Claudine Katan

List of Publications by Year
in descending order

161	15,896	22132	16636
papers	citations	59 h-index	123 g-index

167	167	167	13129
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. Science, 2017, 355, 1288-1292.	6.0	830
3	Hybrid Dionâ€“Jacobson 2D Lead Iodide Perovskites. Journal of the American Chemical Society, 2018, 140, 3775-3783.	6.6	686
4	Light-activated photocurrent degradation and self-healing in perovskite solar cells. Nature Communications, 2016, 7, 11574.	5.8	584
5	Scaling law for excitons in 2D perovskite quantum wells. Nature Communications, 2018, 9, 2254.	5.8	559
6	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
7	Quantum and Dielectric Confinement Effects in Lower-Dimensional Hybrid Perovskite Semiconductors. Chemical Reviews, 2019, 119, 3140-3192.	23.0	525
8	Enhanced Twoâ€Photon Absorption of Organic Chromophores: Theoretical and Experimental Assessments. Advanced Materials, 2008, 20, 4641-4678.	11.1	502
9	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
10	Charge Instability in Quadrupolar Chromophores:Â Symmetry Breaking and Solvatochromism. Journal of the American Chemical Society, 2006, 128, 15742-15755.	6.6	379
11	New Type of 2D Perovskites with Alternating Cations in the Interlayer Space, (C(NH₂)₃)(CH₃NH₃)_nPb_nI<sub>3n Structure, Properties, and Photovoltaic Performance. Journal of the American Chemical Society, 2017, 139, 16297-16309.	6.6	374
12	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
13	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. ACS Nano, 2016, 10, 9776-9786.	7.3	351
14	Structural Diversity in White-Light-Emitting Hybrid Lead Bromide Perovskites. Journal of the American Chemical Society, 2018, 140, 13078-13088.	6.6	351
15	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
16	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
17	Rashba and Dresselhaus Effects in Hybrid Organicâ€“Inorganic Perovskites: From Basics to Devices. ACS Nano, 2015, 9, 11557-11567.	7.3	304
18	Polaron Stabilization by Cooperative Lattice Distortion and Cation Rotations in Hybrid Perovskite Materials. Nano Letters, 2016, 16, 3809-3816.	4.5	245

#	Article	IF	Citations
19	Enhanced Two-Photon Absorption with Novel Octupolar Propeller-Shaped Fluorophores Derived from Triphenylamine. Organic Letters, 2004, 6, 47-50.	2.4	244
20	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
21	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
22	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
23	Understanding Quantum Confinement of Charge Carriers in Layered 2D Hybrid Perovskites. ChemPhysChem, 2014, 15, 3733-3741.	1.0	211
24	Solid-State Physics Perspective on Hybrid Perovskite Semiconductors. Journal of Physical Chemistry C, 2015, 119, 10161-10177.	1.5	205
25	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
26	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
27	Two-Dimensional Halide Perovskites Incorporating Straight Chain Symmetric Diammonium Ions, (NH₃C_mH_{2m}NH₃)(CH₃NH₃)_nPb_nI_{3n+1} (m = 4â€“9; n = 1â€“4). Journal of the American Chemical Society, 2018, 140, 12226-12238.	6.6	184
28	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
29	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
30	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. ACS Nano, 2018, 12, 3321-3332.	7.3	146
31	Quantum confinement and dielectric profiles of colloidal nanoplatelets of halide inorganic and hybrid organicâ€“inorganic perovskites. Nanoscale, 2016, 8, 6369-6378.	2.8	136
32	Two-Photon Transitions in Quadrupolar and Branched Chromophores:â€‰ Experiment and Theory. Journal of Physical Chemistry B, 2007, 111, 9468-9483.	1.2	127
33	Molecular disorder and translation/rotation coupling in the plastic crystal phase of hybrid perovskites. Nanoscale, 2016, 8, 6222-6236.	2.8	119
34	Elastic Softness of Hybrid Lead Halide Perovskites. Physical Review Letters, 2018, 121, 085502.	2.9	116
35	Decreasing the electronic confinement in layered perovskites through intercalation. Chemical Science, 2017, 8, 1960-1968.	3.7	114
36	Effect of Branching on Two-Photon Absorption in Triphenylbenzene Derivatives. ChemPhysChem, 2007, 8, 723-734.	1.0	108

