

Claudine Katan

List of Publications by Year in descending order

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161
papers

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25423

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#	ARTICLE	IF	CITATIONS
1	Importance of Spin-Orbit Coupling in Hybrid Organic/Inorganic Perovskites for Photovoltaic Applications. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 2999-3005.	2.1	1,021
2	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. <i>Science</i> , 2017, 355, 1288-1292.	6.0	830
3	Hybrid Dion-Jacobson 2D Lead Iodide Perovskites. <i>Journal of the American Chemical Society</i> , 2018, 140, 3775-3783.	6.6	686
4	Light-activated photocurrent degradation and self-healing in perovskite solar cells. <i>Nature Communications</i> , 2016, 7, 11574.	5.8	584
5	Scaling law for excitons in 2D perovskite quantum wells. <i>Nature Communications</i> , 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. <i>ACS Nano</i> , 2018, 12, 3477-3486.	7.3	546
7	Quantum and Dielectric Confinement Effects in Lower-Dimensional Hybrid Perovskite Semiconductors. <i>Chemical Reviews</i> , 2019, 119, 3140-3192.	23.0	525
8	Enhanced Two-Photon Absorption of Organic Chromophores: Theoretical and Experimental Assessments. <i>Advanced Materials</i> , 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. <i>Journal of Physical Chemistry C</i> , 2014, 118, 11566-11572.	1.5	463
10	Charge Instability in Quadrupolar Chromophores: Symmetry Breaking and Solvatochromism. <i>Journal of the American Chemical Society</i> , 2006, 128, 15742-15755.	6.6	379
11	New Type of 2D Perovskites with Alternating Cations in the Interlayer Space, $(\text{C}(\text{NH}_2)_3)_3(\text{CH}_3)_3(\text{NH}_3)_3(\text{PbI}_3)_3$. Structure, Properties, and Photovoltaic Performance. <i>Journal of the American Chemical Society</i> , 2017, 139, 16297-16309.	6.6	374
12	High Members of the 2D Ruddlesden-Popper Halide Perovskites: Synthesis, Optical Properties, and Solar Cells of $(\text{CH}_3(\text{CH}_2)_3\text{NH}_3)_2(\text{CH}_3\text{NH}_3)_4\text{Pb}_5\text{I}_{16}$. <i>Chem</i> , 2017, 2, 427-440.	5.8	354
13	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. <i>ACS Nano</i> , 2016, 10, 9776-9786.	7.3	351
14	Structural Diversity in White-Light-Emitting Hybrid Lead Bromide Perovskites. <i>Journal of the American Chemical Society</i> , 2018, 140, 13078-13088.	6.6	351
15	Tunable White-Light Emission in Single-Cation-Templated Three-Layered 2D Perovskites $(\text{CH}_3)_3\text{CH}_2\text{NH}_3)_4(\text{Pb}_3\text{Br}_{10})_2$. <i>Journal of the American Chemical Society</i> , 2017, 139, 11956-11963.	6.6	349
16	Effects of (Multi)branching of Dipolar Chromophores on Photophysical Properties and Two-Photon Absorption. <i>Journal of Physical Chemistry A</i> , 2005, 109, 3024-3037.	1.1	341
17	Rashba and Dresselhaus Effects in Hybrid Organic-Inorganic Perovskites: From Basics to Devices. <i>ACS Nano</i> , 2015, 9, 11557-11567.	7.3	304
18	Polaron Stabilization by Cooperative Lattice Distortion and Cation Rotations in Hybrid Perovskite Materials. <i>Nano Letters</i> , 2016, 16, 3809-3816.	4.5	245

