Claudine Katan

List of Publications by Year
in descending order

161	15,896	25423 59	18944 123
papers	citations	h-index	g-index

167	167	167	15099
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Light-activated interlayer contraction in two-dimensional perovskites for high-efficiency solar cells. Nature Nanotechnology, 2022, 17, 45-52.	15.6	52
2	Expanding the Cage of 2D Bromide Perovskites by Large A-Site Cations. Chemistry of Materials, 2022, 34, 1132-1142.	3.2	22
3	Pseudospin-phonon pretransitional dynamics in lead halide hybrid perovskites. Physical Review B, 2022, 105, .	1.1	5
4	Band gap, effective masses, and energy level alignment of 2D and 3D halide perovskites and heterostructures using DFT-1/2. Physical Review Materials, 2022, 6, .	0.9	13
5	A Theoretical Framework for Microscopic Surface and Interface Dipoles, Work Functions, and Valence Band Alignments in 2D and 3D Halide Perovskite Heterostructures. ACS Energy Letters, 2022, 7, 349-357.	8.8	17
6	Tolerance Factor for Stabilizing 3D Hybrid Halide Perovskitoids Using Linear Diammonium Cations. Journal of the American Chemical Society, 2022, 144, 3902-3912.	6.6	36
7	Pb-free halide perovskites for solar cells, light-emitting diodes, and photocatalysts. APL Materials, 2022, 10, .	2.2	11
8	Synthesis and Characterization of (FA)₃(HEA)₂Pb₃I₁₁: A Rare Example of <1 1 0>-Oriented Multilayered Halide Perovskites. Chemistry of Materials, 2022, 34, 5780-5790.	3.2	2
9	Ordered Mixed-Spacer 2D Bromide Perovskites and the Dual Role of 1,2,4-Triazolium Cation. Chemistry of Materials, 2022, 34, 6541-6552.	3.2	5
10	Effect of protonation on the photophysical properties of 4-substituted and 4,7-disubstituted quinazoline push-pull chromophores. Dyes and Pigments, 2021, 185, 108948.	2.0	17
11	Influence of (de)protonation on the photophysical properties of phenol-substituted diazine chromophores: experimental and theoretical studies. New Journal of Chemistry, 2021, 45, 19132-19144.	1.4	2
12	Tetrazine molecules as an efficient electronic diversion channel in 2D organicâ€“inorganic perovskites. Materials Horizons, 2021, 8, 1547-1560.	6.4	24
13	DFT Simulations as Valuable Tool to Support NMR Characterization of Halide Perovskites: the Case of Pure and Mixed Halide Perovskites. Helvetica Chimica Acta, 2021, 104, e2000231.	1.0	8
14	Memory Seeds Enable High Structural Phase Purity in 2D Perovskite Films for Highâ€Efficiency Devices. Advanced Materials, 2021, 33, e2007176.	11.1	50
15	Bismuth/Silver-Based Two-Dimensional Iodide Double and One-Dimensional Bi Perovskites: Interplay between Structural and Electronic Dimensions. Chemistry of Materials, 2021, 33, 6206-6216.	3.2	27
16	m-Phenylenediammonium as a New Spacer for Dionâ€“Jacobson Two-Dimensional Perovskites. Journal of the American Chemical Society, 2021, 143, 12063-12073.	6.6	71
17	High-phase purity two-dimensional perovskites with 17.3% efficiency enabled by interface engineering of hole transport layer. Cell Reports Physical Science, 2021, 2, 100601.	2.8	17
18	From Zero- to One-Dimensional, Opportunities and Caveats of Hybrid Iodobismuthates for Optoelectronic Applications. Inorganic Chemistry, 2021, 60, 17123-17131.	1.9	13

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19	Electronic structure and stability of Cs2TiX6 and Cs2ZrX6 (X = Br, I) vacancy ordered double perovskites. Applied Physics Letters, 2021, 119, .	1.5	28
