Yi Luo

List of Publications by Year
in descending order

645	34,882	3919 88	6818 155
papers	citations	h-index	g-index

662	662	662	33885
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Singleâ€Atom Pt as Coâ€Catalyst for Enhanced Photocatalytic H₂ Evolution. Advanced Materials, 2016, 28, 2427-2431.	11.1	1,156
2	Nickelâ€“vanadium monolayer double hydroxide for efficient electrochemical water oxidation. Nature Communications, 2016, 7, 11981.	5.8	808
3	Occurrence and Transport of Tetracycline, Sulfonamide, Quinolone, and Macrolide Antibiotics in the Haihe River Basin, China. Environmental Science & Technology, 2011, 45, 1827-1833.	4.6	786
4	Defect-Mediated Electronâ€“Hole Separation in One-Unit-Cell ZnIn₂S₄ Layers for Boosted Solar-Driven CO₂ Reduction. Journal of the American Chemical Society, 2017, 139, 7586-7594.	6.6	764
5	Atomically dispersed platinum supported on curved carbon supports for efficient electrocatalytic hydrogen evolution. Nature Energy, 2019, 4, 512-518.	19.8	756
6	Trends in Antibiotic Resistance Genes Occurrence in the Haihe River, China. Environmental Science & Technology, 2010, 44, 7220-7225.	4.6	661
7	Single Pt Atoms Confined into a Metalâ€“Organic Framework for Efficient Photocatalysis. Advanced Materials, 2018, 30, 1705112.	11.1	599
8	Conversion of Dinitrogen to Ammonia by FeN₃-Embedded Graphene. Journal of the American Chemical Society, 2016, 138, 8706-8709.	6.6	562
9	Occurrence of sulfonamide and tetracycline-resistant bacteria and resistance genes in aquaculture environment. Water Research, 2012, 46, 2355-2364.	5.3	556
10	Boosting Photocatalytic Hydrogen Production of a Metalâ€“Organic Framework Decorated with Platinum Nanoparticles: The Platinum Location Matters. Angewandte Chemie - International Edition, 2016, 55, 9389-9393.	7.2	513
11	Prevalence and proliferation of antibiotic resistance genes in two municipal wastewater treatment plants. Water Research, 2015, 85, 458-466.	5.3	448
12	Versatile Roomâ€Temperatureâ€Phosphorescent Materials Prepared from Nâ€Substituted Naphthalimides: Emission Enhancement and Chemical Conjugation. Angewandte Chemie - International Edition, 2016, 55, 9872-9876.	7.2	343
13	Dinitrogen Cleavage and Hydrogenation by a Trinuclear Titanium Polyhydride Complex. Science, 2013, 340, 1549-1552.	6.0	327
14	Tuning Chemical Enhancement of SERS by Controlling the Chemical Reduction of Graphene Oxide Nanosheets. ACS Nano, 2011, 5, 952-958.	7.3	324
15	How Graphene Is Cut upon Oxidation?. Journal of the American Chemical Society, 2009, 131, 6320-6321.	6.6	323
16	Ultrathin amorphous cobaltâ€“vanadium hydr(oxy)oxide catalysts for the oxygen evolution reaction. Energy and Environmental Science, 2018, 11, 1736-1741.	15.6	310
17	Visualizing coherent intermolecular dipoleâ€“dipole coupling in real space. Nature, 2016, 531, 623-627.	13.7	284
18	Cationic Alkyl Rare-Earth Metal Complexes Bearing an Ancillary Bis(phosphinophenyl)amido Ligand: A Catalytic System for Livingcis-1,4-Polymerization and Copolymerization of Isoprene and Butadiene. Angewandte Chemie - International Edition, 2007, 46, 1909-1913.	7.2	263

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19	New Mechanism for Photocatalytic Reduction of CO₂ on the Anatase TiO₂(101) Surface: The Essential Role of Oxygen Vacancy. Journal of the American Chemical Society, 2016, 138, 15896-15902.	6.6	256
20	Distinguishing adjacent molecules on a surface using plasmon-enhanced Raman scattering. Nature Nanotechnology, 2015, 10, 865-869.	15.6	239
21	Distribution, sources and composition of antibiotics in sediment, overlying water and pore water from Taihu Lake, China. Science of the Total Environment, 2014, 497-498, 267-273.	3.9	234
22	Electronic and vibronic contributions to two-photon absorption of molecules with multi-branched structures. Journal of Chemical Physics, 2000, 113, 7055-7061.	1.2	226