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19	Enhanced Two-Photon Absorption with Novel Octupolar Propeller-Shaped Fluorophores Derived from Triphenylamine. <i>Organic Letters</i> , 2004, 6, 47-50.	2.4	244
20	Two-Dimensional Dionâ€“Jacobson Hybrid Lead Iodide Perovskites with Aromatic Diammonium Cations. <i>Journal of the American Chemical Society</i> , 2019, 141, 12880-12890.	6.6	241
21	Structural and thermodynamic limits of layer thickness in 2D halide perovskites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 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. <i>Chemistry - A European Journal</i> , 2007, 13, 1481-1498.	1.7	233
23	Understanding Quantum Confinement of Charge Carriers in Layered 2D Hybrid Perovskites. <i>ChemPhysChem</i> , 2014, 15, 3733-3741.	1.0	211
24	Solid-State Physics Perspective on Hybrid Perovskite Semiconductors. <i>Journal of Physical Chemistry C</i> , 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. <i>Advanced Materials</i> , 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. <i>Chemistry - A European Journal</i> , 2009, 15, 198-208.	1.7	196
27	Two-Dimensional Halide Perovskites Incorporating Straight Chain Symmetric Diammonium Ions, (NH ₃ C _m H _{2m} NH ₃)(CH ₃) ₃ N ₃ (m = 4, 9; n = 1, 4). <i>Journal of the American Chemical Society</i> , 2018, 140, 12226-12238.	1.2	177
28	DFT and <i>k</i> - <i>p</i> modelling of the phase transitions of lead and tin halide perovskites for photovoltaic cells. <i>Physica Status Solidi - Rapid Research Letters</i> , 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. <i>Physical Review B</i> , 2012, 86, .	1.1	173
30	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. <i>ACS Nano</i> , 2018, 12, 3321-3332.	7.3	146
31	Quantum confinement and dielectric profiles of colloidal nanoplatelets of halide inorganic and hybrid organicâ€“inorganic perovskites. <i>Nanoscale</i> , 2016, 8, 6369-6378.	2.8	136
32	Two-Photon Transitions in Quadrupolar and Branched Chromophores: Experiment and Theory. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9468-9483.	1.2	127
33	Molecular disorder and translation/rotation coupling in the plastic crystal phase of hybrid perovskites. <i>Nanoscale</i> , 2016, 8, 6222-6236.	2.8	119
34	Elastic Softness of Hybrid Lead Halide Perovskites. <i>Physical Review Letters</i> , 2018, 121, 085502.	2.9	116
35	Decreasing the electronic confinement in layered perovskites through intercalation. <i>Chemical Science</i> , 2017, 8, 1960-1968.	3.7	114
36	Effect of Branching on Two-Photon Absorption in Triphenylbenzene Derivatives. <i>ChemPhysChem</i> , 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. <i>Tetrahedron Letters</i> , 2003, 44, 8121-8125.	0.7	103
38	Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. <i>Nano Letters</i> , 2018, 18, 5603-5609.	4.5	103
39	Interplay of spin-orbit coupling and lattice distortion in metal substituted 3D tri-chloride hybrid perovskites. <i>Journal of Materials Chemistry A</i> , 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. <i>Chemistry of Materials</i> , 2019, 31, 3582-3590.	3.2	101
41	Cation Engineering in Two-Dimensional Ruddlesden-Popper Lead Iodide Perovskites with Mixed Large A-Site Cations in the Cages. <i>Journal of the American Chemical Society</i> , 2020, 142, 4008-4021.	6.6	101
42	Elastic Constants, Optical Phonons, and Molecular Relaxations in the High Temperature Plastic Phase of the $\text{CH}_3\text{NH}_3\text{PbBr}_3$ Hybrid Perovskite. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3776-3784.	2.1	89
43	Luminescence Behavior of Protonated Methoxy-Substituted Diazine Derivatives: Toward White Light Emission. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26986-26995.	1.5	85
44	Experimental and Theoretical Studies of Quadrupolar Oligothiophene-Cored Chromophores Containing Dimesitylboryl Moieties as π -Accepting End Groups: Syntheses, Structures, Fluorescence, and One- and Two-Photon Absorption. <i>Chemistry - A European Journal</i> , 2014, 20, 13618-13635.	1.7	84
45	Negative Pressure Engineering with Large Cage Cations in 2D Halide Perovskites Causes Lattice Softening. <i>Journal of the American Chemical Society</i> , 2020, 142, 11486-11496.	6.6	84
46	Entropy in halide perovskites. <i>Nature Materials</i> , 2018, 17, 377-379.	13.3	82
47	Three-Dimensional Lead Iodide Perovskitoid Hybrids with High X-ray Photoresponse. <i>Journal of the American Chemical Society</i> , 2020, 142, 6625-6637.	6.6	82
48	New chromophores from click chemistry for two-photon absorption and tuneable photoluminescence. <i>Chemical Communications</i> , 2005, , 2029.	2.2	79
49	Seven-Layered 2D Hybrid Lead Iodide Perovskites. <i>CheM</i> , 2019, 5, 2593-2604.	5.8	79
50	Multinuclear NMR as a tool for studying local order and dynamics in $\text{CH}_3\text{NH}_3\text{PbX}_3$ (X = Cl, Br, I) hybrid perovskites. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27133-27142.	1.3	78
51	Charge carrier dynamics in two-dimensional hybrid perovskites: Dion-Jacobson vs. Ruddlesden-Popper phases. <i>Journal of Materials Chemistry A</i> , 2020, 8, 22009-22022.	5.2	72
52	<i>m</i> -Phenylenediammonium as a New Spacer for Dion-Jacobson Two-Dimensional Perovskites. <i>Journal of the American Chemical Society</i> , 2021, 143, 12063-12073.	6.6	71
53	Numerical computation of critical properties and atomic basins from three-dimensional grid electron densities. <i>Journal of Applied Crystallography</i> , 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. <i>Journal of the American Chemical Society</i> , 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. <i>Journal of the American Chemical Society</i> , 2020, 142, 5060-5067.	6.6	65
