	
41	25th anniversary article: high-mobility hole and electron transport conjugated polymers: how structure defines function. *Advanced Materials*, **2014**, 26, 2119-36	24	182

40	Polymorphism in Bulk and Thin Films: The Curious Case of Dithiophene-DPP(Boc)-Dithiophene. *Journal of Physical Chemistry C*, **2014**, 118, 657-669	3.8	26
39	Charge dissociation at interfaces between discotic liquid crystals: the surprising role of column mismatch. *Journal of the American Chemical Society*, **2014**, 136, 2911-20	16.4	51
38	What Currently Limits Charge Carrier Mobility in Crystals of Molecular Semiconductors?. *Israel Journal of Chemistry*, **2014**, 54, 595-620	3.4	81
37	Quinquephenyl: the simplest rigid-rod-like nematic liquid crystal, or is it? An atomistic simulation. *ChemPhysChem*, **2014**, 15, 1345-55	3.2	27
36	Approaching disorder-free transport in high-mobility conjugated polymers. *Nature*, **2014**, 515, 384-8	50.4	692
35	Maximizing Singlet Fission by Intermolecular Packing. *Journal of Physical Chemistry Letters*, **2014**, 5, 3345-53	6.4	113
34	Structure Influence on Charge Transport in Naphthalenediimide-Thiophene Copolymers. *Chemistry of Materials*, **2014**, 26, 6796-6804	9.6	44
33	Charge Transport in Organic Semiconductors: A Multiscale Modeling **2014**, 1-38		
32	Tuning of the Photovoltaic Parameters of Molecular Donors by Covalent Bridging. *Advanced Functional Materials*, **2013**, 23, n/a-n/a	15.6	5
31	On the Supramolecular Packing of High Electron Mobility Naphthalene Diimide Copolymers: The Perfect Registry of Asymmetric Branched Alkyl Side Chains. *Macromolecules*, **2013**, 46, 8171-8178	5.5	37
30	Roles of local and nonlocal electron-phonon couplings in triplet exciton diffusion in the anthracene crystal. *Physical Review B*, **2013**, 88,	3.3	16
29	Exploring the energy landscape of the charge transport levels in organic semiconductors at the molecular scale. *Accounts of Chemical Research*, **2013**, 46, 434-43	24.3	59
28	Free radical scavenging by natural polyphenols: atom versus electron transfer. *Journal of Physical Chemistry A*, **2013**, 117, 2082-92	2.8	172
27	Charge-transfer excitations steer the Davydov splitting and mediate singlet exciton fission in pentacene. *Physical Review Letters*, **2013**, 110, 226402	7.4	217
26	Conjugated poly(azomethine)s via simple one-step polycondensation chemistry: synthesis, thermal and optoelectronic properties. *Polymer Chemistry*, **2013**, 4, 4182	4.9	37
25	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. *Journal of Chemical Physics*, **2013**, 138, 204304	3.9	17
24	Unraveling the mechanism of molecular doping in organic semiconductors. *Advanced Materials*, **2012**, 24, 1535-9	24	101
23	Asymmetric electron and hole transport in a high-mobility n-type conjugated polymer. *Physical Review B*, **2012**, 86,	3.3	58

22	Reliable DFT-based estimates of cohesive energies of organic solids: the anthracene crystal. *Journal of Chemical Physics*, **2012**, 137, 194311	3.9	12
21	Polarizability and internal charge transfer in thiophene-triphenylamine hybrid π-conjugated systems. *Journal of Physical Chemistry B*, **2011**, 115, 9379-86	3.4	48
20	Hall-effect measurements probing the degree of charge-carrier delocalization in solution-processed crystalline molecular semiconductors. *Physical Review Letters*, **2011**, 107, 066601	7.4	94
19	Electronic and structural characterisation of a tetrathiafulvalene compound as a potential candidate for ambipolar transport properties. *CrystEngComm*, **2011**, 13, 6597	3.3	16
18	The nature of singlet excitons in oligoacene molecular crystals. *Journal of Chemical Physics*, **2011**, 134, 204703	3.9	208
17	Electron-Withdrawing Substituted Tetrathiafulvalenes as Ambipolar Semiconductors. *Chemistry of Materials*, **2011**, 23, 851-861	9.6	29
16	Supramolecular organization and charge transport properties of self-assembled π-stacks of perylene diimide dyes. *Journal of Physical Chemistry B*, **2011**, 115, 5593-603	3.4	43
15	Benzodicarbomethoxytetrathiafulvalene derivatives as soluble organic semiconductors. *Journal of Organic Chemistry*, **2011**, 76, 154-63	4.2	15
14	Structural and Charge-Transport Properties of a Liquid-Crystalline 2,5-Disubstituted Thiophene Derivative: A Joint Experimental and Theoretical Study. *Journal of Physical Chemistry C*, **2010**, 114, 4617-4627	3.8	17
13	Molecular packing and charge transport parameters in crystalline organic semiconductors from first-principles calculations. *Physical Chemistry Chemical Physics*, **2010**, 12, 9381-8	3.6	56
12	Theoretical characterization of charge transport in one-dimensional collinear arrays of organic conjugated molecules. *ChemPhysChem*, **2010**, 11, 1062-8	3.2	34
11	Deposition of Functional Organic Thin Films by Pulsed Plasma Polymerization: A Joint Theoretical and Experimental Study. *Plasma Processes and Polymers*, **2010**, 7, 172-181	3.4	47
10	Modeling Polymer Dielectric/Pentacene Interfaces: On the Role of Electrostatic Energy Disorder on Charge Carrier Mobility. *Advanced Functional Materials*, **2009**, 19, 3254-3261	15.6	72
9	Influence of intermolecular vibrations on the electronic coupling in organic semiconductors: the case of anthracene and perfluoropentacene. *ChemPhysChem*, **2009**, 10, 2265-73	3.2	69
8	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	
7	Theoretical characterization of the structural and hole transport dynamics in liquid-crystalline phthalocyanine stacks. *Journal of Physical Chemistry B*, **2009**, 113, 14102-11	3.4	82
6	Charge Transport in Conjugated Materials: From Theoretical Models to Experimental Systems. *AIP Conference Proceedings*, **2008**,	0	2
5	Depolarization Effects in Self-Assembled Monolayers: A Quantum-Chemical Insight. *Advanced Functional Materials*, **2007**, 17, 1143-1148	15.6	96

4	Charge transport in organic semiconductors. *Chemical Reviews*, **2007**, 107, 926-52	68.1	3363
3	Charge hopping in organic semiconductors: influence of molecular parameters on macroscopic mobilities in model one-dimensional stacks. *Journal of Physical Chemistry A*, **2006**, 110, 6356-64	2.8	139
2	Photoluminescence and Electrochemiluminescence of Thermally Activated Delayed Fluorescence (TADF) Emitters Containing Diphenylphosphine Chalcogenide-Substituted Carbazole Donors. *Journal of Materials Chemistry C*,	7.1	3
1	Substitution Effects on a New Pyridylbenzimidazole Acceptor for Thermally Activated Delayed Fluorescence and Their Use in Organic Light-Emitting Diodes. *Advanced Optical Materials*,2100846	8.1	0