23	Occurrence and distribution of antibiotics, antibiotic resistance genes in the urban rivers in Beijing, China. Environmental Pollution, 2016, 213, 833-840.	3.7	226
24	Isoprene Polymerization with Yttrium Amidinate Catalysts: Switching the Regioâ€and Stereoselectivity by Addition of AlMe₃. Angewandte Chemie - International Edition, 2008, 47, 2642-2645.	7.2	225
25	Graphene nanoribbon as a negative differential resistance device. Applied Physics Letters, 2009, 94, .	1.5	219
26	Hollow Ironâ€“Vanadium Composite Spheres: A Highly Efficient Ironâ€Based Water Oxidation Electrocatalyst without the Need for Nickel or Cobalt. Angewandte Chemie - International Edition, 2017, 56, 3289-3293.	7.2	216
27	Unprecedented Isospecific 3,4-Polymerization of Isoprene by Cationic Rare Earth Metal Alkyl Species Resulting from a Binuclear Precursor. Journal of the American Chemical Society, 2005, 127, 14562-14563.	6.6	215
28	Tracking Structural Selfâ€Reconstruction and Identifying True Active Sites toward Cobalt Oxychloride Precatalyst of Oxygen Evolution Reaction. Advanced Materials, 2019, 31, e1805127.	11.1	211
29	Optically Switchable Photocatalysis in Ultrathin Black Phosphorus Nanosheets. Journal of the American Chemical Society, 2018, 140, 3474-3480.	6.6	210
30	Nonlocal Exchange Interaction Removes Half-Metallicity in Graphene Nanoribbons. Nano Letters, 2007, 7, 2211-2213.	4.5	202
31	Effects of Ï€ centers and symmetry on two-photon absorption cross sections of organic chromophores. Journal of Chemical Physics, 2001, 114, 9813-9820.	1.2	193
32	Role of point defects on the reactivity of reconstructed anatase titanium dioxide (001) surface. Nature Communications, 2013, 4, 2214.	5.8	184
33	Spatial and temporal variations in the relationship between lake water surface temperatures and water quality - A case study of Dianchi Lake. Science of the Total Environment, 2018, 624, 859-871.	3.9	184
34	Simulations of vibronic profiles in two-photon absorption. Chemical Physics Letters, 2000, 330, 447-456.	1.2	178
35	Aggregationâ€Induced Dualâ€Phosphorescence from Organic Molecules for Nondoped Lightâ€Emitting Diodes. Advanced Materials, 2019, 31, e1904273.	11.1	177
36	Designing pâ€Type Semiconductorâ€“Metal Hybrid Structures for Improved Photocatalysis. Angewandte Chemie - International Edition, 2014, 53, 5107-5111.	7.2	176

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37	Simultaneous removal of antibiotics and antibiotic resistance genes from pharmaceutical wastewater using the combinations of up-flow anaerobic sludge bed, anoxic-oxic tank, and advanced oxidation technologies. Water Research, 2019, 159, 511-520.	5.3	175
38	Molecular co-catalyst accelerating hole transfer for enhanced photocatalytic H2 evolution. Nature Communications, 2015, 6, 8647.	5.8	172
39	Realizing a Not-Strong-Not-Weak Polarization Electric Field in Single-Atom Catalysts Sandwiched by Boron Nitride and Graphene Sheets for Efficient Nitrogen Fixation. Journal of the American Chemical Society, 2020, 142, 19308-19315.	6.6	170
40	Observation of Photocatalytic Dissociation of Water on Terminal Ti Sites of TiO₂(110)-1 Ã— 1 Surface. Journal of the American Chemical Society, 2012, 134, 9978-9985.	6.6	160
41	A Secondâ€Coordinationâ€Sphere Strategy to Modulate Nickelâ€•and Palladiumâ€Catalyzed Olefin Polymerization and Copolymerization. Angewandte Chemie - International Edition, 2017, 56, 11604-11609.	7.2	159
42	Atomicâ€Layerâ€Confined Doping for Atomicâ€Level Insights into Visibleâ€Light Water Splitting. Angewandte Chemie - International Edition, 2015, 54, 9266-9270.	7.2	158
43	Sub-nanometre control of the coherent interaction between a single molecule and a plasmonic nanocavity. Nature Communications, 2017, 8, 15225.	5.8	158