20	Nonadiabatic molecular dynamics analysis of hybrid Dionâ€“Jacobson 2D leads iodide perovskites. Applied Physics Letters, 2021, 119, .	1.5	9
21	A 3D Lead Iodide Hybrid Based on a 2D Perovskite Subnetwork. Crystals, 2021, 11, 1570.	1.0	2
22	Interstitial Nature of Mn²⁺ Doping in 2D Perovskites. ACS Nano, 2021, 15, 20550-20561.	7.3	19
23	Importance of Vacancies and Doping in the Hole-Transporting Nickel Oxide Interface with Halide Perovskites. ACS Applied Materials & Interfaces, 2020, 12, 6633-6640.	4.0	21
24	Charge carrier dynamics in two-dimensional hybrid perovskites: Dionâ€“Jacobson vs. Ruddlesdenâ€“Popper phases. Journal of Materials Chemistry A, 2020, 8, 22009-22022.	5.2	72
25	Negative Pressure Engineering with Large Cage Cations in 2D Halide Perovskites Causes Lattice Softening. Journal of the American Chemical Society, 2020, 142, 11486-11496.	6.6	84
26	Three-Dimensional Lead Iodide Perovskitoid Hybrids with High X-ray Photoresponse. Journal of the American Chemical Society, 2020, 142, 6625-6637.	6.6	82
27	Pushâ€“Pull (Iso)quinoline Chromophores: Synthesis, Photophysical Properties, and Use for Whiteâ€Light Emission. Chemistry - A European Journal, 2020, 26, 8153-8161.	1.7	23
28	Cation Engineering in Two-Dimensional Ruddlesdenâ€“Popper Lead Iodide Perovskites with Mixed Large A-Site Cations in the Cages. Journal of the American Chemical Society, 2020, 142, 4008-4021.	6.6	101
29	Control of Crystal Symmetry Breaking with Halogen-Substituted Benzylammonium in Layered Hybrid Metal-Halide Perovskites. Journal of the American Chemical Society, 2020, 142, 5060-5067.	6.6	65
30	Effects of Chlorine Mixing on Optoelectronics, Ion Migration, and Gamma-Ray Detection in Bromide Perovskites. Chemistry of Materials, 2020, 32, 1854-1863.	3.2	46
31	Branching effect on the linear and nonlinear optical properties of styrylpyrimidines. Physical Chemistry Chemical Physics, 2020, 22, 4165-4176.	1.3	16
32	Direct evidence of weakly dispersed and strongly anharmonic optical phonons in hybrid perovskites. Communications Physics, 2020, 3, .	2.0	49
33	Organic Cation Alloying on Intralayer A and Interlayer Aâ€™ sites in 2D Hybrid Dionâ€“Jacobson Lead Bromide Perovskites (Aâ€™)(A)Pb₂Br₇. Journal of the American Chemical Society, 2020, 142, 8342-8351.	6.6	64
34	Physical properties of bulk, defective, 2D and 0D metal halide perovskite semiconductors from a symmetry perspective. JPhys Materials, 2020, 3, 042001.	1.8	29
35	Two-Dimensional Dionâ€“Jacobson Hybrid Lead Iodide Perovskites with Aromatic Diammonium Cations. Journal of the American Chemical Society, 2019, 141, 12880-12890.	6.6	241
36	Tuning Electronic Structure in Layered Hybrid Perovskites with Organic Spacer Substitution. Nano Letters, 2019, 19, 8732-8740.	4.5	41

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37	Halide Perovskite High-k Field Effect Transistors with Dynamically Reconfigurable Ambipolarity. , 2019, 1, 633-640.		29
38	Halide Perovskites: Low Dimensions for Devices. ACS Energy Letters, 2019, 4, 2902-2904.	8.8	0
39	Seven-Layered 2D Hybrid Lead Iodide Perovskites. CheM, 2019, 5, 2593-2604.	5.8	79
40	Efficient and accurate calculation of band gaps of halide perovskites with the Tran-Blaha modified Becke-Johnson potential. Physical Review B, 2019, 99, .	1.1	61
