

Ke-Li Han

List of Publications by Year in descending order

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512
papers

32,076
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3874

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citing authors

#	ARTICLE	IF	CITATIONS
1	Doped all-inorganic cesium zirconium halide perovskites with high-efficiency and tunable emission. <i>Journal of Energy Chemistry</i> , 2022, 65, 600-604.	7.1	37
2	Unblocked intramolecular charge transfer for enhanced CO ₂ photoreduction enabled by an imidazolium-based ionic conjugated microporous polymer. <i>Applied Catalysis B: Environmental</i> , 2022, 300, 120719.	10.8	25
3	Lead-Free All-Inorganic Indium Chloride Perovskite Variant Nanocrystals for Efficient Luminescence. <i>Advanced Optical Materials</i> , 2022, 10, 2101344.	3.6	26
4	ESIPT-based AIE luminogens: Design strategies, applications, and mechanisms. <i>Aggregate</i> , 2022, 3, .	5.2	100
5	Germanium Halides Serving as Ideal Precursors: Designing a More Effective and Less Toxic Route to High-Optoelectronic-Quality Metal Halide Perovskite Nanocrystals. <i>Nano Letters</i> , 2022, 22, 636-643.	4.5	15
6	The Second Excited Triplet State Facilitates TADF and Triplet-Triplet Annihilation Photon Upconversion via a Thermally Activated Reverse Internal Conversion. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	7
7	Excitation-Dependent Emission in All-Inorganic Lead-Free Cs ₂ ScCl ₅ H ₂ O Perovskite Crystals. <i>Laser and Photonics Reviews</i> , 2022, 16, .	4.4	26
8	Colloidal Synthesis and Tunable Multicolor Emission of Vacancy-Ordered Cs ₂ HfCl ₆ Perovskite Nanocrystals. <i>Laser and Photonics Reviews</i> , 2022, 16, .	4.4	38
9	Profiling Cystathionine β -Lyase in Complex Biosamples Using Novel Activatable Fluorogens. <i>Analytical Chemistry</i> , 2022, 94, 1203-1210.	3.2	5
10	Tuning Exciton Recombination Pathways in Inorganic Bismuth-Based Perovskite for Broadband Emission. <i>Energy Material Advances</i> , 2022, 2022, .	4.7	22
11	Organo-Metal Halide Scintillator with Weak Thermal Quenching Up to 200 °C. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5794-5800.	2.1	16
12	Unraveling the Key Role of the Benzyl Group in the Synthesis of CL-20 Precursor HBIW. <i>ACS Omega</i> , 2022, 7, 21912-21924.	1.6	3
13	New Cy5 photosensitizers for cancer phototherapy: a low singlet-triplet gap provides high quantum yield of singlet oxygen. <i>Chemical Science</i> , 2021, 12, 13809-13816.	3.7	19
14	Band-Gap Engineering of Lead-Free Iron-Based Halide Double-Perovskite Single Crystals and Nanocrystals by an Alloying or Doping Strategy. <i>Journal of Physical Chemistry C</i> , 2021, 125, 11743-11749.	1.5	24
15	New Protocol-Guided Exploitation of a Lysosomal Sulfatase Inhibitor to Suppress Cell Growth in Glioblastoma Multiforme. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 8599-8606.	2.9	4
16	All-Inorganic Rare-Earth Halide Double Perovskite Single Crystals with Highly Efficient Photoluminescence. <i>Advanced Optical Materials</i> , 2021, 9, 2100689.	3.6	53
17	Lead-free rare-earth double perovskite Cs ₂ Agn _{1-x} BixLa ₃ Cl ₆ nanocrystals with highly efficient warm-white emission. <i>Science China Materials</i> , 2021, 64, 2667-2674.	3.5	18
18	Phase Engineering of Cesium Manganese Bromides Nanocrystals with Color-Tunable Emission. <i>Angewandte Chemie</i> , 2021, 133, 19805-19811.	1.6	12