44	First-principle study of electronic and optical properties of two-dimensional materials-based heterostructures based on transition metal dichalcogenides and boron phosphide. Applied Surface Science, 2019, 476, 70-75.	3.1	154
45	Sub-nanometre resolution in single-molecule photoluminescence imaging. Nature Photonics, 2020, 14, 693-699.	15.6	152
46	Mechanism for Negative Differential Resistance in Molecular Electronic Devices: Local Orbital Symmetry Matching. Physical Review Letters, 2007, 99, 146803.	2.9	150
47	Theoretical Study on the Mechanism of Photoreduction of CO₂ to CH₄ on the Anatase TiO₂(101) Surface. ACS Catalysis, 2016, 6, 2018-2025.	5.5	149
48	The occurrence and fate of tetracyclines in two pharmaceutical wastewater treatment plants of Northern China. Environmental Science and Pollution Research, 2016, 23, 1722-1731.	2.7	147
49	Effect of the selective pressure of sub-lethal level of heavy metals on the fate and distribution of ARGs in the catchment scale. Environmental Pollution, 2017, 220, 900-908.	3.7	144
50	Enhanced Asymmetric Induction for the Copolymerization of CO₂ and Cyclohexene Oxide with Unsymmetric Enantiopure SalenCo(III) Complexes: Synthesis of Crystalline CO₂-Based Polycarbonate. Journal of the American Chemical Society, 2012, 134, 5682-5688.	6.6	140
51	Ammonia formation by a thiolate-bridged diiron amide complex as a nitrogenase mimic. Nature Chemistry, 2013, 5, 320-326.	6.6	139
52	Unraveling Surface Plasmon Decay in Coreâ€“Shell Nanostructures toward Broadband Light-Driven Catalytic Organic Synthesis. Journal of the American Chemical Society, 2016, 138, 6822-6828.	6.6	136
53	Insights into the excitonic processes in polymeric photocatalysts. Chemical Science, 2017, 8, 4087-4092.	3.7	136
54	A Unique Semiconductorâ€“Metalâ€“Graphene Stack Design to Harness Charge Flow for Photocatalysis. Advanced Materials, 2014, 26, 5689-5695.	11.1	134

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55	Proliferation of Multidrug-Resistant New Delhi Metallo-Î²-lactamase Genes in Municipal Wastewater Treatment Plants in Northern China. Environmental Science and Technology Letters, 2014, 1, 26-30.	3.9	133
56	Ionic Liquid Facilitates the Conjugative Transfer of Antibiotic Resistance Genes Mediated by Plasmid RP4. Environmental Science & Technology, 2015, 49, 8731-8740.	4.6	132
57	Heteroatom-assisted olefin polymerization by rare-earth metal catalysts. Science Advances, 2017, 3, e1701011.	4.7	122
58	Catalysed low temperature H2 release from nitrogen heterocycles. New Journal of Chemistry, 2006, 30, 1675.	1.4	121
59	Fate and proliferation of typical antibiotic resistance genes in five full-scale pharmaceutical wastewater treatment plants. Science of the Total Environment, 2015, 526, 366-373.	3.9	121
60	Insight into Electrocatalysts as Co-catalysts in Efficient Photocatalytic Hydrogen Evolution. ACS Catalysis, 2016, 6, 4253-4257.	5.5	120
61	Conjugative multi-resistant plasmids in Haihe River and their impacts on the abundance and spatial distribution of antibiotic resistance genes. Water Research, 2017, 111, 81-91.	5.3	114
62	Wide-bandgap organicâ€“inorganic hybrid and all-inorganic perovskite solar cells and their application in all-perovskite tandem solar cells. Energy and Environmental Science, 2021, 14, 5723-5759.	15.6	114
63	Aggregation-enhanced luminescence and vibronic coupling of silole molecules from first principles. Physical Review B, 2006, 73, .	1.1	113
64	Unraveling the formation mechanism of graphitic nitrogen-doping in thermally treated graphene with ammonia. Scientific Reports, 2016, 6, 23495.	1.6	111
65	Single Crystalline Submicrotubes from Small Organic Molecules. Chemistry of Materials, 2005, 17, 6430-6435.	3.2	110
66	First-Principles Study on Transition-Metal Dichalcogenide/BSe van der Waals Heterostructures: A Promising Water-Splitting Photocatalyst. Journal of Physical Chemistry C, 2019, 123, 22742-22751.	1.5	110