41	Cation Alloying Delocalizes Polarons in Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 3516-3524.	2.1	33
42	From 2D to 1D Electronic Dimensionality in Halide Perovskites with Stepped and Flat Layers Using Propylammonium as a Spacer. Journal of the American Chemical Society, 2019, 141, 10661-10676.	6.6	66
43	Charge Trap Formation and Passivation in Methylammonium Lead Tribromide. Journal of Physical Chemistry C, 2019, 123, 13812-13817.	1.5	9
44	Enhanced Stability and Band Gap Tuning of Î±-[HC(NH₂)₂]PbI₃ Hybrid Perovskite by Large Cation Integration. ACS Applied Materials & Interfaces, 2019, 11, 20743-20751.	4.0	52
45	Small Cyclic Diammonium Cation Templated (110)-Oriented 2D Halide (X = I, Br, Cl) Perovskites with White-Light Emission. Chemistry of Materials, 2019, 31, 3582-3590.	3.2	101
46	Guanidinium and Mixed Cesiumâ€“Guanidinium Tin(II) Bromides: Effects of Quantum Confinement and Out-of-Plane Octahedral Tilting. Chemistry of Materials, 2019, 31, 2121-2129.	3.2	24
47	The importance of relativistic effects on two-photon absorption spectra in metal halide perovskites. Nature Communications, 2019, 10, 5342.	5.8	30
48	Electronic properties of Pb-I deficient lead halide perovskites. Journal of Chemical Physics, 2019, 151, 234704.	1.2	7
49	Structural and thermodynamic limits of layer thickness in 2D halide perovskites. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 58-66.	3.3	236
50	Quantum and Dielectric Confinement Effects in Lower-Dimensional Hybrid Perovskite Semiconductors. Chemical Reviews, 2019, 119, 3140-3192.	23.0	525
51	Influence of Disorder and Anharmonic Fluctuations on the Dynamical Rashba Effect in Purely Inorganic Lead-Halide Perovskites. Journal of Physical Chemistry C, 2019, 123, 291-298.	1.5	32
52	Hybrid Dionâ€“Jacobson 2D Lead Iodide Perovskites. Journal of the American Chemical Society, 2018, 140, 3775-3783.	6.6	686
53	Density of States Broadening in CH₃NH₃PbI₃ Hybrid Perovskites Understood from ab Initio Molecular Dynamics Simulations. ACS Energy Letters, 2018, 3, 787-793.	8.8	28
54	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. ACS Nano, 2018, 12, 3321-3332.	7.3	146

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55	On the contribution of f electrons to the quadratic hyperpolarizability: the case of lanthanide terpyridyl complexes. Physical Chemistry Chemical Physics, 2018, 20, 7401-7406.	1.3	2
56	Entropy in halide perovskites. Nature Materials, 2018, 17, 377-379.	13.3	82
57	Enhancement of Pushâ€“Pull Properties of Pentafulvene and Pentafulvalene Derivatives by Protonation at Carbon. European Journal of Organic Chemistry, 2018, 2018, 739-749.	1.2	7
58	Computational analysis of hybrid perovskite on silicon 2-T tandem solar cells based on a Si tunnel junction. Optical and Quantum Electronics, 2018, 50, 1.	1.5	26
59	Anharmonicity and Disorder in the Black Phases of Cesium Lead Iodide Used for Stable Inorganic Perovskite Solar Cells. ACS Nano, 2018, 12, 3477-3486.	7.3	546
60	Does Rashba splitting in CH₃NH₃PbBr₃ arise from 2 Ã— 2 surface reconstruction?. Physical Chemistry Chemical Physics, 2018, 20, 9638-9643.	1.3	29
61	Critical Role of Interface and Crystallinity on the Performance and Photostability of Perovskite Solar Cell on Nickel Oxide. Advanced Materials, 2018, 30, 1703879.	11.1	198
62	Anharmonicity and Disorder in the Black Phases of CsPbI3 used for Stable Inorganic Perovskite Solar Cells. , 2018, , .		1
