Masayoshi Nakano

List of Publications by Year
in descending order

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430 papers	12,595 citations	25014 57 h-index	37183 96 g-index
454 all docs	454 docs citations	454 times ranked	5037 citing authors

#	Article	IF	Citations
1	Theoretical Study on Second Hyperpolarizabilities of Phenylacetylene Dendrimer:Â Toward an Understanding of Structureâ"Property Relation in NLO Responses of Fractal Antenna Dendrimers. Journal of the American Chemical Society, 2002, 124, 9648-9655.	6.6	373
2	Synthesis, Intermolecular Interaction, and Semiconductive Behavior of a Delocalized Singlet Biradical Hydrocarbon. Angewandte Chemie - International Edition, 2005, 44, 6564-6568.	7.2	312
3	Diindeno-fusion of an anthracene as a design strategy for stable organic biradicals. Nature Chemistry, 2016, 8, 753-759.	6.6	302
4	Second Hyperpolarizability (Î³) of Singlet Diradical System:Â Dependence of Î³ on the Diradical Character. Journal of Physical Chemistry A, 2005, 109, 885-891.	1.1	296
5	Synthesis and Characterization of Teranthene: A Singlet Biradical Polycyclic Aromatic Hydrocarbon Having KekulÃ© Structures. Journal of the American Chemical Society, 2010, 132, 11021-11023.	6.6	285
6	Strong Two-Photon Absorption of Singlet Diradical Hydrocarbons. Angewandte Chemie - International Edition, 2007, 46, 3544-3546.	7.2	261
7	Relationship between Third-Order Nonlinear Optical Properties and Magnetic Interactions in Open-Shell Systems: A New Paradigm for Nonlinear Optics. Physical Review Letters, 2007, 99, 033001.	2.9	258
8	Diradical Character View of Singlet Fission. Journal of Physical Chemistry Letters, 2012, 3, 145-150.	2.1	252
9	Sizeâ€consistent approach and density analysis of hyperpolarizability: Second hyperpolarizabilities of polymeric systems with and without defects. Journal of Chemical Physics, 1995, 103, 4175-4191.	1.2	250
10	Synthesis and Characterization of Quarteranthene: Elucidating the Characteristics of the Edge State of Graphene Nanoribbons at the Molecular Level. Journal of the American Chemical Society, 2013, 135, 1430-1437.	6.6	237
11	Indeno[2,1â€b]fluorene: A 20â€Ïâ€Electron Hydrocarbon with Very Lowâ€Energy Light Absorption. Angewandte Chemie - International Edition, 2013, 52, 6076-6079.	7.2	228
12	Singlet Diradical Character from Experiment. Journal of Physical Chemistry Letters, 2010, 1, 937-940.	2.1	181
13	Alternating Covalent Bonding Interactions in a One-Dimensional Chain of a Phenalenyl-Based Singlet Biradical Molecule Having KekulÃ© Structures. Journal of the American Chemical Society, 2010, 132, 14421-14428.	6.6	162
14	Singlet Biradical Character of Phenalenyl-Based KekulÃ© Hydrocarbon with Naphthoquinoid Structure. Organic Letters, 2007, 9, 81-84.	2.4	148
15	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. Journal of Physical Chemistry Letters, 2015, 6, 3236-3256.	2.1	142
16	Basis set and electron correlation effects on the polarizability and second hyperpolarizability of model open-shell Ï€-conjugated systems. Journal of Chemical Physics, 2005, 122, 114315.	1.2	141
17	Resonance Balance Shift in Stacks of Delocalized Singlet Biradicals. Angewandte Chemie - International Edition, 2009, 48, 5482-5486.	7.2	140
18	Second hyperpolarizabilities of polycyclic aromatic hydrocarbons involving phenalenyl radical units. Chemical Physics Letters, 2006, 418, 142-147.	1.2	139