67	High-efficiency photocatalyst for water splitting: a Janus MoSSe/XN (Xâ€‰â€‰=â€‰â€‰Ga, Al) van der Waals heterostructure. Journal Physics D: Applied Physics, 2020, 53, 185504.	1.3	110
68	Coherent Random Fiber Laser Based on Nanoparticles Scattering in the Extremely Weakly Scattering Regime. Physical Review Letters, 2012, 109, 253901.	2.9	108
69	Spatialâ€Temporal Variation of Lake Surface Water Temperature and Its Driving Factors in Yunnanâ€Guizhou Plateau. Water Resources Research, 2019, 55, 4688-4703.	1.7	108
70	Grapheneâ€“boron nitride hybrid-supported single Mo atom electrocatalysts for efficient nitrogen reduction reaction. Journal of Materials Chemistry A, 2019, 7, 15173-15180.	5.2	107
71	Computational Study of Titanocene-Catalyzed Dehydrocoupling of the Adduct Me2NHÂ·BH3:Â An Intramolecular, Stepwise Mechanism. Organometallics, 2007, 26, 3597-3600.	1.1	106
72	Accurate Determination of Interfacial Protein Secondary Structure by Combining Interfacial-Sensitive Amide I and Amide III Spectral Signals. Journal of the American Chemical Society, 2014, 136, 1206-1209.	6.6	106

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73	Transition-metal dichalcogenides/Mg(OH)₂ van der Waals heterostructures as promising water-splitting photocatalysts: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 1791-1796.	1.3	106
74	Ultrahigh Carrier Mobility in the Two-Dimensional Semiconductors B₈Si₄, B₈Ge₄, and B₈Sn₄. Chemistry of Materials, 2021, 33, 6475-6483.	3.2	104
75	Arctic antibiotic resistance gene contamination, a result of anthropogenic activities and natural origin. Science of the Total Environment, 2018, 621, 1176-1184.	3.9	102
76	Oxyhydroxide Nanosheets with Highly Efficient Electronâ€“Hole Pair Separation for Hydrogen Evolution. Angewandte Chemie - International Edition, 2016, 55, 2137-2141.	7.2	99
77	Large two-photon absorption cross sections in two-dimensional, charge-transfer, cumulene-containing aromatic molecules. Journal of Chemical Physics, 1999, 111, 7758-7765.	1.2	98
78	The Microscopic Structure of Liquid Methanol from Raman Spectroscopy. Journal of Physical Chemistry B, 2010, 114, 3567-3573.	1.2	98
79	Inâ€…situ Integration of a Metallic 1Tâ€MoS₂/CdS Heterostructure as a Means to Promote Visibleâ€Lightâ€Driven Photocatalytic Hydrogen Evolution. ChemCatChem, 2016, 8, 2614-2619.	1.8	98
80	Narrowband Emission from Organic Fluorescent Emitters with Dominant Lowâ€Frequency Vibronic Coupling. Advanced Optical Materials, 2021, 9, 2001845.	3.6	98
81	Solvent effects on the electronic structure of a newly synthesized two-photon polymerization initiator. Journal of Chemical Physics, 2003, 119, 1208-1213.	1.2	97
82	A quantum chemistry approach for currentÃ¢â‚¬â€œvoltage characterization of molecular junctions. Physical Chemistry Chemical Physics, 2001, 3, 5017-5023.	1.3	95
83	Lighting Up the Invisible Twisted Intramolecular Charge Transfer State by High Pressure. Journal of Physical Chemistry Letters, 2019, 10, 748-753.	2.1	95
84	Unusual Thiolate-Bridged Diiron Clusters Bearing the cis-HNâ•NH Ligand and Their Reactivities with Terminal Alkynes. Journal of the American Chemical Society, 2011, 133, 1147-1149.	6.6	94
85	A New Cubic Phase for a NaYF₄ Host Matrix Offering High Upconversion Luminescence Efficiency. Advanced Materials, 2015, 27, 5528-5533.	11.1	94
86	Role of the co-catalyst in the asymmetric coupling of racemic epoxides with CO2 using multichiral Co(iii) complexes: product selectivity and enantioselectivity. Chemical Science, 2012, 3, 2094.	3.7	93
87	Theoretical Modeling of Plasmon-Enhanced Raman Images of a Single Molecule with Subnanometer Resolution. Journal of the American Chemical Society, 2015, 137, 9515-9518.	6.6	92
88	Electrically driven single-photon emission from an isolated single molecule. Nature Communications, 2017, 8, 580.	5.8	92