63	Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Substitution in Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 7130-7136.	2.1	52
64	Structural Diversity in White-Light-Emitting Hybrid Lead Bromide Perovskites. Journal of the American Chemical Society, 2018, 140, 13078-13088.	6.6	351
65	Two-Dimensional Halide Perovskites Incorporating Straight Chain Symmetric Diammonium Ions, (NH₃C_mH_{2m}NH₃)(CH₃NH₃)_{n-1} (m = 4â€“9; n = 1â€“4). Journal of the American Chemical Society, 2018, 140, 12226-12238.	6.6	184
66	Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. Nano Letters, 2018, 18, 5603-5609.	4.5	103
67	Elastic Softness of Hybrid Lead Halide Perovskites. Physical Review Letters, 2018, 121, 085502.	2.9	116
68	Scaling law for excitons in 2D perovskite quantum wells. Nature Communications, 2018, 9, 2254.	5.8	559
69	Influence of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï€</mml:mi></mml:math> -conjugated cations and halogen substitution on the optoelectronic and excitonic properties of layered hybrid perovskites. Physical Review Materials, 2018, 2, .	0.9	24
70	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. Science, 2017, 355, 1288-1292.	6.0	830
71	Design and Synthesis of a Caged Carboxylic Acid with a Donorâ^Ï€â€“Donor Coumarin Structure: One-photon and Two-photon Uncaging Reactions Using Visible and Near-Infrared Lights. Organic Letters, 2017, 19, 2622-2625.	2.4	39
72	High Members of the 2D Ruddlesden-Popper Halide Perovskites: Synthesis, Optical Properties, and Solar Cells of (CH3(CH2)3NH3)2(CH3NH3)4Pb5I16. CheM, 2017, 2, 427-440.	5.8	354

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73	Computational design of high performance hybrid perovskite on silicon 2-T tandem solar cells based on a tunnel junction. , 2017, , .		2
74	Critical Fluctuations and Anharmonicity in Lead Iodide Perovskites from Molecular Dynamics Supercell Simulations. Journal of Physical Chemistry C, 2017, 121, 20729-20738.	1.5	62
75	Tunable White-Light Emission in Single-Cation-Templated Three-Layered 2D Perovskites (CH₃CH₂NH₃)₄Pb₃Br_{10â€“x}Cl_x Journal of the American Chemical Society, 2017, 139, 11956-11963.	6.6	349
76	New Type of 2D Perovskites with Alternating Cations in the Interlayer Space, (C(NH₂)₃)(CH₃NH₃)_nPb_nI_{3n} Structure, Properties, and Photovoltaic Performance. Journal of the American Chemical Society, 2017, 139, 16297-16309.	6.6	374
77	Decreasing the electronic confinement in layered perovskites through intercalation. Chemical Science, 2017, 8, 1960-1968.	3.7	114
78	A close examination of the structure and dynamics of HC(NH₂)₂PbI₃ by MD simulations and group theory. Physical Chemistry Chemical Physics, 2016, 18, 27109-27118.	1.3	48
79	Polaron Stabilization by Cooperative Lattice Distortion and Cation Rotations in Hybrid Perovskite Materials. Nano Letters, 2016, 16, 3809-3816.	4.5	245
80	Elastic Constants, Optical Phonons, and Molecular Relaxations in the High Temperature Plastic Phase of the CH₃NH₃PbBr₃ Hybrid Perovskite. Journal of Physical Chemistry Letters, 2016, 7, 3776-3784.	2.1	89
81	Design and Synthesis of a 4-Nitrobromobenzene Derivative Bearing an Ethylene Glycol Tetraacetic Acid Unit for a New Generation of Caged Calcium Compounds with Two-Photon Absorption Properties in the Near-IR Region and Their Application in Vivo. ACS Omega, 2016, 1, 193-201.	1.6	23