56	On the accurate estimation of intermolecular interactions and charge transfer: the case of TTF-CA. <i>Faraday Discussions</i> , 2007, 135, 217-235.	1.6	64
57	Organic Cation Alloying on Intralayer A and Interlayer A sites in 2D Hybrid Dion-Jacobson Lead Bromide Perovskites (A)(Pb ₂ Br ₇). <i>Journal of the American Chemical Society</i> , 2020, 142, 8342-8351.	6.6	64
58	Improved transparency/nonlinearity trade-off with boroxine-based octupolar molecules. <i>Chemical Communications</i> , 2003, , 2766-2767.	2.2	63
59	Critical Fluctuations and Anharmonicity in Lead Iodide Perovskites from Molecular Dynamics Supercell Simulations. <i>Journal of Physical Chemistry C</i> , 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. <i>Physical Review B</i> , 2019, 99, .	1.1	61
61	Electronic properties of 2D and 3D hybrid organic/inorganic perovskites for optoelectronic and photovoltaic applications. <i>Optical and Quantum Electronics</i> , 2014, 46, 1225-1232.	1.5	60
62	Symmetry-Based Tight Binding Modeling of Halide Perovskite Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3833-3840.	2.1	57
63	Simultaneous Control of Emission Localization and Two-Photon Absorption Efficiency in Dissymmetrical Chromophores. <i>Journal of Physical Chemistry B</i> , 2010, 114, 3152-3169.	1.2	52
64	Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Substitution in Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 7130-7136.	2.1	52
65	Enhanced Stability and Band Gap Tuning of [HC(NH ₂) ₂] ₂ PbI ₃ Hybrid Perovskite by Large Cation Integration. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 20743-20751.	4.0	52
66	Light-activated interlayer contraction in two-dimensional perovskites for high-efficiency solar cells. <i>Nature Nanotechnology</i> , 2022, 17, 45-52.	15.6	52
67	Memory Seeds Enable High Structural Phase Purity in 2D Perovskite Films for High-Efficiency Devices. <i>Advanced Materials</i> , 2021, 33, e2007176.	11.1	50
68	Direct evidence of weakly dispersed and strongly anharmonic optical phonons in hybrid perovskites. <i>Communications Physics</i> , 2020, 3, .	2.0	49
69	High-Yield Formation of Substituted Tetracyanobutadienes from Reaction of Ynamides with Tetracyanoethylene. <i>Chemistry - A European Journal</i> , 2014, 20, 9553-9557.	1.7	48
70	A close examination of the structure and dynamics of HC(NH ₂) ₂ PbI ₃ by MD simulations and group theory. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1407-1413.	1.1	47
72	Effects of Chlorine Mixing on Optoelectronics, Ion Migration, and Gamma-Ray Detection in Bromide Perovskites. <i>Chemistry of Materials</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Chemical Communications</i> , 2016, 52, 331-334.	2.2	41
75	Tuning Electronic Structure in Layered Hybrid Perovskites with Organic Spacer Substitution. <i>Nano Letters</i> , 2019, 19, 8732-8740.	4.5	41
76	Design and Synthesis of a Caged Carboxylic Acid with a Donor- π -Donor Coumarin Structure: One-photon and Two-photon Uncaging Reactions Using Visible and Near-Infrared Lights. <i>Organic Letters</i> , 2017, 19, 2622-2625.	2.4	39
77	Tolerance Factor for Stabilizing 3D Hybrid Halide Perovskitoids Using Linear Diammonium Cations. <i>Journal of the American Chemical Society</i> , 2022, 144, 3902-3912.	6.6	36
78	Effects of Dipolar Interactions on Linear and Nonlinear Optical Properties of Multichromophore Assemblies: A Case Study. <i>Chemistry - A European Journal</i> , 2006, 12, 3089-3102.	1.7	34
79	First-principles molecular-dynamics simulations for neutral-p-chloranil and its radical anion. <i>Physical Review B</i> , 1996, 53, 12112-12120.	1.1	33
80	Neutral-ionic phase transition: a thorough study of TTF-CA. <i>Physical Review B</i> , 2003, 67, .	1.1	33
81	Caged Glutamates with π -Extended 1,2-Dihydronaphthalene Chromophore: Design, Synthesis, Two-Photon Absorption Property, and Photochemical Reactivity. <i>Journal of Organic Chemistry</i> , 2014, 79, 7822-7830.	1.7	33
82	Cation Alloying Delocalizes Polarons in Lead Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3516-3524.	2.1	33
83	Designing a New Two-Dimensional Molecular Layout by Hydrogen Bonding. <i>ChemPhysChem</i> , 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. <i>Journal of Physical Chemistry C</i> , 2019, 123, 291-298.	1.5	32
85	The importance of relativistic effects on two-photon absorption spectra in metal halide perovskites. <i>Nature Communications</i> , 2019, 10, 5342.	5.8	30
86	On the entanglement of electrostriction and non-linear piezoelectricity in non-centrosymmetric materials. <i>Applied Physics Letters</i> , 2012, 100, .	1.5	29
87	Absorption and fluorescence signatures of 1,2,3-triazole based regioisomers: challenging compounds for TD-DFT. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9064-9073.	1.3	29
88	Does Rashba splitting in $\text{CH}_3\text{NH}_3\text{PbBr}_3$ arise from $2\sqrt{2}$ surface reconstruction?. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 9638-9643.	1.3	29
89	Halide Perovskite High- k Field Effect Transistors with Dynamically Reconfigurable Ambipolarity. <i>Nature Communications</i> , 2019, 1, 633-640.		29
90	Physical properties of bulk, defective, 2D and 0D metal halide perovskite semiconductors from a symmetry perspective. <i>JPhys Materials</i> , 2020, 3, 042001.	1.8	29