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19	Impact of Diradical Character on Two-Photon Absorption: Bis(acridine) Dimers Synthesized from an Allenic Precursor. Journal of the American Chemical Society, 2013, 135, 232-241.	6.6	135
20	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. Theoretical Chemistry Accounts, 2011, 130, 711-724.	0.5	125
21	Open-Shell-Character-Based Molecular Design Principles: Applications to Nonlinear Optics and Singlet Fission. Chemical Record, 2017, 17, 27-62.	2.9	124
22	A proposal of new organic third-order nonlinear optical compounds. Centrosymmetric systems with large negative third-order hyperpolarizabilities. Chemical Physics Letters, 1993, 206, 285-292.	1.2	119
23	Thiophene and its sulfur inhibit indenoindenodibenzothiophene diradicals from low-energy lying thermal triplets. Nature Chemistry, 2018, 10, 1134-1140.	6.6	119
24	Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Polyaromatic Diphenalenyl Diradicaloids by an External Electric Field and Donorâ€“Acceptor Substitution. Journal of Physical Chemistry Letters, 2011, 2, 1094-1098.	2.1	111
25	A new type of organicâ€“inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. Dalton Transactions, 2013, 42, 15053.	1.6	111
26	Fundamental of Diradical-Character-Based Molecular Design for Singlet Fission. Journal of Physical Chemistry Letters, 2013, 4, 2133-2137.	2.1	110
27	Excitation Energies and Properties of Open-Shell Singlet Molecules. Springer Briefs in Molecular Science, 2014, , .	0.1	101
28	Second Hyperpolarizabilities (Î³) of Bisimidazole and Bistriazole Benzenes:Â Diradical Character, Charged State, and Spin State Dependences. Journal of Physical Chemistry A, 2006, 110, 4238-4243.	1.1	100
29	Molecular design for efficient singlet fission. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2018, 34, 85-120.	5.6	99
30	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. Chemical Physics Letters, 2008, 467, 120-125.	1.2	96
31	Pushâ€“Pull Type Oligo(N-annulated perylene)quinodimethanes: Chain Length and Solvent-Dependent Ground States and Physical Properties. Journal of the American Chemical Society, 2015, 137, 8572-8583.	6.6	93
32	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. Chemical Physics Letters, 2010, 489, 212-218.	1.2	90
33	Diradical Character Based Design for Singlet Fission of Condensed-Ring Systems with 4nÏ€ Electrons. Journal of Physical Chemistry C, 2012, 116, 19729-19736.	1.5	89
34	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. Journal of Chemical Physics, 2006, 125, 074113.	1.2	88
35	EHF theory of chemical reactions Part 4. UNO CASSCF, UNO CASPT2 and R(U)HF coupled-cluster (CC) wavefunctions. Journal of Molecular Structure, 1994, 310, 205-218.	1.8	87
36	Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: A Potential Tetraradicaloid Hydrocarbon. Angewandte Chemie - International Edition, 2015, 54, 2090-2094.	7.2	87

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37	Theoretical Study on the Second Hyperpolarizabilities of Phenalenyl Radical Systems Involving Acetylene and Vinylene Linkers:Â Diradical Character and Spin Multiplicity Dependences. Journal of Physical Chemistry A, 2007, 111, 3633-3641.	1.1	84
38	Role of a singlet diradical character in carbon nanomaterials: a novel hot spot for efficient nonlinear optical materials. Nanoscale, 2016, 8, 17998-18020.	2.8	83
39	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. Journal of Chemical Physics, 2010, 132, 094107.	1.2	82
40	Tuned CAM-B3LYP functional in the time-dependent density functional theory scheme for excitation energies and properties of diarylethene derivatives. Journal of Photochemistry and Photobiology A: Chemistry, 2012, 235, 29-34.	2.0	82
41	Theoretical Study of Singlet Fission in Oligorylenes. Journal of Physical Chemistry Letters, 2012, 3, 2719-2723.	2.1	81
42	Synthesis of the Unknown Indeno[1,2â€a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. Angewandte Chemie - International Edition, 2017, 56, 15363-15367.	7.2	81
43	Spin Multiplicity Effects on the Second Hyperpolarizability of an Open-Shell Neutral Ï€-Conjugated System. Journal of Physical Chemistry A, 2004, 108, 4105-4111.	1.1	80
44	Many-electron hyperpolarizability density analysis: Application to the dissociation processof one-dimensionalH2s. Physical Review A, 1997, 55, 1503-1513.	1.0	76
45	Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. Chemical Physics Letters, 2009, 477, 355-359.	1.2	74
46	MO theoretical studies of magnetic interactions in clusters of nitronyl nitroxide and related species. Chemical Physics Letters, 1992, 190, 353-360.	1.2	72
47	Size dependences of the diradical character and the second hyperpolarizabilities in dicyclopenta-fused acenes: relationships with their aromaticity/antiaromaticity. Physical Chemistry Chemical Physics, 2011, 13, 20575.	1.3	69
48	Molecule Isomerism Modulates the Diradical Properties of Stable Singlet Diradicaloids. Journal of the American Chemical Society, 2020, 142, 1548-1555.	6.6	65
49	Biphenalenylidene: Isolation and Characterization of the Reactive Intermediate on the Decomposition Pathway of Phenalenyl Radical. Journal of the American Chemical Society, 2016, 138, 2399-2410.	6.6	64
50	Nonlinear optical properties in openâ€shell molecular systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 198-210.	6.2	63
51	Halide Ion Complexes of Decaborane (B₁₀H₁₄) and Their Derivatives: Noncovalent Charge Transfer Effect on Second-Order Nonlinear Optical Properties. Journal of Physical Chemistry A, 2012, 116, 1417-1424.	1.1	62
52	Impact of Antidot Structure on the Multiradical Characters, Aromaticities, and Third-Order Nonlinear Optical Properties of Hexagonal Graphene Nanoflakes. Journal of Physical Chemistry C, 2012, 116, 17787-17795.	1.5	61
53	Second Hyperpolarizability of Zethrenes. Computing Letters, 2007, 3, 333-338.	0.5	60
54	Theoretical investigation on the second hyperpolarizabilities of open-shell singlet systems by spin-unrestricted density functional theory with long-range correction: Range separating parameter dependence. Chemical Physics Letters, 2010, 493, 195-199.	1.2	59