82	Multinuclear NMR as a tool for studying local order and dynamics in CH₃NH₃PbX₃ (X = Cl, Br, I) hybrid perovskites. Physical Chemistry Chemical Physics, 2016, 18, 27133-27142.	1.3	78
83	Symmetry-Based Tight Binding Modeling of Halide Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 3833-3840.	2.1	57
84	Design, Synthesis, and Reaction of Ï€-Extended Coumarin-based New Caged Compounds with Two-photon Absorption Character in the Near-IR Region. Chemistry Letters, 2016, 45, 1186-1188.	0.7	19
85	Vibronic coupling to simulate the phosphorescence spectra of Ir(III)-based OLED systems: TD-DFT results meet experimental data. Journal of Molecular Modeling, 2016, 22, 265.	0.8	11
86	Luminescence Behavior of Protonated Methoxy-Substituted Diazine Derivatives: Toward White Light Emission. Journal of Physical Chemistry C, 2016, 120, 26986-26995.	1.5	85
87	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. ACS Nano, 2016, 10, 9776-9786.	7.3	351
88	Light-activated photocurrent degradation and self-healing in perovskite solar cells. Nature Communications, 2016, 7, 11574.	5.8	584
89	Nonlinear optical properties of intriguing Ru Ïƒ-acetylide complexes and the use of a photocrosslinked polymer as a springboard to obtain SHG active thin films. Dalton Transactions, 2016, 45, 11052-11060.	1.6	19
90	Quantum confinement and dielectric profiles of colloidal nanoplatelets of halide inorganic and hybrid organicâ€“inorganic perovskites. Nanoscale, 2016, 8, 6369-6378.	2.8	136

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91	Theoretical insights into hybrid perovskites for photovoltaic applications. , 2016, , .		6
92	Carrier scattering processes and low energy phonon spectroscopy in hybrid perovskites crystals. Proceedings of SPIE, 2016, , .	0.8	10
93	Dielectric properties of hybrid perovskites and drift-diffusion modeling of perovskite cells. Proceedings of SPIE, 2016, , .	0.8	8
94	Theoretical studies of Rashba and Dresselhaus effects in hybrid organic-inorganic perovskites for optoelectronic applications. , 2016, , .		2
95	Molecular disorder and translation/rotation coupling in the plastic crystal phase of hybrid perovskites. Nanoscale, 2016, 8, 6222-6236.	2.8	119
96	Design and synthesis of a new chromophore, 2-(4-nitrophenyl)benzofuran, for two-photon uncaging using near-IR light. Chemical Communications, 2016, 52, 331-334.	2.2	41
97	Chapter 7. Electronic Properties of Metal Halide Perovskites. RSC Energy and Environment Series, 2016, , 202-233.	0.2	2
98	Non-degenerate two photon absorption enhancement for laser dyes by precise lock-in detection. AIP Advances, 2015, 5, 127138.	0.6	3
99	Interplay of spinâ€“orbit coupling and lattice distortion in metal substituted 3D tri-chloride hybrid perovskites. Journal of Materials Chemistry A, 2015, 3, 9232-9240.	5.2	101
100	Solid-State Physics Perspective on Hybrid Perovskite Semiconductors. Journal of Physical Chemistry C, 2015, 119, 10161-10177.	1.5	205
101	Photoisomerisation in Aminoazobenzeneâ€Substituted Ruthenium(II) Tris(bipyridine) Complexes: Influence of the Conjugation Pathway. Chemistry - A European Journal, 2015, 21, 8262-8270.	1.7	25
102	Theoretical insights into multibandgap hybrid perovskites for photovoltaic applications. , 2015, , .		0
