

Hans Ågren

List of Publications by Year in descending order

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491
papers

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9264

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16183

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g-index

498
all docs

498
docs citations

498
times ranked

18988
citing authors

#	ARTICLE	IF	CITATIONS
1	The <sc>D</sc>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	Two-dimensional MXenes: From morphological to optical, electric, and magnetic properties and applications. Physics Reports, 2020, 848, 1-58.	25.6	594
3	Ultrasmall Monodisperse NaYF ₄ :Yb ³⁺ /Tm ³⁺ Nanocrystals with Enhanced Near-Infrared to Near-Infrared Upconversion Photoluminescence. ACS Nano, 2010, 4, 3163-3168.	14.6	586
4	Light upconverting core-shell nanostructures: nanophotonic control for emerging applications. Chemical Society Reviews, 2015, 44, 1680-1713.	38.1	483
5	Resonant X-ray Raman scattering. Physics Reports, 1999, 312, 87-330.	25.6	435
6	Theory and Calculation of the Phosphorescence Phenomenon. Chemical Reviews, 2017, 117, 6500-6537.	47.7	420
7	Principles of phosphorescent organic light emitting devices. Physical Chemistry Chemical Physics, 2014, 16, 1719-1758.	2.8	398
8	Density-functional theory of linear and nonlinear time-dependent molecular properties. Journal of Chemical Physics, 2002, 117, 9630-9645.	3.0	359
9	Energy-Cascaded Upconversion in an Organic Dye-Sensitized Core/Shell Fluoride Nanocrystal. Nano Letters, 2015, 15, 7400-7407.	9.1	341
10	Dye-sensitized lanthanide-doped upconversion nanoparticles. Chemical Society Reviews, 2017, 46, 4150-4167.	38.1	281
11	X-Ray Emission Spectroscopy of Hydrogen Bonding and Electronic Structure of Liquid Water. Physical Review Letters, 2002, 89, 137402.	7.8	242
12	Achieving high-efficiency emission depletion nanoscopy by employing cross relaxation in upconversion nanoparticles. Nature Communications, 2017, 8, 1058.	12.8	239
13	Multicolor Photoluminescence Including White-Light Emission by a Single Host-Guest Complex. Journal of the American Chemical Society, 2016, 138, 13541-13550.	13.7	233
14	Electronic and vibronic contributions to two-photon absorption of molecules with multi-branched structures. Journal of Chemical Physics, 2000, 113, 7055-7061.	3.0	226
15	Effects of ĩ centers and symmetry on two-photon absorption cross sections of organic chromophores. Journal of Chemical Physics, 2001, 114, 9813-9820.	3.0	193
16	Simulations of vibronic profiles in two-photon absorption. Chemical Physics Letters, 2000, 330, 447-456.	2.6	178
17	Applications of Few-Layer Nb ₂ C MXene: Narrow-Band Photodetectors and Femtosecond Mode-Locked Fiber Lasers. ACS Nano, 2021, 15, 954-965.	14.6	176
18	Direct SCF direct static-exchange calculations of electronic spectra. Theoretical Chemistry Accounts, 1997, 97, 14-40.	1.4	171