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55	Theoretical study of the second hyperpolarizabilities of three charged states of pentalene. A consideration of the structure-property correlation for the sensitive second hyperpolarizability. Chemical Physics Letters, 1996, 262, 66-73.	1.2	58
56	Exciton migration dynamics in a dendritic molecular aggregate. Chemical Physics Letters, 2000, 323, 249-256.	1.2	57
57	Nonempirically Tuned Long-Range Corrected Density Functional Theory Study on Local and Charge-Transfer Excitation Energies in a Pentacene/C₆₀ Model Complex. Journal of Physical Chemistry Letters, 2011, 2, 1725-1730.	2.1	57
58	Theoretical Molecular Design of Heteroacenes for Singlet Fission: Tuning the Diradical Character by Modifying Ï€-Conjugation Length and Aromaticity. Journal of Physical Chemistry C, 2015, 119, 148-157.	1.5	56
59	Static second hyperpolarizabilities Î³ of nitroxide radical and formaldehyde: evaluation of spatial contributions to Î³ by a hyperpolarizability density analysis. Chemical Physics Letters, 1996, 254, 158-164.	1.2	55
60	Electronic Structure of Open-Shell Singlet Molecules: Diradical Character Viewpoint. Topics in Current Chemistry, 2017, 375, 47.	3.0	55
61	Remarkable two-photon absorption in open-shell singlet systems. Journal of Chemical Physics, 2009, 131, 114316.	1.2	54
62	Theoretical consideration of singlet open-shell character of polyperiacenes using Clar's aromatic sextet valence bond model and quantum chemical calculations. AIP Conference Proceedings, 2012, , .	0.3	54
63	A Biradical Balancing Act: Redox Amphoterism in a Diindenoanthracene Derivative Results from Quinoidal Acceptor and Aromatic Donor Motifs. Journal of the American Chemical Society, 2016, 138, 12648-12654.	6.6	52
64	Fluoreno[2,3-b]fluorene vs Indeno[2,1-b]fluorene: Unusual Relationship between the Number of Ï€ Electrons and Excitation Energy in m-Quinodimethane-Type Singlet Diradicaloids. Journal of Organic Chemistry, 2017, 82, 1380-1388.	1.7	52
65	Enhancement of Antiaromatic Character via Additional Benzoannulation into Dibenzo[a,f]pentalene: Syntheses and Properties of Benzo[a]naphtho[2,1-f]pentalene and Dinaphtho[2,1-a,f]pentalene. Journal of the American Chemical Society, 2019, 141, 560-571.	6.6	52
66	Diradical character dependences of the first and second hyperpolarizabilities of asymmetric open-shell singlet systems. Journal of Chemical Physics, 2013, 138, 244306.	1.2	51
67	Bis-periazulene (Cyclohepta[def]fluorene) as a Nonalternant Isomer of Pyrene: Synthesis and Characterization of Its Triaryl Derivatives. Journal of the American Chemical Society, 2022, 144, 3370-3375.	6.6	50
68	Theoretical Study on Second Hyperpolarizabilities of Singlet Diradical Square Planar Nickel Complexes Involving o-Semiquinonato Type Ligands. Journal of Physical Chemistry A, 2008, 112, 8423-8429.	1.1	49
69	Third-order nonlinear optical properties of trigonal, rhombic and bow-tie graphene nanoflakes with strong structural dependence of diradical character. Chemical Physics Letters, 2009, 480, 278-283.	1.2	49
70	Design Principles of Electronic Couplings for Intramolecular Singlet Fission in Covalently-Linked Systems. Journal of Physical Chemistry A, 2016, 120, 6236-6241.	1.1	49
71	Theoretical calculations of effective exchange integrals between nitronyl nitroxides with donor and acceptor groups. Chemical Physics Letters, 1992, 191, 237-244.	1.2	48
72	Mechanism of exciton migration of dendritic molecular aggregate: a master equation approach including weak excitonâ€“phonon coupling. Chemical Physics Letters, 2002, 363, 422-428.	1.2	48