89	Visually constructing the chemical structure of a single molecule by scanning Raman picoscopy. National Science Review, 2019, 6, 1169-1175.	4.6	91
90	Design and control of electron transport properties of single molecules. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15259-15263.	3.3	88

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91	Oxidation states of graphene: Insights from computational spectroscopy. Journal of Chemical Physics, 2009, 131, 244505.	1.2	88
92	Synergistic Effect of Surface-Terminated Oxygen Vacancy and Single-Atom Catalysts on Defective MXenes for Efficient Nitrogen Fixation. Journal of Physical Chemistry Letters, 2020, 11, 5051-5058.	2.1	88
93	First-Principles Simulations of Inelastic Electron Tunneling Spectroscopy of Molecular Electronic Devices. Nano Letters, 2005, 5, 1551-1555.	4.5	87
94	Chemical and electronic structures of liquid methanol from x-ray emission spectroscopy and density functional theory. Physical Review B, 2005, 71, .	1.1	87
95	What Are the Adsorption Sites for CO on the Reduced TiO₂(110)-1 Ã— 1 Surface?. Journal of the American Chemical Society, 2009, 131, 7958-7959.	6.6	87
96	ortho-Selective Câ€“H addition of N,N-dimethyl anilines to alkenes by a yttrium catalyst. Chemical Science, 2016, 7, 5265-5270.	3.7	87
97	Non-catalytic hydrogenation of VO2 in acid solution. Nature Communications, 2018, 9, 818.	5.8	87
98	Heavy metal copper accelerates the conjugative transfer of antibiotic resistance genes in freshwater microcosms. Science of the Total Environment, 2020, 717, 137055.	3.9	87
99	Combining photocatalytic hydrogen generation and capsule storage in graphene based sandwich structures. Nature Communications, 2017, 8, 16049.	5.8	86
100	Strain-enhanced properties of van der Waals heterostructure based on blue phosphorus and g-GaN as a visible-light-driven photocatalyst for water splitting. RSC Advances, 2019, 9, 4816-4823.	1.7	86
101	Direct writing of electronic devices on graphene oxide by catalytic scanning probe lithography. Nature Communications, 2012, 3, 1194.	5.8	85
102	Organic field-effect optical waveguides. Nature Communications, 2018, 9, 4790.	5.8	85
103	Dinitrogen Activation by Dihydrogen and a PNP-Ligated Titanium Complex. Journal of the American Chemical Society, 2017, 139, 1818-1821.	6.6	83
104	Occurrence and distribution of clinical and veterinary antibiotics in the faeces of a Chinese population. Journal of Hazardous Materials, 2020, 383, 121129.	6.5	83
105	Active Sites of Pd-Doped Flat and Stepped Cu(111) Surfaces for H₂ Dissociation in Heterogeneous Catalytic Hydrogenation. ACS Catalysis, 2013, 3, 1245-1252.	5.5	79
106	X-ray absorption spectra of graphene from first-principles simulations. Physical Review B, 2010, 82, .	1.1	78
107	An Ionic Liquid Facilitates the Proliferation of Antibiotic Resistance Genes Mediated by Class I Integrons. Environmental Science and Technology Letters, 2014, 1, 266-270.	3.9	78
108	A van der Waals Heterostructure Based on Graphene-like Gallium Nitride and Boron Selenide: A High-Efficiency Photocatalyst for Water Splitting. ACS Omega, 2019, 4, 21689-21697.	1.6	78

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109	Catalytic Activity of Single Transition-Metal Atom Doped in Cu(111) Surface for Heterogeneous Hydrogenation. Journal of Physical Chemistry C, 2013, 117, 14618-14624.	1.5	77
110	Occurrence and reduction of antibiotic resistance genes in conventional and advanced drinking water treatment processes. Science of the Total Environment, 2019, 669, 777-784.	3.9	77
111	Determining structural and chemical heterogeneities of surface species at the single-bond limit. Science, 2021, 371, 818-822.	6.0	77
112	Unraveling the Mechanism for the Sharpâ€Tip Enhanced Electrocatalytic Carbon Dioxide Reduction: The Kinetics Decide. Angewandte Chemie - International Edition, 2017, 56, 15617-15621.	7.2	76