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19	Solvent induced polarizabilities and hyperpolarizabilities of para- ϵ -nitroaniline studied by reaction field linear response theory. <i>Journal of Chemical Physics</i> , 1994, 100, 8240-8250.	3.0	169
20	Femtosecond Dissociation of Core-Excited HCl Monitored by Frequency Detuning. <i>Physical Review Letters</i> , 1997, 79, 3150-3153.	7.8	166
21	Recent Advances in Oxidation Stable Chemistry of 2D MXenes. <i>Advanced Materials</i> , 2022, 34, e2107554.	21.0	163
22	Resonant inelastic x-ray scattering with symmetry-selective excitation. <i>Physical Review A</i> , 1994, 49, 4378-4389.	2.5	154
23	Time-dependent density functional calculations of phosphorescence parameters for fac-tris(2-phenylpyridine) iridium. <i>Chemical Physics</i> , 2007, 333, 157-167.	1.9	154
24	Helical Self-Assembly-Induced Singlet-Triplet Emissive Switching in a Mechanically Sensitive System. <i>Journal of the American Chemical Society</i> , 2017, 139, 785-791.	13.7	153
25	Hetero-MXenes: Theory, Synthesis, and Emerging Applications. <i>Advanced Materials</i> , 2021, 33, e2004129.	21.0	150
26	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. <i>Journal of Chemical Physics</i> , 1992, 97, 9178-9187.	3.0	148
27	Unimolecular Photoconversion of Multicolor Luminescence on Hierarchical Self-Assemblies. <i>Journal of the American Chemical Society</i> , 2013, 135, 5175-5182.	13.7	144
28	Response Theory and Calculations of Spin-Orbit Coupling Phenomena in Molecules. <i>Advances in Quantum Chemistry</i> , 1996, , 71-162.	0.8	137
29	Porphyrins Containing a Triphenylamine Donor and up to Eight Alkoxy Chains for Dye-Sensitized Solar Cells: A High Efficiency of 10.9%. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 27976-27985.	8.0	137
30	Calculations of two-photon absorption cross sections by means of density-functional theory. <i>Chemical Physics Letters</i> , 2003, 374, 446-452.	2.6	136
31	Size-Tunable and Monodisperse Tm^{3+}/Gd^{3+} -Doped Hexagonal $NaYbF_4$ Nanoparticles with Engineered Efficient Near Infrared-to-Near Infrared Upconversion for In Vivo Imaging. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 13884-13893.	8.0	128
32	NIR-Responsive Inorganic 2D Nanomaterials for Cancer Photothermal Therapy: Recent Advances and Future Challenges. <i>Advanced Functional Materials</i> , 2021, 31, 2101625.	14.9	126
33	Quenching of Symmetry Breaking in Resonant Inelastic X-Ray Scattering by Detuned Excitation. <i>Physical Review Letters</i> , 1996, 77, 5035-5038.	7.8	116
34	Nitrogen bonding structure in carbon nitride thin films studied by soft x-ray spectroscopy. <i>Applied Physics Letters</i> , 2001, 79, 4348-4350.	3.3	114
35	SCF and limited CI calculations for assignment of the Auger spectrum and of the satellites in the soft X-ray spectrum of H ₂ O. <i>Chemical Physics Letters</i> , 1975, 35, 336-344.	2.6	113
36	Efficient optimization of large scale MCSCF wave functions with a restricted step algorithm. <i>Journal of Chemical Physics</i> , 1987, 87, 451-466.	3.0	112

