Yoan Olivier

List of Publications by Year in descending order

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117	11,685	38742 50	27406 106
papers	citations	h-index	g-index

123	123	123	11917
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Violation of Hundâ€™s rule in molecules: Predicting the excited-state energy inversion by TD-DFT with double-hybrid methods. Journal of Chemical Physics, 2022, 156, 034105.	3.0	26
2	Diindolocarbazole â€“ achieving multiresonant thermally activated delayed fluorescence without the need for acceptor units. Materials Horizons, 2022, 9, 1068-1080.	12.2	48
3	An S-shaped double helicene showing both multi-resonance thermally activated delayed fluorescence and circularly polarized luminescence. Journal of Materials Chemistry C, 2022, 10, 4861-4870.	5.5	23
4	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.	7.4	30
5	Enhancing Thermally Activated Delayed Fluorescence by Fine-Tuning the Dendron Donor Strength. Journal of Physical Chemistry B, 2022, 126, 552-562.	2.6	7
6	Tuning Short Contacts between Polymer Chains To Enhance Charge Transport in Amorphous Donorâ€“Acceptor Polymers. Journal of Physical Chemistry C, 2022, 126, 3118-3126.	3.1	8
7	Photoluminescence and electrochemiluminescence of thermally activated delayed fluorescence (TADF) emitters containing diphenylphosphine chalcogenide-substituted carbazole donors. Journal of Materials Chemistry C, 2022, 10, 4646-4667.	5.5	20
8	Excited-State Modulation in Donor-Substituted Multiresonant Thermally Activated Delayed Fluorescence Emitters. ACS Applied Materials & Interfaces, 2022, 14, 22341-22352.	8.0	47
9	Multi-Edge Resonant Tender X-ray Diffraction for Probing the Crystalline Packing of Conjugated Polymers. Macromolecules, 2022, 55, 4733-4741.	4.8	4
10	Dynamic self-stabilization in the electronic and nanomechanical properties of an organic polymer semiconductor. Nature Communications, 2022, 13, .	12.8	14
11	Emission and Absorption Tuning in TADF B,Nâ€Doped Heptacenes: Toward Idealâ€Blue Hyperfluorescent OLEDs. Advanced Optical Materials, 2022, 10, .	7.3	28
12	Modeling of Multiresonant Thermally Activated Delayed Fluorescence Emittersâ”€Properly Accounting for Electron Correlation Is Key!. Journal of Chemical Theory and Computation, 2022, 18, 4903-4918.	5.3	32
13	Singletâ€Triplet Excitedâ€State Inversion in Heptazine and Related Molecules: Assessment of TDâ€DFT and ab initio Methods. ChemPhysChem, 2021, 22, 553-560.	2.1	45
14	Negative Singletâ€“Triplet Excitation Energy Gap in Triangle-Shaped Molecular Emitters for Efficient Triplet Harvesting. Journal of Physical Chemistry A, 2021, 125, 513-522.	2.5	41
15	Analysis of External and Internal Disorder to Understand Bandâ€Like Transport in nâ€Type Organic Semiconductors. Advanced Materials, 2021, 33, 2007870.	21.0	24
16	19â€2: Invited Paper: 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
17	Hypsochromic Shift of Multipleâ€Resonanceâ€Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. Angewandte Chemie - International Edition, 2021, 60, 17910-17914.	13.8	152
18	Hypsochromic Shift of Multipleâ€Resonanceâ€Induced Thermally Activated Delayed Fluorescence by Oxygen Atom Incorporation. Angewandte Chemie, 2021, 133, 18054-18058.	2.0	39