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19	Phase Engineering of Cesium Manganese Bromides Nanocrystals with Color-Tunable Emission. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 19653-19659.	7.2	64
20	All-Inorganic Rare-Earth-Based Double Perovskite Nanocrystals with Near-Infrared Emission. <i>Laser and Photonics Reviews</i> , 2021, 15, 2100218.	4.4	42
21	Recent Advances in All-Inorganic Lead-Free Three-Dimensional Halide Double Perovskite Nanocrystals. <i>Energy & Fuels</i> , 2021, 35, 18871-18887.	2.5	30
22	Ultrafast Dynamics of Self-Trapped Excitons in Lead-Free Perovskite Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8256-8262.	2.1	82
23	Controlling Photoluminescence and Photocatalysis Activities in Lead-Free Cs ₂ Pt _x Sn _{1-x} Cl ₆ Perovskites via Ion Substitution. <i>Angewandte Chemie</i> , 2021, 133, 22875-22881.	1.6	13
24	Controlling Photoluminescence and Photocatalysis Activities in Lead-Free Cs ₂ Pt _x Sn _{1-x} Cl ₆ Perovskites via Ion Substitution. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22693-22699.	7.2	44
25	Efficient Luminescent Halide Quadruple-Perovskite Nanocrystals via Trap-Engineering for Highly Sensitive Photodetectors. <i>Advanced Materials</i> , 2021, 33, e2007215.	11.1	49
26	Extending the Legible Time of Light-Responsive Rewritable Papers with a Tunable Photochromic Diarylethene Molecule. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 51414-51425.	4.0	7
27	Directionally Modified Fluorophores for Super-Resolution Imaging of Target Enzymes: A Case Study with Carboxylesterases. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 16177-16186.	2.9	5
28	Bright Triplet Self-Trapped Excitons to Dopant Energy Transfer in Halide Double-Perovskite Nanocrystals. <i>Nano Letters</i> , 2021, 21, 8671-8678.	4.5	53
29	Quasi-Two-Dimensional Perovskite Nanosheets Based on the Triplet Energy Acceptor Molecule with Pure Green Emission Light. <i>Journal of Physical Chemistry C</i> , 2021, 125, 23889-23894.	1.5	5
30	Lead-free B-site bimetallic perovskite photocatalyst for efficient benzylic C-H bond activation. <i>Cell Reports Physical Science</i> , 2021, 2, 100656.	2.8	32
31	First-Principles Screening of Lead-Free Mixed-Anion Perovskites for Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1303-1308.	1.5	8
32	Lead-Free Small-Bandgap Cs ₂ CuSbCl ₆ Double Perovskite Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6463-6467.	2.1	57
33	Quantifying the Fast Dynamics of HClO in Living Cells by a Fluorescence Probe Capable of Responding to Oxidation and Reduction Events within the Time Scale of Milliseconds. <i>Analytical Chemistry</i> , 2020, 92, 12987-12995.	3.2	21
34	Doped Zero-Dimensional Cesium Zinc Halides for High-Efficiency Blue Light Emission. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21414-21418.	7.2	97
35	Doped Zero-Dimensional Cesium Zinc Halides for High-Efficiency Blue Light Emission. <i>Angewandte Chemie</i> , 2020, 132, 21598-21602.	1.6	19
36	A fluorophore's electron-deficiency does matter in designing high-performance near-infrared fluorescent probes. <i>Chemical Science</i> , 2020, 11, 11205-11213.	3.7	10