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37	Theoretical Study of the Cyclometalated Iridium(III) Complexes Used as Chromophores for Organic Light-Emitting Diodes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 726-735.	2.5	111
38	Dirac Magnons in Honeycomb Ferromagnets. <i>Physical Review X</i> , 2018, 8, .	8.9	106
39	Efficient Broadband Upconversion of Near-Infrared Light in Dye-Sensitized Core/Shell Nanocrystals. <i>Advanced Optical Materials</i> , 2016, 4, 1760-1766.	7.3	104
40	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6701-6705.	4.6	103
41	Use of colloidal upconversion nanocrystals for energy relay solar cell light harvesting in the near-infrared region. <i>Journal of Materials Chemistry</i> , 2012, 22, 16709.	6.7	101
42	Sign change of hyperpolarizabilities of solvated water. <i>Journal of Chemical Physics</i> , 1995, 102, 9362-9367.	3.0	100
43	Cosensitizers for simultaneous filling up of both absorption valleys of porphyrins: a novel approach for developing efficient panchromatic dye-sensitized solar cells. <i>Chemical Communications</i> , 2014, 50, 15609-15612.	4.1	99
44	Enhancing dye-sensitized solar cell efficiency through broadband near-infrared upconverting nanoparticles. <i>Nanoscale</i> , 2017, 9, 6711-6715.	5.6	99
45	Large two-photon absorption cross sections in two-dimensional, charge-transfer, cumulene-containing aromatic molecules. <i>Journal of Chemical Physics</i> , 1999, 111, 7758-7765.	3.0	98
46	Cubic response functions in the multiconfiguration self-consistent field approximation. <i>Journal of Chemical Physics</i> , 1996, 105, 6401-6419.	3.0	96
47	X-ray resonant scattering involving dissociative states. <i>Physical Review A</i> , 1996, 54, 379-393.	2.5	95
48	Spin uncoupling in surface chemisorption of unsaturated hydrocarbons. <i>Journal of Chemical Physics</i> , 1998, 108, 1193-1205.	3.0	94
49	Theoretical DFT study of phosphorescence from porphyrins. <i>Chemical Physics</i> , 2005, 315, 215-239.	1.9	94
50	Luminescent Color Conversion on Cyanostilbene-Functionalized Quantum Dots via In-situ Photo-tuning. <i>Advanced Materials</i> , 2012, 24, 4020-4024.	21.0	93
51	Duration of x-ray Raman scattering. <i>Physical Review A</i> , 1999, 59, 380-389.	2.5	91
52	Restricted density functional theory of linear time-dependent properties in open-shell molecules. <i>Journal of Chemical Physics</i> , 2003, 119, 34-46.	3.0	91
53	Spin-orbit coupling constants in a multiconfiguration linear response approach. <i>Journal of Chemical Physics</i> , 1992, 96, 2118-2126.	3.0	90
54	A High Affinity Red Fluorescence and Colorimetric Probe for Amyloid β^2 Aggregates. <i>Scientific Reports</i> , 2016, 6, 23668.	3.3	90

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55	Molecular stacking dependent phosphorescenceâ€“fluorescence dual emission in a single luminophore for self-recoverable mechanoconversion of multicolor luminescence. <i>Chemical Communications</i> , 2017, 53, 2661-2664.	4.1	90
56	Vibronic emission from short-lived core-hole states: Theory and applications for the water molecule. <i>Physical Review A</i> , 1989, 40, 187-206.	2.5	88
57	Spin-flip time dependent density functional theory applied to excited states with single, double, or mixed electron excitation character. <i>Journal of Chemical Physics</i> , 2010, 133, 114104.	3.0	88
58	Surface-Active <i>cis</i> -Pinonic Acid in Atmospheric Droplets: A Molecular Dynamics Study. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 769-773.	4.6	88
59	Chemical and electronic structures of liquid methanol from x-ray emission spectroscopy and density functional theory. <i>Physical Review B</i> , 2005, 71, .	3.2	87
60	Selective Dualâ€“Channel Imaging on Cyanostyrylâ€“Modified Azulene Systems with Unimolecularly Tunable Visibleâ€“Near Infrared Luminescence. <i>Chemistry - A European Journal</i> , 2017, 23, 7642-7647.	3.3	87
61	Breakdown of the first hyperpolarizability/bond-length alternation parameter relationship. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 16453-16458.	7.1	84
62	Efficient Solar Cells Based on Porphyrin Dyes with Flexible Chains Attached to the Auxiliary Benzothiadiazole Acceptor: Suppression of Dye Aggregation and the Effect of Distortion. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 36875-36885.	8.0	84
63	Local structures of liquid water studied by x-ray emission spectroscopy. <i>Physical Review B</i> , 2004, 69, .	3.2	83
64	Multiply Wrapped Porphyrin Dyes with a Phenothiazine Donor: A High Efficiency of 11.7% Achieved through a Synergetic Coadsorption and Cosensitization Approach. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 5046-5054.	8.0	83
65	Theoretical Study of Phosphorescence of Iridium Complexes with Fluorineâ€“Substituted Phenylpyridine Ligands. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2517-2524.	2.0	82
66	Crystal Multiâ€“Conformational Control Through Deformable Carbonâ€“Sulfur Bond for Singletâ€“Triplet Emissive Tuning. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 4328-4333.	13.8	82
67	A theoretical study of xâ€“ray photoelectron spectra of model molecules for polymethylmethacrylate. <i>Journal of Chemical Physics</i> , 1991, 95, 2965-2974.	3.0	80
68	A three-dimensional ratiometric sensing strategy on unimolecular fluorescenceâ€“thermally activated delayed fluorescence dual emission. <i>Nature Communications</i> , 2019, 10, 731.	12.8	80
69	Density functional theory of nonlinear triplet response properties with applications to phosphorescence. <i>Journal of Chemical Physics</i> , 2003, 119, 11024-11034.	3.0	79
70	X-ray absorption spectra of graphene from first-principles simulations. <i>Physical Review B</i> , 2010, 82, .	3.2	78
71	Highly sensitive detection of low-level water content in organic solvents and cyanide in aqueous media using novel solvatochromic AIEE fluorophores. <i>RSC Advances</i> , 2015, 5, 12191-12201.	3.6	78
72	Simultaneous Multiple Wavelength Upconversion in a Coreâ€“Shell Nanoparticle for Enhanced Near Infrared Light Harvesting in a Dye-Sensitized Solar Cell. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 18018-18025.	8.0	77