103	Rashba and Dresselhaus Effects in Hybrid Organicâ€“Inorganic Perovskites: From Basics to Devices. ACS Nano, 2015, 9, 11557-11567.	7.3	304
104	Synthesis of a double-stranded spiroborate helicate bearing stilbene units and its photoresponsive behaviour. New Journal of Chemistry, 2015, 39, 3259-3269.	1.4	16
105	Density Functional Theory Simulations of Semiconductors for Photovoltaic Applications: Hybrid Organic-Inorganic Perovskites and III/V Heterostructures. International Journal of Photoenergy, 2014, 2014, 1-11.	1.4	23
106	Experimental and Theoretical Studies of Quadrupolar Oligothiopheneâ€Cored Chromophores Containing Dimesitylboryl Moieties as Ïâ€Accepting Endâ€Groups: Syntheses, Structures, Fluorescence, and Oneâ€and Twoâ€Photon Absorption. Chemistry - A European Journal, 2014, 20, 13618-13635.	1.7	84
107	Theoretical insights into multibandgap hybrid perovskites for photovoltaic applications. Proceedings of SPIE, 2014, , .	0.8	9
108	Analysis of Multivalley and Multibandgap Absorption and Enhancement of Free Carriers Related to Exciton Screening in Hybrid Perovskites. Journal of Physical Chemistry C, 2014, 118, 11566-11572.	1.5	463

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109	Electronic properties of 2D and 3D hybrid organic/inorganic perovskites for optoelectronic and photovoltaic applications. Optical and Quantum Electronics, 2014, 46, 1225-1232.	1.5	60
110	DFT and k Â· p modelling of the phase transitions of lead and tin halide perovskites for photovoltaic cells. Physica Status Solidi - Rapid Research Letters, 2014, 8, 31-35.	1.2	177
111	Comment on â€œDensity functional theory analysis of structural and electronic properties of orthorhombic perovskite CH3NH3PbI3â€•by Y. Wang et al., Phys. Chem. Chem. Phys., 2014, 16, 1424â€“1429. Physical Chemistry Chemical Physics, 2014, 16, 8697-8698.	1.3	13
112	Understanding Quantum Confinement of Charge Carriers in Layered 2D Hybrid Perovskites. ChemPhysChem, 2014, 15, 3733-3741.	1.0	211
113	Caged Glutamates with Ï€-Extended 1,2-Dihydronaphthalene Chromophore: Design, Synthesis, Two-Photon Absorption Property, and Photochemical Reactivity. Journal of Organic Chemistry, 2014, 79, 7822-7830.	1.7	33
114	Highâ€Yield Formation of Substituted Tetracyanobutadienes from Reaction of Ynamides with Tetracyanoethylene. Chemistry - A European Journal, 2014, 20, 9553-9557.	1.7	48
115	Absorption and fluorescence signatures of 1,2,3-triazole based regioisomers: challenging compounds for TD-DFT. Physical Chemistry Chemical Physics, 2014, 16, 9064-9073.	1.3	29
116	Importance of Spinâ€“Orbit Coupling in Hybrid Organic/Inorganic Perovskites for Photovoltaic Applications. Journal of Physical Chemistry Letters, 2013, 4, 2999-3005.	2.1	1,021
117	Vibrational properties of 2H-PbI2 semiconductors studied via Density Functional Theory calculations. Thin Solid Films, 2013, 541, 9-11.	0.8	6
118	Synthesis and photochemical reactivity of caged glutamates with a Ï€-extended coumarin chromophore as a photolabile protecting group. Tetrahedron Letters, 2013, 54, 7171-7174.	0.7	15
119	Nonâ€linear electroâ€elastic coupling in highly strained zincâ€blende compounds: InGaP/GaP [111] quantum wells. Physica Status Solidi (B): Basic Research, 2013, 250, 765-768.	0.7	0
120	Non-linear electro-elastic coupling in non-centrosymmetric materials. Journal of Physics: Conference Series, 2012, 367, 012005.	0.3	1