113	Thermally Activated Delayed Fluorescence in an Organic Cocrystal: Narrowing the Singletâ€“Triplet Energy Gap via Charge Transfer. Angewandte Chemie - International Edition, 2019, 58, 11311-11316.	7.2	76
114	Versatile Roomâ€Temperatureâ€Phosphorescent Materials Prepared from Nâ€Substituted Naphthalimides: Emission Enhancement and Chemical Conjugation. Angewandte Chemie, 2016, 128, 10026-10030.	1.6	75
115	Fabrication of Graphene Nanomesh and Improved Chemical Enhancement for Raman Spectroscopy. Journal of Physical Chemistry C, 2012, 116, 15741-15746.	1.5	74
116	Effects of dipole alignment and channel interference on two-photon absorption cross sections of two-dimensional charge-transfer systems. Journal of Chemical Physics, 2002, 117, 11102-11106.	1.2	73
117	Location of Trapped Hole on Rutile-TiO2(110) Surface and Its Role in Water Oxidation. Journal of Physical Chemistry C, 2012, 116, 7863-7866.	1.5	73
118	CeO₂ Nanoparticles Regulate the Propagation of Antibiotic Resistance Genes by Altering Cellular Contact and Plasmid Transfer. Environmental Science & Technology, 2020, 54, 10012-10021.	4.6	73
119	Towards high-performance sustainable polymers via isomerization-driven irreversible ring-opening polymerization of five-membered thionolactones. Nature Chemistry, 2022, 14, 294-303.	6.6	73
120	Bioâ€“nano interaction of proteins adsorbed on single-walled carbon nanotubes. Carbon, 2009, 47, 967-973.	5.4	72
121	Analysis on driving factors of lake surface water temperature for major lakes in Yunnan-Guizhou Plateau. Water Research, 2020, 184, 116018.	5.3	72
122	Experimental Identification of Ultrafast Reverse Hole Transfer at the Interface of the Photoexcited Methanol/Graphitic Carbon Nitride System. Angewandte Chemie - International Edition, 2018, 57, 5320-5324.	7.2	71
123	Currentâ€“voltage characteristics of single molecular junction: Dimensionality of metal contacts. Journal of Chemical Physics, 2003, 119, 4923-4928.	1.2	70
124	Density functional theory study of vibronic structure of the first absorption Qx band in free-base porphin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 308-323.	2.0	70
125	Scandium-Catalyzed Regio- and Stereoselective Cyclopolymerization of Functionalized Î±,Ï‰-Dienes and Copolymerization with Ethylene. Journal of the American Chemical Society, 2019, 141, 12624-12633.	6.6	70
126	Municipal Solid Waste Treatment System Increases Ambient Airborne Bacteria and Antibiotic Resistance Genes. Environmental Science & Technology, 2020, 54, 3900-3908.	4.6	70

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127	Novel heterocycle-based organic molecules with two-photon induced blue fluorescent emission. Journal of Materials Chemistry, 2003, 13, 708-711.	6.7	68
128	Solvent effects on two-photon absorption of dialkylamino substituted distyrylbenzene chromophore. Journal of Chemical Physics, 2007, 126, 204509.	1.2	68
129	Two-photon excited hemoglobin fluorescence. Biomedical Optics Express, 2011, 2, 71.	1.5	68
130	CO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>dissociation activated through electron attachment on the reduced rutile TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(110)-1<mml:math xmlns:mml="http://www.w3.org/1998	1.1	68
131	Mechanistic Insights into Scandium-Catalyzed Hydroaminoalkylation of Olefins with Amines: Origin of Regioselectivity and Charge-Based Prediction Model. Organometallics, 2017, 36, 1557-1565.	1.1	67
132	Risk assessment of antibiotic resistance genes in the drinking water system. Science of the Total Environment, 2021, 800, 149650.	3.9	67
133	Mechanistic Investigation on Scandium-Catalyzed Câ€“H Addition of Pyridines to Olefins. Organometallics, 2012, 31, 3930-3937.	1.1	66
134	Exposure to phthalates in patients with diabetes and its association with oxidative stress, adiponectin, and inflammatory cytokines. Environment International, 2017, 109, 53-63.	4.8	66