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91	Density of States Broadening in CH ₃ NH ₃ PbI ₃ 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 Cs ₂ TiX ₆ and Cs ₂ ZrX ₆ (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 Aminoazobenzene-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 Cesium-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 organic-inorganic perovskites. Materials Horizons, 2021, 8, 1547-1560.	6.4	24
99	Influence of π -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 pyridine-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	Push-Pull (Iso)quinoline Chromophores: Synthesis, Photophysical Properties, and Use for White-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 Neutral-to-Ionic Transition. Journal of Physical Chemistry A, 2001, 105, 4300-4307.	1.1	19
108	Design, Synthesis, and Reaction of π -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 π -acetylide complexes and the use of a photocrosslinked polymer as a springboard to obtain SHG active thin films. <i>Dalton Transactions</i> , 2016, 45, 11052-11060.	1.6	19
110	Interstitial Nature of Mn ²⁺ Doping in 2D Perovskites. <i>ACS Nano</i> , 2021, 15, 20550-20561.	7.3	19
111	Theoretical description of two-photon phase conjugation in polar molecules. <i>Physical Review A</i> , 1993, 48, 1564-1572.	1.0	18
112	30-band k -p method for quantum semiconductor heterostructures. <i>Applied Physics Letters</i> , 2011, 98, .	1.5	17
113	Effect of protonation on the photophysical properties of 4-substituted and 4,7-disubstituted quinazoline push-pull chromophores. <i>Dyes and Pigments</i> , 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. <i>Cell Reports Physical Science</i> , 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. <i>ACS Energy Letters</i> , 2022, 7, 349-357.	8.8	17
116	Synthesis of a double-stranded spiroborate helicate bearing stilbene units and its photoresponsive behaviour. <i>New Journal of Chemistry</i> , 2015, 39, 3259-3269.	1.4	16
117	Branching effect on the linear and nonlinear optical properties of styrylpyrimidines. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4165-4176.	1.3	16
118	DFT study of NLO properties of boroxine based octupolar molecules. <i>Computational and Theoretical Chemistry</i> , 2008, 866, 58-62.	1.5	15
119	Position Isomerism on One and Two Photon Absorption in Multibranched Chromophores: A TDDFT Investigation. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3410-3426.	2.3	15
120	Synthesis and photochemical reactivity of caged glutamates with a π -extended coumarin chromophore as a photolabile protecting group. <i>Tetrahedron Letters</i> , 2013, 54, 7171-7174.	0.7	15
121	Comment on "Density functional theory analysis of structural and electronic properties of orthorhombic perovskite CH ₃ NH ₃ PbI ₃ " by Y. Wang et al., <i>Phys. Chem. Chem. Phys.</i> , 2014, 16, 1424-1429. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 8697-8698.	1.3	13
122	From Zero- to One-Dimensional, Opportunities and Caveats of Hybrid Iodobismuthates for Optoelectronic Applications. <i>Inorganic Chemistry</i> , 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. <i>Physical Review Materials</i> , 2022, 6, .	0.9	13
124	Theoretical Investigation of the Ground-State Properties of DMTF ⁺ CA ⁻ : A Step toward the Understanding of Charge Transfer Complexes Undergoing the Neutral-to-Ionic Phase Transition. <i>Journal of Physical Chemistry A</i> , 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. <i>Journal of Molecular Modeling</i> , 2016, 22, 265.	0.8	11
126	Pb-free halide perovskites for solar cells, light-emitting diodes, and photocatalysts. <i>APL Materials</i> , 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 QUADRUPOLE 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
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