121	Electronic model for self-assembled hybrid organic/perovskite semiconductors: Reverse band edge electronic states ordering and spin-orbit coupling. Physical Review B, 2012, 86, .	1.1	173
122	On the entanglement of electrostriction and non-linear piezoelectricity in non-centrosymmetric materials. Applied Physics Letters, 2012, 100, .	1.5	29
123	30-band kâ‹…p method for quantum semiconductor heterostructures. Applied Physics Letters, 2011, 98, .	1.5	17
124	Two-photon transitions in triazole based quadrupolar and octupolar chromophores: a TD-DFT investigation. , 2010, , .		4
125	Simultaneous Control of Emission Localization and Two-Photon Absorption Efficiency in Dissymmetrical Chromophores. Journal of Physical Chemistry B, 2010, 114, 3152-3169.	1.2	52
126	Position Isomerism on One and Two Photon Absorption in Multibranched Chromophores: A TDDFT Investigation. Journal of Chemical Theory and Computation, 2010, 6, 3410-3426.	2.3	15

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127	The Synthesis and Oneâ€•and Twoâ€Photon Optical Properties of Dipolar, Quadrupolar and Octupolar Donorâ€“Acceptor Molecules Containing Dimesitylboryl Groups. Chemistry - A European Journal, 2009, 15, 198-208.	1.7	196
128	Novel chromophores from alternated pyridineâ€“ethylenedioxythiophene unit oligomers: dramatic enhancement of photoluminescence properties in elongated derivatives. Chemical Communications, 2009, , 692-694.	2.2	23
129	Enhanced Twoâ€Photon Absorption of Organic Chromophores: Theoretical and Experimental Assessments. Advanced Materials, 2008, 20, 4641-4678.	11.1	502
130	Inside Front Cover: Enhanced Twoâ€Photon Absorption of Organic Chromophores: Theoretical and Experimental Assessments (Adv. Mater. 24/2008). Advanced Materials, 2008, 20, .	11.1	2
131	DFT study of NLO properties of boroxine based octupolar molecules. Computational and Theoretical Chemistry, 2008, 866, 58-62.	1.5	15
132	On the accurate estimation of intermolecular interactions and charge transfer: the case of TTF-CA. Faraday Discussions, 2007, 135, 217-235.	1.6	64
133	Two-Photon Transitions in Quadrupolar and Branched Chromophores:â€‰ Experiment and Theory. Journal of Physical Chemistry B, 2007, 111, 9468-9483.	1.2	127
134	Synthesis, Fluorescence, and Two-Photon Absorption of a Series of Elongated Rodlike and Banana-Shaped Quadrupolar Fluorophores: A Comprehensive Study of Structureâ€“Property Relationships. Chemistry - A European Journal, 2007, 13, 1481-1498.	1.7	233
135	Effect of Branching on Two-Photon Absorption in Triphenylbenzene Derivatives. ChemPhysChem, 2007, 8, 723-734.	1.0	108
136	Charge Instability in Quadrupolar Chromophores:Â Symmetry Breaking and Solvatochromism. Journal of the American Chemical Society, 2006, 128, 15742-15755.	6.6	379
137	Effects of Dipolar Interactions on Linear and Nonlinear Optical Properties of Multichromophore Assemblies: A Case Study. Chemistry - A European Journal, 2006, 12, 3089-3102.	1.7	34
138	Designing a New Two-Dimensional Molecular Layout by Hydrogen Bonding. ChemPhysChem, 2006, 7, 82-85.	1.0	32
139	Nonlinear Optical Response and Photodynamics of Conjugated Molecules. , 2006, , 1266-1269.		0
140	Branching of dipolar chromophores: effects on linear and nonlinear optical properties. , 2005, , .		2
141	Effects of (Multi)branching of Dipolar Chromophores on Photophysical Properties and Two-Photon Absorption. Journal of Physical Chemistry A, 2005, 109, 3024-3037.	1.1	341