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37	Efficient Thermally Activated Delayed Fluorescence from All-Inorganic Cesium Zirconium Halide Perovskite Nanocrystals. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21925-21929.	7.2	126
38	Efficient Thermally Activated Delayed Fluorescence from All-Inorganic Cesium Zirconium Halide Perovskite Nanocrystals. <i>Angewandte Chemie</i> , 2020, 132, 22109-22113.	1.6	24
39	Vertical Phase Separated Cesium Fluoride Doping Organic Electron Transport Layer: A Facile and Efficient σ -Bridge-Linked Heterojunction for Perovskite Solar Cells. <i>Advanced Functional Materials</i> , 2020, 30, 2001418.	7.8	44
40	Enhancing Intersystem Crossing to Achieve Thermally Activated Delayed Fluorescence in a Water-Soluble Fluorescein Derivative with a Flexible Propenyl Group. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5692-5698.	2.1	18
41	Manganese-Doped, Lead-Free Double Perovskite Nanocrystals for Bright Orange-Red Emission. <i>ACS Central Science</i> , 2020, 6, 566-572.	5.3	102
42	A Lead-Free All-Inorganic Metal Halide with Near-Unity Green Luminescence. <i>Laser and Photonics Reviews</i> , 2020, 14, 2000027.	4.4	66
43	Self-trapped exciton engineering for white-light emission in colloidal lead-free double perovskite nanocrystals. <i>Science Bulletin</i> , 2020, 65, 1078-1084.	4.3	73
44	Direct observation of charge transfer between molecular heterojunctions based on inorganic semiconductor clusters. <i>Chemical Science</i> , 2020, 11, 4085-4096.	3.7	16
45	Thermochemistry and Initial Decomposition Pathways of Triazole Energetic Materials. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2951-2960.	1.1	20
46	Carrier Multiplication and Hot-Carrier Cooling Dynamics in Quantum-Confined CsPb ₃ Perovskite Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1921-1926.	2.1	37
47	Detection of atherosclerosis-related hypochlorous acid produced in foam cells with a localized endoplasmic reticulum probe. <i>Chemical Communications</i> , 2020, 56, 2610-2613.	2.2	36
48	Unraveling the Mechanism of <i>cyclo</i> -N ₅ ⁺ Production through Selective C-N Bond Cleavage of Arylpentazole with Ferrous Bisglycinate and <i>m</i> -Chloroperbenzoic Acid: A Theoretical Perspective. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1030-1037.	2.1	26
49	Salen-Based Conjugated Microporous Polymers for Efficient Oxygen Evolution Reaction. <i>Chemistry - A European Journal</i> , 2020, 26, 7720-7726.	1.7	16
50	All-Inorganic Lead-Free OD Perovskites by a Doping Strategy to Achieve a PLQY Boost from 2% to 90%. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12709-12713.	7.2	162
51	All-Inorganic Lead-Free OD Perovskites by a Doping Strategy to Achieve a PLQY Boost from 2% to 90%. <i>Angewandte Chemie</i> , 2020, 132, 12809-12813.	1.6	38
52	Semi-Quantitatively Designing Two-Photon High-Performance Fluorescent Probes for Glutathione S-Transferases. <i>Research</i> , 2020, 2020, 7043124.	2.8	6
53	Substitution Dependent Ultrafast Ultraviolet Energy Dissipation Mechanisms of Plant Sunscreens. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5244-5249.	2.1	22
54	Hetero-bichromophore Dyad as a Highly Efficient Triplet Acceptor for Polarity Tuned Triplet-Triplet Annihilation Upconversion. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4368-4373.	2.1	11