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73	Enhanced Upconversion Luminescence in Yb ³⁺ /Tm ³⁺ -Codoped Fluoride Active Core/Active Shell/Inert Shell Nanoparticles through Directed Energy Migration. <i>Nanomaterials</i> , 2014, 4, 55-68.	4.1	76
74	Systematic Investigations on the Roles of the Electron Acceptor and Neighboring Ethynylene Moiety in Porphyrins for Dye-Sensitized Solar Cells. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 21956-21965.	8.0	76
75	On the decay time of upconversion luminescence. <i>Nanoscale</i> , 2019, 11, 4959-4969.	5.6	76
76	Anti-Kasha's Rule Emissive Switching Induced by Intermolecular H-Bonding. <i>Chemistry of Materials</i> , 2018, 30, 8008-8016.	6.7	75
77	Collision-induced $b1\hat{1}g+â€“a1\hat{1}g$, $b1\hat{1}g+â€“X3\hat{1}g$ - and $a1\hat{1}g+â€“X3\hat{1}g$ - transition probabilities in molecular oxygen. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 2231-2239.	1.7	74
78	A comparison of density-functional-theory and coupled-cluster frequency-dependent polarizabilities and hyperpolarizabilities. <i>Molecular Physics</i> , 2005, 103, 439-450.	1.7	74
79	Density Functional Theory Study of Photophysical Properties of Iridium(III) Complexes with Phenylisoquinoline and Phenylpyridine Ligands. <i>Journal of Physical Chemistry C</i> , 2011, 115, 20724-20731.	3.1	74
80	Helicity Inversion of Supramolecular Hydrogels Induced by Achiral Substituents. <i>ACS Nano</i> , 2017, 11, 11880-11889.	14.6	74
81	Cross-interaction of tau PET tracers with monoamine oxidase B: evidence from in silico modelling and in vivo imaging. <i>European Journal of Nuclear Medicine and Molecular Imaging</i> , 2019, 46, 1369-1382.	6.4	74
82	Effects of dipole alignment and channel interference on two-photon absorption cross sections of two-dimensional charge-transfer systems. <i>Journal of Chemical Physics</i> , 2002, 117, 11102-11106.	3.0	73
83	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. <i>Chemical Physics</i> , 2009, 358, 245-257.	1.9	73
84	Activation of Triplet Dioxygen by Glucose Oxidase:â€‰ Spin-Orbit Coupling in the Superoxide Ion. <i>Journal of Physical Chemistry B</i> , 2002, 106, 3742-3750.	2.6	71
85	One-step solvothermal synthesis of high-emissive amphiphilic carbon dots <i>via</i> rigidity derivation. <i>Chemical Science</i> , 2018, 9, 1323-1329.	7.4	71
86	Density functional theory study of vibronic structure of the first absorption Qx band in free-base porphyrin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 308-323.	3.9	70
87	Different Positron Emission Tomography Tau Tracers Bind to Multiple Binding Sites on the Tau Fibril: Insight from Computational Modeling. <i>ACS Chemical Neuroscience</i> , 2018, 9, 1757-1767.	3.5	69
88	Chirality Control for in Situ Preparation of Gold Nanoparticle Superstructures Directed by a Coordinatable Organogelator. <i>Journal of the American Chemical Society</i> , 2013, 135, 9174-9180.	13.7	68
89	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20765-20774.	8.0	68
90	A theoretical study of the near-edge x-ray absorption spectra of some larger amino acids. <i>Journal of Chemical Physics</i> , 1998, 109, 1456-1464.	3.0	66