142	New chromophores from click chemistry for two-photon absorption and tuneable photoluminescence. Chemical Communications, 2005, , 2029.	2.2	79
143	Improved transparency-nonlinearity trade-off with boroxine-based octupolar molecules. , 2004, 5517, 26.		0
144	TWO-PHOTON ABSORPTION AND FLUORESCENCE WITH QUADRUPOLAR AND BRANCHED CHROMOPHORESâ€”EFFECT OF STRUCTURE AND BRANCHING. Journal of Nonlinear Optical Physics and Materials, 2004, 13, 451-460.	1.1	8

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145	Two-photon absorption and fluorescence in nanoscale multipolar chromophores: effect of dimensionality and charge-symmetry. Journal of Molecular Structure, 2004, 704, 17-24.	1.8	43
146	Accuracy of topological analysis of gridded electron densities. Journal of Physics and Chemistry of Solids, 2004, 65, 1951-1955.	1.9	10
147	Enhanced Two-Photon Absorption with Novel Octupolar Propeller-Shaped Fluorophores Derived from Triphenylamine. Organic Letters, 2004, 6, 47-50.	2.4	244
148	Theoretical Investigation of the Ground-State Properties of DMTTFâˆ’CA:Â A Step toward the Understanding of Charge Transfer Complexes Undergoing the Neutral-to-Ionic Phase Transition. Journal of Physical Chemistry A, 2004, 108, 11049-11055.	1.1	11
149	Nanoscale multipolar chromophores for optical limiting in the visible-NIR range based on multiphoton absorption. , 2004, , .		0
150	Synthesis and two-photon absorption of highly soluble three-branched fluorenylene-vinylene derivatives. Tetrahedron Letters, 2003, 44, 8121-8125.	0.7	103
151	Numerical computation of critical properties and atomic basins from three-dimensional grid electron densities. Journal of Applied Crystallography, 2003, 36, 65-73.	1.9	67
152	Improved transparencyâ€“nonlinearity trade-off with boroxine-based octupolar molecules. Chemical Communications, 2003, , 2766-2767.	2.2	63
153	Neutral-ionic phase transition:â€ƒA thoroughab initiostudy of TTF-CA. Physical Review B, 2003, 67, .	1.1	33
154	Intramolecular Electronic Redistribution Coupled to Hydrogen Bonding: An Important Mechanism for the â€œNeutral-to-Ionicâ€•Transition. Journal of Physical Chemistry A, 2001, 105, 4300-4307.	1.1	19
155	Charge-transfer variation caused by symmetry breaking in a mixed-stack organic compound: TTF-2, 5Cl2BQ. Journal of Physics Condensed Matter, 1999, 11, 4163-4177.	0.7	6
156	First-Principles Study of the Structures and Vibrational Frequencies for Tetrathiafulvalene TTF and TTF-d4 in Different Oxidation States. Journal of Physical Chemistry A, 1999, 103, 1407-1413.	1.1	47
157	First principles investigations of a â€œquasi-one-dimensionalâ€•charge-transfer molecular crystal: TTF-2,5Cl2BQ. Computational Materials Science, 1998, 10, 325-329.	1.4	5
158	Ab-initio calculations of one-dimensional band structures of mixed-stack molecular crystals. Solid State Communications, 1997, 102, 589-594.	0.9	19
159	First-principles molecular-dynamics simulations for neutralp-chloranil and its radical anion. Physical Review B, 1996, 53, 12112-12120.	1.1	33
160	Theoretical description of two-photon phase conjugation in polar molecules. Physical Review A, 1993, 48, 1564-1572.	1.0	18
161	Effects of permanent dipole moments in degenerate four-wave-mixing processes. Physical Review A, 1991, 44, 5947-5957.	1.0	26