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19	Identification of the Key Parameters for Horizontal Transition Dipole Orientation in Fluorescent and TADF Organic Lightâ€Emitting Diodes. Advanced Materials, 2021, 33, e2100677.	21.0	99
20	Substitution Effects on a New Pyridylbenzimidazole Acceptor for Thermally Activated Delayed Fluorescence and Their Use in Organic Lightâ€Emitting Diodes. Advanced Optical Materials, 2021, 9, 2100846.	7.3	6
21	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.	8.0	15
22	peri-Acenoacene molecules: tuning of the singlet and triplet excitation energies by modifying their radical character. Physical Chemistry Chemical Physics, 2021, 23, 24016-24028.	2.8	5
23	Spontaneous exciton dissociation enables spin state interconversion in delayed fluorescence organic semiconductors. Nature Communications, 2021, 12, 6640.	12.8	18
24	Intramolecular Borylation via Sequential Bâ^'Mes Bond Cleavage for the Divergent Synthesis of B,N,Bâ€Doped Benzo[4]helicenes. Angewandte Chemie - International Edition, 2020, 59, 3156-3160.	13.8	90
25	Divergente Synthese von B,N,Bâ€Benzo[4]helicenen durch intramolekulare Borylierung unter sequenzieller Bâ€Mesâ€Bindungsspaltung. Angewandte Chemie, 2020, 132, 3181-3185.	2.0	30
26	Improving Processability and Efficiency of Resonant TADF Emitters: A Design Strategy. Advanced Optical Materials, 2020, 8, 1901627.	7.3	182
27	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.	5.5	15
28	Luminescent Dinuclear Copper(I) Complexes Bearing an Imidazolylpyrimidine Bridging Ligand. Inorganic Chemistry, 2020, 59, 14772-14784.	4.0	26
29	Carbeneâ€“Metalâ€“Amide Polycrystalline Materials Feature Blue Shifted Energy yet Unchanged Kinetics of Emission. Chemistry of Materials, 2020, 32, 4743-4753.	6.7	25
30	The design of an extended multiple resonance TADF emitter based on a polycyclic amine/carbonyl system. Materials Chemistry Frontiers, 2020, 4, 2018-2022.	5.9	81
31	Multiresonant Thermally Activated Delayed Fluorescence Emitters Based on Heteroatomâ€Doped Nanographenes: Recent Advances and Prospects for Organic Lightâ€Emitting Diodes. Advanced Functional Materials, 2020, 30, 1908677.	14.9	385
32	A Deep Blue B,N-Doped Heptacene Emitter That Shows Both Thermally Activated Delayed Fluorescence and Delayed Fluorescence by Tripletâ€“Triplet Annihilation. Journal of the American Chemical Society, 2020, 142, 6588-6599.	13.7	189
33	Computational Studies of Molecular Materials for Unconventional Energy Conversion: The Challenge of Light Emission by Thermally Activated Delayed Fluorescence. Molecules, 2020, 25, 1006.	3.8	18
34	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.	5.5	27
35	Tuning conformation, assembly, and charge transport properties of conjugated polymers by printing flow. Science Advances, 2019, 5, eaaw7757.	10.3	105
36	Crossed 2D versus Slipped 1D Ï€â€Stacking in Polymorphs of Crystalline Organic Thin Films: Impact on the Electronic and Optical Response. Advanced Optical Materials, 2019, 7, 1900749.	7.3	13

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37	Resilience to Conformational Fluctuations Controls Energetic Disorder in Conjugated Polymer Materials: Insights from Atomistic Simulations. Chemistry of Materials, 2019, 31, 6889-6899.	6.7	30
38	Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules. Nature Communications, 2019, 10, 597.	12.8	253
39	Multiple Charge Transfer States in Donorâ€“Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. Chemistry of Materials, 2019, 31, 6808-6817.	6.7	20
40	Polaron spin dynamics in high-mobility polymeric semiconductors. Nature Physics, 2019, 15, 814-822.	16.7	40
41	Short contacts between chains enhancing luminescence quantum yields and carrier mobilities in conjugated copolymers. Nature Communications, 2019, 10, 2614.	12.8	60
42	Impact of structural anisotropy on electro-mechanical response in crystalline organic semiconductors. Journal of Materials Chemistry C, 2019, 7, 4382-4391.	5.5	10
43	Photoluminescence Quenching Probes Spin Conversion and Exciton Dynamics in Thermally Activated Delayed Fluorescence Materials. Advanced Materials, 2019, 31, e1804490.	21.0	31
44	Comprehensive modelling study of singlet exciton diffusion in donorâ€“acceptor dyads: when small changes in chemical structure matter. Physical Chemistry Chemical Physics, 2019, 21, 25023-25034.	2.8	14
45	Robust singlet fission in pentacene thin films with tuned charge transfer interactions. Nature Communications, 2018, 9, 954.	12.8	76
46	Carbeneâ€“Metalâ€“Amide Bond Deformation, Rather Than Ligand Rotation, Drives Delayed Fluorescence. Journal of Physical Chemistry Letters, 2018, 9, 1620-1626.	4.6	57
47	Unusual electromechanical response in rubrene single crystals. Materials Horizons, 2018, 5, 41-50.	12.2	28
48	Nâ€doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. International Journal of Quantum Chemistry, 2018, 118, e25562.	2.0	9
49	Application of Rubrene Air-Gap Transistors as Sensitive MEMS Physical Sensors. ACS Applied Materials & Interfaces, 2018, 10, 41570-41577.	8.0	10
50	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. Journal of Physical Chemistry Letters, 2018, 9, 6149-6163.	4.6	121
51	Deep-Blue Oxadiazole-Containing Thermally Activated Delayed Fluorescence Emitters for Organic Light-Emitting Diodes. ACS Applied Materials & Interfaces, 2018, 10, 33360-33372.	8.0	67
52	20â€1: Invited Paper: Towards Deepâ€Blue Materials with Efficient Triplet Harvesting. Digest of Technical Papers SID International Symposium, 2018, 49, 239-242.	0.3	1
53	Vibrationally Assisted Intersystem Crossing in Benchmark Thermally Activated Delayed Fluorescence Molecules. Journal of Physical Chemistry Letters, 2018, 9, 4053-4058.	4.6	69
54	Collective molecular switching in hybrid superlattices for light-modulated two-dimensional electronics. Nature Communications, 2018, 9, 2661.	12.8	53