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91	Einsteinâ€“Bohr recoiling double-slit gedanken experiment performed at the molecular level. Nature Photonics, 2015, 9, 120-125.	31.4	66
92	Phase angle encoded upconversion luminescent nanocrystals for multiplexing applications. Nanoscale, 2017, 9, 1676-1686.	5.6	66
93	Internal and external heavy-atom effects on phosphorescence radiative lifetimes calculated using a mean-field spinâ€“orbit Hamiltonian. Chemical Physics Letters, 1999, 310, 215-221.	2.6	65
94	Engineering Topochemical Polymerizations Using Block Copolymer Templates. Journal of the American Chemical Society, 2014, 136, 13381-13387.	13.7	65
95	Ultrafast photonics applications of emerging 2D-Xenes beyond graphene. Nanophotonics, 2022, 11, 1261-1284.	6.0	65
96	Ab initio calculations of the polarizability and the hyperpolarizability of C60. Journal of Chemical Physics, 1997, 106, 8788-8791.	3.0	64
97	Hydrogen Bonding to Tyrosyl Radical Analyzed by Ab Initio g-Tensor Calculations. Journal of Physical Chemistry A, 2000, 104, 5149-5153.	2.5	64
98	Contribution of TADF and exciplex emission for efficient â€“warm-whiteâ€“OLEDs. Journal of Materials Chemistry C, 2018, 6, 1543-1550.	5.5	64
99	Femtosecond nuclear motion of HCl probed by resonant x-ray Raman scattering in the Cl 1s region. Physical Review A, 2006, 73, .	2.5	63
100	Collapse of vibrational structure in spectra of resonant x-ray Raman scattering. Physical Review A, 1997, 56, 256-264.	2.5	61
101	Relativistic effects on linear and nonlinear polarizabilities studied by effective-core potential, Douglasâ€“Kroll, and Diracâ€“Hartreeâ€“Fock response theory. Journal of Chemical Physics, 2002, 116, 6914-6923.	3.0	60
102	Huge upconversion luminescence enhancement by a cascade optical field modulation strategy facilitating selective multispectral narrow-band near-infrared photodetection. Light: Science and Applications, 2020, 9, 184.	16.6	60
103	Nonlinear optical response of molecules in a nonequilibrium solvation model. Journal of Chemical Physics, 1998, 109, 5576-5584.	3.0	58
104	Integrating Timeâ€“Resolved Imaging Information by Singleâ€“Luminophore Dual Thermally Activated Delayed Fluorescence. Angewandte Chemie - International Edition, 2020, 59, 17018-17025.	13.8	58
105	Magnetic phosphorescence of molecular oxygen. A study of the $b^1\Sigma_g^+ \rightarrow X^3\Sigma_g^-$ transition probability using multiconfiguration response theory. Chemical Physics, 1996, 208, 299-311.	1.9	57
106	Tuning for Visible Fluorescence and Near-Infrared Phosphorescence on a Unimolecular Mechanically Sensitive Platform via Adjustable CHâ€“â€“ Interaction. ACS Applied Materials & Interfaces, 2017, 9, 3865-3872.	8.0	56
107	Novel Zinc Complex with an Ethylenediamine Schiff Base for High-Luminance Blue Fluorescent OLED Applications. Journal of Physical Chemistry C, 2019, 123, 11850-11859.	3.1	56
108	Molecular Structure â€“ Optical Property Relationships for a Series of Non-Centrosymmetric Two-photon Absorbing Push-Pull Triarylamine Molecules. Scientific Reports, 2014, 4, 4447.	3.3	55