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55	Size effect of lead-free halide double perovskite on luminescence property. <i>Science China Chemistry</i> , 2019, 62, 1405-1413.	4.2	95
56	New Insight into the Photoprotection Mechanism of Plant Sunscreens: Adiabatic Relaxation Competing with Nonadiabatic Relaxation in the <i>cis</i> \rightarrow <i>trans</i> Photoisomerization of Methyl Sinapate. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4197-4202.	2.1	26
57	Asynchronous Photoexcited Electronic and Structural Relaxation in Lead-Free Perovskites. <i>Journal of the American Chemical Society</i> , 2019, 141, 13074-13080.	6.6	39
58	Restriction of Flip-flop Motion as a Mechanism for Aggregation-Induced Emission. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6929-6935.	2.1	80
59	Lead-Free Sodium-Indium Double Perovskite Nanocrystals through Doping Silver Cations for Bright Yellow Emission. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 17231-17235.	7.2	166
60	Colloidal Synthesis and Optical Properties of All-Inorganic Low-Dimensional Cesium Copper Halide Nanocrystals. <i>Angewandte Chemie</i> , 2019, 131, 16233-16237.	1.6	78
61	Charge-Carrier Dynamics of Lead-Free Halide Perovskite Nanocrystals. <i>Accounts of Chemical Research</i> , 2019, 52, 3188-3198.	7.6	164
62	Lead-Free Sodium-Indium Double Perovskite Nanocrystals through Doping Silver Cations for Bright Yellow Emission. <i>Angewandte Chemie</i> , 2019, 131, 17391-17395.	1.6	36
63	Colloidal Synthesis and Optical Properties of All-Inorganic Low-Dimensional Cesium Copper Halide Nanocrystals. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16087-16091.	7.2	192
64	Theoretical perspective on the reaction mechanism from arylpentazenes to arylpentazoles: new insights into the enhancement of <i>cyclo</i> -N ₅ production. <i>Chemical Communications</i> , 2019, 55, 2628-2631.	2.2	20
65	Air-Stable, Lead-Free Zero-Dimensional Mixed Bismuth-Antimony Perovskite Single Crystals with Ultra-broadband Emission. <i>Angewandte Chemie</i> , 2019, 131, 2751-2755.	1.6	41
66	Rational design of a visible-light photochromic diarylethene: a simple strategy by extending conjugation with electron donating groups. <i>Science China Chemistry</i> , 2019, 62, 451-459.	4.2	19
67	Air-Stable, Lead-Free Zero-Dimensional Mixed Bismuth-Antimony Perovskite Single Crystals with Ultra-broadband Emission. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2725-2729.	7.2	199
68	Surface-Halogenation-Induced Atomic Site Activation and Local Charge Separation for Superb CO ₂ Photoreduction. <i>Advanced Materials</i> , 2019, 31, e1900546.	11.1	343
69	Broad-Band Emission in a Zero-Dimensional Hybrid Organic [PbBr ₆] Trimer with Intrinsic Vacancies. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1337-1341.	2.1	86
70	Differentiation between Enamines and Tautomerizable Imines Oxidation Reaction Mechanism using Electron-Vibration-Vibration Two Dimensional Infrared Spectroscopy. <i>Molecules</i> , 2019, 24, 869.	1.7	6
71	Three-One Oxygen Vacancies: Whole Visible Spectrum Absorption, Efficient Charge Separation, and Surface Site Activation for Robust CO ₂ Photoreduction. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3880-3884.	7.2	483
72	Colloidal Synthesis and Charge-Carrier Dynamics of Cs ₂ AgSb _{1-x} Bi _x X ₆ (X: Br, Cl; 0 \leq x \leq 1) Tj 110q0 0 0 BT /Over		