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37	Synthesis and two-photon absorption of highly soluble three-branched fluorenylene-vinylene derivatives. Tetrahedron Letters, 2003, 44, 8121-8125.	0.7	103
38	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
39	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
40	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
41	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
42	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
43	Luminescence Behavior of Protonated Methoxy-Substituted Diazine Derivatives: Toward White Light Emission. Journal of Physical Chemistry C, 2016, 120, 26986-26995.	1.5	85
44	Experimental and Theoretical Studies of Quadrupolar Oligothiopheneâ€Cored Chromophores Containing Dimesitylboryl Moieties as Ï€â€Accepting Endâ€Groups: Syntheses, Structures, Fluorescence, and Oneâ€•and Twoâ€Photon Absorption. Chemistry - A European Journal, 2014, 20, 13618-13635.	1.7	84
45	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
46	Entropy in halide perovskites. Nature Materials, 2018, 17, 377-379.	13.3	82
47	Three-Dimensional Lead Iodide Perovskitoid Hybrids with High X-ray Photoresponse. Journal of the American Chemical Society, 2020, 142, 6625-6637.	6.6	82
48	New chromophores from click chemistry for two-photon absorption and tuneable photoluminescence. Chemical Communications, 2005, , 2029.	2.2	79
49	Seven-Layered 2D Hybrid Lead Iodide Perovskites. CheM, 2019, 5, 2593-2604.	5.8	79
50	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
51	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
52	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
53	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
54	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

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55	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
56	On the accurate estimation of intermolecular interactions and charge transfer: the case of TTF-CA. Faraday Discussions, 2007, 135, 217-235.	1.6	64
57	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
58	Improved transparencyâ€“nonlinearity trade-off with boroxine-based octupolar molecules. Chemical Communications, 2003, , 2766-2767.	2.2	63
59	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
60	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
61	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
62	Symmetry-Based Tight Binding Modeling of Halide Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 3833-3840.	2.1	57
63	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
64	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
65	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
66	Light-activated interlayer contraction in two-dimensional perovskites for high-efficiency solar cells. Nature Nanotechnology, 2022, 17, 45-52.	15.6	52
67	Memory Seeds Enable High Structural Phase Purity in 2D Perovskite Films for Highâ€Efficiency Devices. Advanced Materials, 2021, 33, e2007176.	11.1	50
68	Direct evidence of weakly dispersed and strongly anharmonic optical phonons in hybrid perovskites. Communications Physics, 2020, 3, .	2.0	49
69	Highâ€Yield Formation of Substituted Tetracyanobutadienes from Reaction of Ynamides with Tetracyanoethylene. Chemistry - A European Journal, 2014, 20, 9553-9557.	1.7	48
70	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
71	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
72	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

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73	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
74	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
75	Tuning Electronic Structure in Layered Hybrid Perovskites with Organic Spacer Substitution. Nano Letters, 2019, 19, 8732-8740.	4.5	41
76	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
77	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
78	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
79	First-principles molecular-dynamics simulations for neutralp-chloranil and its radical anion. Physical Review B, 1996, 53, 12112-12120.	1.1	33
80	Neutral-ionic phase transition:â€ƒA thoroughab initiostudy of TTF-CA. Physical Review B, 2003, 67, .	1.1	33
81	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
82	Cation Alloying Delocalizes Polarons in Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 3516-3524.	2.1	33
83	Designing a New Two-Dimensional Molecular Layout by Hydrogen Bonding. ChemPhysChem, 2006, 7, 82-85.	1.0	32
84	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
85	The importance of relativistic effects on two-photon absorption spectra in metal halide perovskites. Nature Communications, 2019, 10, 5342.	5.8	30
86	On the entanglement of electrostriction and non-linear piezoelectricity in non-centrosymmetric materials. Applied Physics Letters, 2012, 100, .	1.5	29
87	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
88	Does Rashba splitting in CH₃NH₃PbBr₃ arise from 2 Ã— 2 surface reconstruction?. Physical Chemistry Chemical Physics, 2018, 20, 9638-9643.	1.3	29
89	Halide Perovskite High-k Field Effect Transistors with Dynamically Reconfigurable Ambipolarity. , 2019, 1, 633-640.		29
90	Physical properties of bulk, defective, 2D and 0D metal halide perovskite semiconductors from a symmetry perspective. JPhys Materials, 2020, 3, 042001.	1.8	29

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91	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
92	Electronic structure and stability of Cs2TiX6 and Cs2ZrX6 (X = Br, I) vacancy ordered double perovskites. Applied Physics Letters, 2021, 119, .	1.5	28
93	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
94	Effects of permanent dipole moments in degenerate four-wave-mixing processes. Physical Review A, 1991, 44, 5947-5957.	1.0	26
95	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
96	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
97	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
98	Tetrazine molecules as an efficient electronic diversion channel in 2D organicâ€“inorganic perovskites. Materials Horizons, 2021, 8, 1547-1560.	6.4	24
99	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
100	Novel chromophores from alternated pyridineâ€“ethylenedioxythiophene unit oligomers: dramatic enhancement of photoluminescence properties in elongated derivatives. Chemical Communications, 2009, , 692-694.	2.2	23
101	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
102	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
103	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
104	Expanding the Cage of 2D Bromide Perovskites by Large A-Site Cations. Chemistry of Materials, 2022, 34, 1132-1142.	3.2	22
105	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
106	Ab-initio calculations of one-dimensional band structures of mixed-stack molecular crystals. Solid State Communications, 1997, 102, 589-594.	0.9	19
107	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
108	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