135	Using van der Waals heterostructures based on two-dimensional blue phosphorus and XC (X = Ge, Si) for water-splitting photocatalysis: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 9949-9956.	1.3	66
136	Metal-Free Boron Nitride Nanoribbon Catalysts for Electrochemical CO₂ Reduction: Combining High Activity and Selectivity. ACS Applied Materials & Interfaces, 2019, 11, 906-915.	4.0	66
137	Making silole photovoltaically active by attaching carbazolyl donor groups to the silolyl acceptor core. Chemical Communications, 2005, , 3583.	2.2	65
138	Quantum Chemistry Study of H⁺(H₂O)₈:â€‰ A Global Search for Its Isomers by the Scaled Hypersphere Search Method, and Its Thermal Behavior. Journal of Physical Chemistry A, 2007, 111, 10732-10737.	1.1	65
139	Tunable Hydrogen Doping of Metal Oxide Semiconductors with Acidâ€“Metal Treatment at Ambient Conditions. Journal of the American Chemical Society, 2020, 142, 4136-4140.	6.6	65
140	Electric Dipole Descriptor for Machine Learning Prediction of Catalyst Surfaceâ€“Molecular Adsorbate Interactions. Journal of the American Chemical Society, 2020, 142, 7737-7743.	6.6	65
141	Solvent dependence of solvatochromic shifts and the first hyperpolarizability of para-nitroaniline: A nonmonotonic behavior. Journal of Chemical Physics, 2003, 119, 4409-4412.	1.2	64
142	Water-catalyzed gas-phase reaction of formic acid with hydroxyl radical: A computational investigation. Chemical Physics Letters, 2009, 469, 57-61.	1.2	64
143	The Realistic Domain Structure of As-Synthesized Graphene Oxide from Ultrafast Spectroscopy. Journal of the American Chemical Society, 2013, 135, 12468-12474.	6.6	64
144	Dehydrogenation of Propane to Propylene by a Pd/Cu Single-Atom Catalyst: Insight from First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 1016-1023.	1.5	64

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145	A generalized quantum chemical approach for elastic and inelastic electron transports in molecular electronics devices. Journal of Chemical Physics, 2006, 124, 034708.	1.2	63
146	Antibiotic Resistance Gene-Carrying Plasmid Spreads into the Plant Endophytic Bacteria using Soil Bacteria as Carriers. Environmental Science & Technology, 2021, 55, 10462-10470.	4.6	63
147	Regulating Electronic Spin Moments of Single-Atom Catalyst Sites via Single-Atom Promoter Tuning on S-Vacancy MoS₂ for Efficient Nitrogen Fixation. Journal of Physical Chemistry Letters, 2021, 12, 8355-8362.	2.1	63
148	Electrically Driven Single-Photon Superradiance from Molecular Chains in a Plasmonic Nanocavity. Physical Review Letters, 2019, 122, 233901.	2.9	62
149	Observation of inhomogeneous plasmonic field distribution in a nanocavity. Nature Nanotechnology, 2020, 15, 922-926.	15.6	62
150	Evidence of van Hove Singularities in Ordered Grain Boundaries of Graphene. Physical Review Letters, 2014, 112, 226802.	2.9	61
151	QM/MM Studies on Scandium-Catalyzed Syndiospecific Copolymerization of Styrene and Ethylene. Organometallics, 2011, 30, 2908-2919.	1.1	60
152	Machine Learning Protocol for Surface-Enhanced Raman Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 6026-6031.	2.1	60
153	Integrated Design of Organic Hole Transport Materials for Efficient Solidâ€State Dyeâ€Sensitized Solar Cells. Advanced Energy Materials, 2015, 5, 1401185.	10.2	59
154	Pd₄S₃Se₃, Pd₄S₃Te₃, and Pd₄Se₃Te₃: Candidate Two-Dimensional Janus Materials for Photocatalytic Water Splitting. Chemistry of Materials, 2021, 33, 4128-4134.	3.2	59
155	Misfolding of a Human Islet Amyloid Polypeptide at the Lipid Membrane Populates through Î²-Sheet Conformers without Involving Î±-Helical Intermediates. Journal of the American Chemical Society, 2019, 141, 1941-1948.	6.6	58
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