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109	Mechanism for the Extremely Efficient Sensitization of Yb ³⁺ Luminescence in CsPbCl ₃ Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 487-492.	4.6	55
110	Effects of Graphene Nanopore Geometry on DNA Sequencing. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1602-1607.	4.6	54
111	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28040-28051.	2.8	54
112	The interpretation of the Wulf absorption band of ozone. <i>Chemical Physics Letters</i> , 1994, 217, 531-538.	2.6	53
113	Black Phosphorus/Polymers: Status and Challenges. <i>Advanced Materials</i> , 2021, 33, e2100113.	21.0	53
114	Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13349-13357.	2.6	52
115	Neo-Fused Hexaphyrin: A Molecular Puzzle Containing an N-Linked Pentaphyrin. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 14069-14073.	13.8	52
116	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. <i>Vibrational Spectroscopy</i> , 2012, 61, 156-166.	2.2	51
117	Red turn-on fluorescent phenazine-cyanine chemodosimeters for cyanide anion in aqueous solution and its application for cell imaging. <i>Sensors and Actuators B: Chemical</i> , 2014, 203, 833-847.	7.8	51
118	On the interpretation of the external heavy atom effect on singlet-triplet transitions. <i>Chemical Physics</i> , 1994, 181, 15-28.	1.9	50
119	Lanthanide-Doped Fluoride Core/Multishell Nanoparticles for Broadband Upconversion of Infrared Light. <i>Advanced Optical Materials</i> , 2015, 3, 575-582.	7.3	50
120	Selective gating to vibrational modes through resonant X-ray scattering. <i>Nature Communications</i> , 2017, 8, 14165.	12.8	50
121	Ultra-Small 2D PbS Nanoplatelets: Liquid-Phase Exfoliation and Emerging Applications for Photo-Electrochemical Photodetectors. <i>Small</i> , 2021, 17, e2005913.	10.0	50
122	Quasiparticle electronic structure and optical spectra of single-layer and bilayer PdSe ₂ : Proximity and defect-induced band gap renormalization. <i>Physical Review B</i> , 2019, 99, .	10.2	49
123	Investigation of the Binding Profiles of AZD2184 and Thioflavin T with Amyloid- β (1-42) Fibril by Molecular Docking and Molecular Dynamics Methods. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11560-11567.	2.6	48
124	Near infrared harvesting dye-sensitized solar cells enabled by rare-earth upconversion materials. <i>Dalton Transactions</i> , 2018, 47, 8526-8537.	3.3	48
125	The vibronically induced phosphorescence in benzene. <i>Chemical Physics</i> , 1993, 175, 245-254.	1.9	47
126	Fluorescence and FTIR Spectra Analysis of Trans-A2B2-Substituted Di- and Tetra-Phenyl Porphyrins. <i>Materials</i> , 2010, 3, 4446-4475.	2.9	47