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109	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
110	Interstitial Nature of Mn²⁺ Doping in 2D Perovskites. ACS Nano, 2021, 15, 20550-20561.	7.3	19
111	Theoretical description of two-photon phase conjugation in polar molecules. Physical Review A, 1993, 48, 1564-1572.	1.0	18
112	30-band kâ‹…p method for quantum semiconductor heterostructures. Applied Physics Letters, 2011, 98, .	1.5	17
113	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
114	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
115	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
116	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
117	Branching effect on the linear and nonlinear optical properties of styrylpyrimidines. Physical Chemistry Chemical Physics, 2020, 22, 4165-4176.	1.3	16
118	DFT study of NLO properties of boroxine based octupolar molecules. Computational and Theoretical Chemistry, 2008, 866, 58-62.	1.5	15
119	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
120	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
121	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
122	From Zero- to One-Dimensional, Opportunities and Caveats of Hybrid Iodobismuthates for Optoelectronic Applications. Inorganic Chemistry, 2021, 60, 17123-17131.	1.9	13
123	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
124	Theoretical Investigation of the Ground-State Properties of DMTTFâ¯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
125	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
126	Pb-free halide perovskites for solar cells, light-emitting diodes, and photocatalysts. APL Materials, 2022, 10, .	2.2	11

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127	Accuracy of topological analysis of gridded electron densities. Journal of Physics and Chemistry of Solids, 2004, 65, 1951-1955.	1.9	10
128	Carrier scattering processes and low energy phonon spectroscopy in hybrid perovskites crystals. Proceedings of SPIE, 2016, , .	0.8	10
129	Theoretical insights into multibandgap hybrid perovskites for photovoltaic applications. Proceedings of SPIE, 2014, , .	0.8	9
130	Charge Trap Formation and Passivation in Methylammonium Lead Tribromide. Journal of Physical Chemistry C, 2019, 123, 13812-13817.	1.5	9
131	Nonadiabatic molecular dynamics analysis of hybrid Dionâ€“Jacobson 2D leads iodide perovskites. Applied Physics Letters, 2021, 119, .	1.5	9
132	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
133	Dielectric properties of hybrid perovskites and drift-diffusion modeling of perovskite cells. Proceedings of SPIE, 2016, , .	0.8	8
134	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
135	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
136	Electronic properties of Pb-I deficient lead halide perovskites. Journal of Chemical Physics, 2019, 151, 234704.	1.2	7
137	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
138	Vibrational properties of 2H-PbI2 semiconductors studied via Density Functional Theory calculations. Thin Solid Films, 2013, 541, 9-11.	0.8	6
139	Theoretical insights into hybrid perovskites for photovoltaic applications. , 2016, , .		6
140	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
141	Pseudospin-phonon pretransitional dynamics in lead halide hybrid perovskites. Physical Review B, 2022, 105, .	1.1	5
142	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
143	Two-photon transitions in triazole based quadrupolar and octupolar chromophores: a TD-DFT investigation. , 2010, , .		4
144	Non-degenerate two photon absorption enhancement for laser dyes by precise lock-in detection. AIP Advances, 2015, 5, 127138.	0.6	3

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145	Branching of dipolar chromophores: effects on linear and nonlinear optical properties. , 2005, , .		2
146	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
147	Theoretical studies of Rashba and Dresselhaus effects in hybrid organic-inorganic perovskites for optoelectronic applications. , 2016, , .		2
148	Computational design of high performance hybrid perovskite on silicon 2-T tandem solar cells based on a tunnel junction. , 2017, , .		2
149	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
150	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
151	Chapter 7. Electronic Properties of Metal Halide Perovskites. RSC Energy and Environment Series, 2016, , 202-233.	0.2	2
152	A 3D Lead Iodide Hybrid Based on a 2D Perovskite Subnetwork. Crystals, 2021, 11, 1570.	1.0	2
153	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
154	Non-linear electro-elastic coupling in non-centrosymmetric materials. Journal of Physics: Conference Series, 2012, 367, 012005.	0.3	1
155	Anharmonicity and Disorder in the Black Phases of CsPbI3 used for Stable Inorganic Perovskite Solar Cells. , 2018, , .		1
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