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73	Colloidal Synthesis and Charge Carrier Dynamics of Cs ₂ AgSb ₃ Bi ₂ X ₆ (X: Br, Cl; O) Ternary Perovskites. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1237-1247.	7.1	108
74	Three Oxygen Vacancies: Whole Visible Spectrum Absorption, Efficient Charge Separation, and Surface Site Activation for Robust CO ₂ Photoreduction. <i>Angewandte Chemie</i> , 2019, 131, 3920-3924.	1.6	45
75	Ionization and Electron Attachment for Nucleobases in Water. <i>Journal of Physical Chemistry B</i> , 2019, 123, 1237-1247.	1.2	24
76	Different types of hydrogen-bonded complexes would accelerate or delay the excited state proton transfer in 3-hydroxyflavone. <i>Journal of Luminescence</i> , 2019, 206, 46-52.	1.5	26
77	Bismuth doped lead-free two-dimensional tin based halide perovskite single crystals. <i>Journal of Energy Chemistry</i> , 2019, 36, 1-6.	7.1	42
78	Black phosphorus-CdS-La ₂ Ti ₂ O ₇ ternary composite: Effective noble metal-free photocatalyst for full solar spectrum activated H ₂ production. <i>Applied Catalysis B: Environmental</i> , 2019, 242, 441-448.	10.8	105
79	Lead-Free Silver-Bismuth Halide Double Perovskite Nanocrystals. <i>Angewandte Chemie</i> , 2018, 130, 5457-5461.	1.6	132
80	Lead-Free Silver-Bismuth Halide Double Perovskite Nanocrystals. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 5359-5363.	7.2	281
81	Reaction between C ₄ H ₃ Radical and Acetylene (C ₂ H ₂): Is Phenyl (C ₆ H ₅) the Primary Product? <i>Energy & Fuels</i> , 2018, 32, 5581-5587.	2.5	2
82	Molecular dynamics simulation of the high-temperature pyrolysis of methylcyclohexane. <i>Fuel</i> , 2018, 217, 185-192.	3.4	44
83	Diabatic potential energy surfaces of MgH ₂ ⁺ and dynamic studies for the Mg ⁺ (3p) + H ₂ → MgH ⁺ + H reaction. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 6638-6647.	1.3	30
84	Reconsideration of the Detection and Fluorescence Mechanism of a Pyrene-Based Chemosensor for TNT. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1400-1405.	1.1	32
85	A Revisit to the Orthogonal Bodipy Dimers: Experimental Evidence for the Symmetry Breaking Charge Transfer-Induced Intersystem Crossing. <i>Journal of Physical Chemistry C</i> , 2018, 122, 2502-2511.	1.5	79
86	Lead-Free, Two-Dimensional Mixed Germanium and Tin Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2518-2522.	2.1	92
87	First-Principles Screening of All-Inorganic Lead-Free ABX ₃ Perovskites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 7670-7675.	1.5	98
88	Ultrafast Charge Separation for Full Solar Spectrum-Activated Photocatalytic H ₂ Generation in a Black Phosphorus-Au-CdS Heterostructure. <i>ACS Energy Letters</i> , 2018, 3, 932-939.	8.8	122
89	Unveiling excited state energy transfer and charge transfer in a host/guest coordination cage. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 2205-2210.	1.3	13
90	Development of a Reactive Force Field for Hydrocarbons and Application to Iso-octane Thermal Decomposition. <i>Energy & Fuels</i> , 2018, 32, 901-907.	2.5	21