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55	Donorâ€“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.	7.4	64
56	Ultrafast Excitonâ€toâ€Polaron Conversion in Densely Packed Small Organic Semiconducting Molecules. Advanced Optical Materials, 2017, 5, 1700024.	7.3	16
57	Estimation of Ï€â€“Ï€ Electronic Couplings from Current Measurements. Nano Letters, 2017, 17, 3215-3224.	9.1	35
58	Periodic potentials in hybrid van der Waals heterostructures formed by supramolecular lattices on graphene. Nature Communications, 2017, 8, 14767.	12.8	68
59	Dynamic nature of excited states of donorâ€“acceptor TADF materials for OLEDs: how theory can reveal structureâ€“property relationships. Journal of Materials Chemistry C, 2017, 5, 5718-5729.	5.5	97
60	Measurements of Ambipolar Seebeck Coefficients in Highâ€Mobility Diketopyrrolopyrrole Donorâ€“Acceptor Copolymers. Advanced Electronic Materials, 2017, 3, 1700225.	5.1	26
61	Pressure sensor based on organic single crystal air-gap transistor. , 2017, , .		1
62	Highly Luminescent 2Dâ€Type Slab Crystals Based on a Molecular Chargeâ€Transfer Complex as Promising Organic Lightâ€Emitting Transistor Materials. Advanced Materials, 2017, 29, 1701346.	21.0	111
63	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. Physical Review Materials, 2017, 1, .	2.4	102
64	Temperature Dependence of Charge Localization in Highâ€Mobility, Solutionâ€Crystallized Small Molecule Semiconductors Studied by Charge Modulation Spectroscopy. Advanced Functional Materials, 2016, 26, 2326-2333.	14.9	29
65	Unraveling Unprecedented Charge Carrier Mobility through Structure Property Relationship of Four Isomers of Didodecyl[1]benzothieno[3,2â€b][1]benzothiophene. Advanced Materials, 2016, 28, 7106-7114.	21.0	138
66	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 rgBT /Overlock 10 Tf 5	21.0	0
67	Electronic Structure and Charge Transport in Nanostripped Graphene. Journal of Physical Chemistry C, 2016, 120, 20024-20032.	3.1	10
68	Liquid-Phase Exfoliation of Graphite into Single- and Few-Layer Graphene with Î±-Functionalized Alkanes. Journal of Physical Chemistry Letters, 2016, 7, 2714-2721.	4.6	73
69	Charge Separation and Recombination at Polymerâ€“Fullerene Heterojunctions: Delocalization and Hybridization Effects. Journal of Physical Chemistry Letters, 2016, 7, 536-540.	4.6	93
70	Do charges delocalize over multiple molecules in fullerene derivatives?. Journal of Materials Chemistry C, 2016, 4, 3747-3756.	5.5	44
71	Ultrafast Charge Dynamics in Novel Star-Shaped Small Molecules: the Effect of Donor and Acceptor Groups. , 2016, , .		0
72	First-Principles Quantum Dynamics of Singlet Fission: Coherent versus Thermally Activated Mechanisms Governed by Molecular<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï€</mml:mi></mml:math>Stacking. Physical Review Letters, 2015, 115, 107401.	7.8	137