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127	2-Diphenylaminothiophene as the donor of porphyrin sensitizers for dye-sensitized solar cells. <i>New Journal of Chemistry</i> , 2014, 38, 3227-3235.	2.8	47
128	Response theory for static and dynamic polarizabilities of excited states. <i>Journal of Chemical Physics</i> , 1996, 105, 581-587.	3.0	46
129	Dual-Phase Thermally Activated Delayed Fluorescence Luminogens: A Material for Time-Resolved Imaging Independent of Probe Pretreatment and Probe Concentration. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 7548-7554.	13.8	46
130	Simultaneous anchoring of Ni nanoparticles and single-atom Ni on BCN matrix promotes efficient conversion of nitrate in water into high-value-added ammonia. <i>Chemical Engineering Journal</i> , 2022, 433, 133190.	12.7	46
131	Optical Properties of Few-Layer Ti_3CN MXene: From Experimental Observations to Theoretical Calculations. <i>ACS Nano</i> , 2022, 16, 3059-3069.	14.6	46
132	An efficient method for calculating molecular radiative intensities in the VUV and soft X-ray wavelength regions. <i>Physica Scripta</i> , 1989, 40, 745-750.	2.5	45
133	Spin-catalysis phenomena. <i>International Journal of Quantum Chemistry</i> , 1996, 57, 519-532.	2.0	45
134	A Fluorescence-Phosphorescence-Phosphorescence Triple-Channel Emission Strategy for Full-Color Luminescence. <i>Small</i> , 2020, 16, e1906475.	10.0	45
135	Theoretical study of triplet state properties of free-base porphyrin. <i>Chemical Physics</i> , 2005, 312, 299-309.	1.9	44
136	Potassium ions promote electrochemical nitrogen reduction on nano-Au catalysts triggered by bifunctional boron supramolecular assembly. <i>Journal of Materials Chemistry A</i> , 2020, 8, 13086-13094.	10.3	44
137	Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 272-276.	4.6	43
138	Fast upconversion super-resolution microscopy with 10 ¹⁴ s per pixel dwell times. <i>Nanoscale</i> , 2019, 11, 1563-1569.	5.6	43
139	Photoinduced Radical Emission in a Coassembly System. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 23842-23848.	13.8	43
140	Modeling of dynamic molecular solvent properties using local and cavity field approaches. <i>Journal of Chemical Physics</i> , 2000, 112, 1868-1875.	3.0	42
141	Substituent effects on the photophysical properties of fluorescent 2-benzoylmethylenequinoline difluoroboranes: A combined experimental and quantum chemical study. <i>Dyes and Pigments</i> , 2013, 99, 957-965.	3.7	42
142	Photon Upconversion Kinetic Nanosystems and Their Optical Response. <i>Laser and Photonics Reviews</i> , 2018, 12, 1700144.	8.7	42
143	Copper confined in vesicle-like BCN cavities promotes electrochemical reduction of nitrate to ammonia in water. <i>Journal of Materials Chemistry A</i> , 2021, 9, 23675-23686.	10.3	42
144	The X-ray emission spectrum of water. <i>Journal of Physics B: Atomic and Molecular Physics</i> , 1975, 8, L18-L19.	1.6	41

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145	Influence of electron-acceptor strength on the resonant two-photon absorption cross sections of diphenylaminofluorene-based chromophores. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 3869-3873.	2.8	41
146	Type-II colloidal quantum dot sensitized solar cells with a thiourea based organic redox couple. <i>Journal of Materials Chemistry</i> , 2012, 22, 6032.	6.7	41
147	Dioxygen spectra and bioactivation. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1847-1867.	2.0	41
148	Theoretical study on key factors in DNA sequencing with graphene nanopores. <i>RSC Advances</i> , 2013, 3, 2445.	3.6	41
149	A protected excitation-energy reservoir for efficient upconversion luminescence. <i>Nanoscale</i> , 2018, 10, 250-259.	5.6	41
150	Micro lens array enhanced upconversion luminescence at low excitation irradiance. <i>Nanoscale</i> , 2019, 11, 14070-14078.	5.6	41
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