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91	The sensing mechanism studies of the fluorescent probes with electronically excited state calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1351.	6.2	78
92	Lead-Free Direct Band Gap Double-Perovskite Nanocrystals with Bright Dual-Color Emission. Journal of the American Chemical Society, 2018, 140, 17001-17006.	6.6	399
93	Constructing Sensitive and Fast Lead-Free Single-Crystalline Perovskite Photodetectors. Journal of Physical Chemistry Letters, 2018, 9, 3087-3092.	2.1	92
94	New insights into the sensing mechanism of a phosphonate pyrene chemosensor for TNT. Physical Chemistry Chemical Physics, 2018, 20, 19539-19545.	1.3	20
95	Significant effects of vibrational excitation of reactant in $K + H_2 \rightarrow H + KH$ reaction based on a new neural network potential energy surface. Physical Chemistry Chemical Physics, 2018, 20, 20641-20649.	1.3	14
96	Mechanism of Efficient Viologen Radical Generation by Ultrafast Electron Transfer from CdS Quantum Dots. Journal of Physical Chemistry C, 2018, 122, 17136-17142.	1.5	34
97	High Resolution Mapping of Two-Photon Excited Photocurrent in Perovskite Microplate Photodetector. Journal of Physical Chemistry Letters, 2018, 9, 5017-5022.	2.1	35
98	Unraveling the Detailed Mechanism of Excited-State Proton Transfer. Accounts of Chemical Research, 2018, 51, 1681-1690.	7.6	432
99	Long-wavelength chromophores with thermally activated delayed fluorescence based on fluorescein derivatives. Journal of Photonics for Energy, 2018, 8, 1.	0.8	6
100	Ultrafast Barrierless Photoisomerization and Strong Ultraviolet Absorption of Photoproducts in Plant Sunscreens. Journal of Physical Chemistry Letters, 2017, 8, 1025-1030.	2.1	76
101	Perovskite $CH_3NH_3PbI_3$ Single Crystals with Charge-Carrier Lifetimes Exceeding 260 ns. ACS Applied Materials & Interfaces, 2017, 9, 14827-14832.	4.0	58
102	Size- and Wavelength-Dependent Two-Photon Absorption Cross-Section of $CsPbBr_3$ Perovskite Quantum Dots. Journal of Physical Chemistry Letters, 2017, 8, 2316-2321.	2.1	173
103	Probing Charge-Transfer and Short-Lived Triplet States of a Biosensitive Molecule, 2,6-ANS: Transient Absorption and Time-Resolved Spectroscopy. ACS Omega, 2017, 2, 6782-6785.	1.6	1
104	Intraligand Charge Transfer Sensitization on Self-Assembled Europium Tetrahedral Cage Leads to Dual-Selective Luminescent Sensing toward Anion and Cation. Journal of the American Chemical Society, 2017, 139, 12474-12479.	6.6	128
105	$(C_6H_5)_2C_2H_4NH_3$: A Layered Two-Dimensional Perovskite with Potential for Photovoltaic Applications. Journal of Physical Chemistry Letters, 2017, 8, 4402-4406.	2.1	98
106	Ultrasensitive and Fast All-Inorganic Perovskite-Based Photodetector via Fast Carrier Diffusion. Advanced Materials, 2017, 29, 1703758.	11.1	255
107	Lead-Free, Air-Stable All-Inorganic Cesium Bismuth Halide Perovskite Nanocrystals. Angewandte Chemie, 2017, 129, 12645-12649.	1.6	88
108	Lead-Free, Air-Stable All-Inorganic Cesium Bismuth Halide Perovskite Nanocrystals. Angewandte Chemie - International Edition, 2017, 56, 12471-12475.	7.2	487