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73	Theoretical Rationalization of the Singletâ€“Triplet Gap in OLEDs Materials: Impact of Charge-Transfer Character. Journal of Chemical Theory and Computation, 2015, 11, 168-177.	5.3	108
74	Determining the cohesive energy of coronene by dispersion-corrected DFT methods: Periodic boundary conditions vs. molecular pairs. Journal of Chemical Physics, 2015, 142, 054702.	3.0	10
75	Bis(arylene-ethynylene)-s-tetrazines: A Promising Family of n-Type Organic Semiconductors?. Journal of Physical Chemistry C, 2015, 119, 18945-18955.	3.1	18
76	Cost-Effective Force Field Tailored for Solid-Phase Simulations of OLED Materials. Journal of Chemical Theory and Computation, 2015, 11, 3383-3392.	5.3	17
77	Bulky Endâ€Capped [1]Benzothieno[3,2â€b]benzothiophenes: Reaching Highâ€Mobility Organic Semiconductors by Fine Tuning of the Crystalline Solidâ€State Order. Advanced Materials, 2015, 27, 3066-3072.	21.0	155
78	Ultrafast Charge Generation Pathways in Photovoltaic Blends Based on Novel Starâ€Shaped Conjugated Molecules. Advanced Energy Materials, 2015, 5, 1401657.	19.5	35
79	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.	5.5	62
80	25th Anniversary Article: Highâ€Mobility Hole and Electron Transport Conjugated Polymers: How Structure Defines Function. Advanced Materials, 2014, 26, 2119-2136.	21.0	199
81	Polymorphism in Bulk and Thin Films: The Curious Case of Dithiophene-DPP(Boc)-Dithiophene. Journal of Physical Chemistry C, 2014, 118, 657-669.	3.1	26
82	Charge Dissociation at Interfaces between Discotic Liquid Crystals: The Surprising Role of Column Mismatch. Journal of the American Chemical Society, 2014, 136, 2911-2920.	13.7	55
83	What Currently Limits Charge Carrier Mobility in Crystals of Molecular Semiconductors?. Israel Journal of Chemistry, 2014, 54, 595-620.	2.3	97
84	Quinquephenyl: The Simplest Rigidâ€Rodâ€Like Nematic Liquid Crystal, or is it? An Atomistic Simulation. ChemPhysChem, 2014, 15, 1345-1355.	2.1	30
85	Approaching disorder-free transport in high-mobility conjugated polymers. Nature, 2014, 515, 384-388.	27.8	844
86	Maximizing Singlet Fission by Intermolecular Packing. Journal of Physical Chemistry Letters, 2014, 5, 3345-3353.	4.6	135
87	Structure Influence on Charge Transport in Naphthalenediimideâ€“Thiophene Copolymers. Chemistry of Materials, 2014, 26, 6796-6804.	6.7	51
88	Tuning of the Photovoltaic Parameters of Molecular Donors by Covalent Bridging. Advanced Functional Materials, 2013, 23, 4854-4861.	14.9	20
89	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.	4.8	44
90	Roles of local and nonlocal electron-phonon couplings in triplet exciton diffusion in the anthracene crystal. Physical Review B, 2013, 88, .	3.2	22

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91	Exploring the Energy Landscape of the Charge Transport Levels in Organic Semiconductors at the Molecular Scale. Accounts of Chemical Research, 2013, 46, 434-443.	15.6	64
92	Free Radical Scavenging by Natural Polyphenols: Atom versus Electron Transfer. Journal of Physical Chemistry A, 2013, 117, 2082-2092.	2.5	224
93	Charge-Transfer Excitations Steer the Davydov Splitting and Mediate Singlet Exciton Fission in Pentacene. Physical Review Letters, 2013, 110, 226402.	7.8	253
94	Conjugated poly(azomethine)s via simple one-step polycondensation chemistry: synthesis, thermal and optoelectronic properties. Polymer Chemistry, 2013, 4, 4182.	3.9	41
95	Obtaining the lattice energy of the anthracene crystal by modern yet affordable first-principles methods. Journal of Chemical Physics, 2013, 138, 204304.	3.0	17
96	Asymmetric electron and hole transport in a high-mobility<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type conjugated polymer. Physical Review B, 2012, 86, .	3.2	63
97	Reliable DFT-based estimates of cohesive energies of organic solids: The anthracene crystal. Journal of Chemical Physics, 2012, 137, 194311.	3.0	12
98	Unraveling the Mechanism of Molecular Doping in Organic Semiconductors. Advanced Materials, 2012, 24, 1535-1539.	21.0	114
99	Electronic and structural characterisation of a tetrathiafulvalene compound as a potential candidate for ambipolar transport properties. CrystEngComm, 2011, 13, 6597.	2.6	19
100	The nature of singlet excitons in oligoacene molecular crystals. Journal of Chemical Physics, 2011, 134, 204703.	3.0	233
101	Electron-Withdrawing Substituted Tetrathiafulvalenes as Ambipolar Semiconductors. Chemistry of Materials, 2011, 23, 851-861.	6.7	32
102	Supramolecular Organization and Charge Transport Properties of Self-Assembled Ï€â^Ï€ Stacks of Perylene Diimide Dyes. Journal of Physical Chemistry B, 2011, 115, 5593-5603.	2.6	54
103	Benzodicarbomethoxytetrathiafulvalene Derivatives as Soluble Organic Semiconductors. Journal of Organic Chemistry, 2011, 76, 154-163.	3.2	19
104	Polarizability and Internal Charge Transfer in Thiopheneâ€“Triphenylamine Hybrid Ï€-Conjugated Systems. Journal of Physical Chemistry B, 2011, 115, 9379-9386.	2.6	50
105	Hall-Effect Measurements Probing the Degree of Charge-Carrier Delocalization in Solution-Processed Crystalline Molecular Semiconductors. Physical Review Letters, 2011, 107, 066601.	7.8	101
106	Theoretical Characterization of Charge Transport in Oneâ€Dimensional Collinear Arrays of Organic Conjugated Molecules. ChemPhysChem, 2010, 11, 1062-1068.	2.1	37
107	Deposition of Functional Organic Thin Films by Pulsed Plasma Polymerization: A Joint Theoretical and Experimental Study. Plasma Processes and Polymers, 2010, 7, 172-181.	3.0	55
108	Structural and Charge-Transport Properties of a Liquid-Crystalline Î±,Ï‰-Disubstituted Thiophene Derivative: A Joint Experimental and Theoretical Study. Journal of Physical Chemistry C, 2010, 114, 4617-4627.	3.1	18

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109	Molecular packing and charge transport parameters in crystalline organic semiconductors from first-principles calculations. Physical Chemistry Chemical Physics, 2010, 12, 9381.	2.8	57
110	Modeling Polymer Dielectric/Pentacene Interfaces: On the Role of Electrostatic Energy Disorder on Charge Carrier Mobility. Advanced Functional Materials, 2009, 19, 3254-3261.	14.9	81
111	Influence of Intermolecular Vibrations on the Electronic Coupling in Organic Semiconductors: The Case of Anthracene and Perfluoropentacene. ChemPhysChem, 2009, 10, 2265-2273.	2.1	77
112	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.	2.1	0
113	Theoretical Characterization of the Structural and Hole Transport Dynamics in Liquid-Crystalline Phthalocyanine Stacks. Journal of Physical Chemistry B, 2009, 113, 14102-14111.	2.6	83
114	Charge Transport in Conjugated Materials: From Theoretical Models to Experimental Systems. AIP Conference Proceedings, 2008, , .	0.4	2
115	Depolarization Effects in Self-Assembled Monolayers: A Quantum-Chemical Insight. Advanced Functional Materials, 2007, 17, 1143-1148.	14.9	97
116	Charge Transport in Organic Semiconductors. Chemical Reviews, 2007, 107, 926-952.	47.7	3,853
117	Charge Hopping in Organic Semiconductors:Â Influence of Molecular Parameters on Macroscopic Mobilities in Model One-Dimensional Stacks. Journal of Physical Chemistry A, 2006, 110, 6356-6364.	2.5	155