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109	Combining theory and experiment in the design of a lead-free ((CH ₃) ₃ NH) ₃ AgBi ₂ double perovskite. <i>New Journal of Chemistry</i> , 2017, 41, 9598-9601.	1.4	72
110	Direct Observation of a Triplet-State Absorption-Emission Conversion in a Fullerene-Functionalized Pt(II) Metallacycle. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14975-14980.	1.5	9
111	Orientation hydrogen-bonding effect on vibronic spectra of isoquinoline in water solvent: Franck-Condon simulation and interpretation. <i>Journal of Chemical Physics</i> , 2016, 145, 164314.	1.2	33
112	Potential Energy Surfaces for the First Two Lowest-Lying Electronic States of the LiH ₂ ⁺ System, and Dynamics of the H ⁺ + LiH → H ₂ ⁺ + Li + Reactions. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2459-2470.	1.1	17
113	Synthesis and Characterization of Phenothiazine-Based Platinum(II)-Acetylide Photosensitizers for Efficient Dye-Sensitized Solar Cells. <i>Chemistry - A European Journal</i> , 2016, 22, 3750-3757.	1.7	27
114	Free energy profiles of cocaine esterase-cocaine binding process by molecular dynamics and potential of mean force simulations. <i>Chemico-Biological Interactions</i> , 2016, 259, 142-147.	1.7	1
115	High-Efficiency Microiterative Optimization in QM/MM Simulations of Large Flexible Systems. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4632-4643.	2.3	8
116	Rational Design of a Profluorescent Substrate for S-adenosylhomocysteine Hydrolase and its Applications in Bioimaging and Inhibitor Screening. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 25818-25824.	4.0	16
117	The Effects of Heteroatoms Si and S on Tuning the Optical Properties of Rhodamine and Fluorescein-Based Fluorescence Probes: A Theoretical Analysis. <i>ChemPhysChem</i> , 2016, 17, 3139-3145.	1.0	37
118	Low Threshold Two-Photon-Pumped Amplified Spontaneous Emission in CH ₃ NH ₃ PbBr ₃ Microdisks. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 19587-19592.	4.0	54
119	A versatile two-photon fluorescent probe for ratiometric imaging E. coli β-galactosidase in live cells and in vivo. <i>Chemical Communications</i> , 2016, 52, 8283-8286.	2.2	69
120	Effects of Solvent Dielectric Constant and Viscosity on Two Rotational Relaxation Paths of Excited 9-(Dicyanovinyl) Julolidine. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4961-4965.	1.1	44
121	Molecular engineering of starburst triarylamine donor with selenophene containing π-linker for dye-sensitized solar cells. <i>Journal of Materials Chemistry C</i> , 2016, 4, 713-726.	2.7	23
122	A turn-on fluorescent chemodosimeter based on detelluration for detecting ferrous iron (Fe ²⁺) in living cells. <i>Journal of Materials Chemistry B</i> , 2016, 4, 887-892.	2.9	38
123	AMP/GMP Analogs as Affinity ESIPT Probes for Highly Selective Sensing of Alkaline Phosphatase Activity in Living Systems. <i>Chemistry - an Asian Journal</i> , 2015, 10, 2444-2451.	1.7	19
124	Accurate high level <i>ab initio</i> -based global potential energy surface and dynamics calculations for ground state of CH ₂ ⁺ . <i>Journal of Chemical Physics</i> , 2015, 142, 124302.	1.2	38
125	Effect of the Hydrogen Bond on Photochemical Synthesis of Silver Nanoparticles. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12579-12585.	1.1	10
126	Comprehensive Studies on Excited-State Proton Transfer of a Series of 2-(2-Hydroxyphenyl)benzothiazole Derivatives: Synthesis, Optical Properties, and Theoretical Calculations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4242-4251.	1.5	99

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127	Mechanism of the collision energy and reagent vibration TM s effects on the collision time for the reaction Ca+HCl. Computational and Theoretical Chemistry, 2015, 1056, 1-10.	1.1	4
128	<sc>GQSD</sc>: The program for the graphic processing units accelerated quantum scattering dynamics. International Journal of Quantum Chemistry, 2015, 115, 738-743.	1.0	14
129	Theoretical Investigations on Rh(III)-Catalyzed Cross-Dehydrogenative Aryl TM Aryl Coupling via C TM H Bond Activation. Journal of Physical Chemistry A, 2015, 119, 2989-2997.	1.1	13
130	Redox-Responsive Fluorescent Probes with Different Design Strategies. Accounts of Chemical Research, 2015, 48, 1358-1368.	7.6	433
131	Mechanistic studies on C TM reductive coupling of five-coordinate Rh(<sc>iii</sc>) complexes. Organic Chemistry Frontiers, 2015, 2, 783-791.	2.3	7
132	Photophysical Properties of a Post-Self-Assembly Host/Guest Coordination Cage: Visible Light Driven Core-to-Cage Charge Transfer. Journal of Physical Chemistry Letters, 2015, 6, 1942-1947.	2.1	56
133	Quantitative prediction of charge mobilities of π -stacked systems by first-principles simulation. Nature Protocols, 2015, 10, 632-642.	5.5	187
134	Spin mixed charge transfer states of iridium complex Ir(ppy) ₃ : transient absorption and time-resolved photoluminescence. RSC Advances, 2015, 5, 34094-34099.	1.7	30
135	Switching of the Triplet Excited State of Rhodamine/Naphthaleneimide Dyads: An Experimental and Theoretical Study. Journal of Organic Chemistry, 2015, 80, 568-581.	1.7	24
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