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73	Photochromic Switching of Diradical Character: Design of Efficient Nonlinear Optical Switches. Journal of Physical Chemistry Letters, 2013, 4, 2418-2422.	2.1	48
74	Density Analysis of Intra- and Intermolecular Vibronic Couplings toward Bath Engineering for Singlet Fission. Journal of Physical Chemistry Letters, 2015, 6, 4972-4977.	2.1	47
75	Coupled-Hartreeâ€"Fock calculations of the third-order hyperpolarizabilities of substituted polydiacetylenes. Chemical Physics Letters, 1991, 185, 550-554.	1.2	46
76	Openâ€Shell Characters and Second Hyperpolarizabilities of Oneâ€Dimensional Graphene Nanoflakes Composed of Trigonal Graphene Units. ChemPhysChem, 2011, 12, 1697-1707.	1.0	46
77	Thirdâ€Order Nonlinear Optical Properties of Oneâ€Dimensional Openâ€Shell Molecular Aggregates Composed of Phenalenyl Radicals. Chemistry - A European Journal, 2014, 20, 11129-11136.	1.7	46
78	Diindenoanthracene Diradicaloids Enable Rational, Incremental Tuning of Their Singlet-Triplet Energy Gaps. CheM, 2020, 6, 1353-1368.	5.8	46
79	EHF theory of chemical reactions Part 4. UNO CASSCF, UNO CASPT2 and R(U)HF coupled-cluster (CC) wavefunctions. Computational and Theoretical Chemistry, 1994, 310, 205-218.	1.5	45
80	Numerical Liouville approach: A calculation method for nonlinear optical susceptibilities ofN-state systems. Physical Review A, 1994, 50, 2989-3004.	1.0	44
81	First and second hyperpolarizabilities of donorâ€"acceptor disubstituted diphenalenyl radical systems. Chemical Physics Letters, 2007, 443, 95-101.	1.2	43
82	Monoradicals and Diradicals of Dibenzofluoreno[3,2-b]fluorene Isomers: Mechanisms of Electronic Delocalization. Journal of the American Chemical Society, 2020, 142, 20444-20455.	6.6	43
83	Interplay between Open-Shell Character, Aromaticity, and Second Hyperpolarizabilities in Indenofluorenes. Journal of Physical Chemistry A, 2015, 119, 10620-10627.	1.1	42
84	Quantum Master Equation Approach to Singlet Fission Dynamics of Realistic/Artificial Pentacene Dimer Models: Relative Relaxation Factor Analysis. Journal of Physical Chemistry C, 2016, 120, 22803-22815.	1.5	42
85	Finite-Field Spin-Flip Configuration Interaction Calculation of the Second Hyperpolarizabilities of Singlet Diradical Systems. Journal of Chemical Theory and Computation, 2007, 3, 1699-1707.	2.3	41
86	Extended Hubbard Models for Transition Metal Oxides and Halides: Importance of Spin and Charge Fluctuations in Charge Transfer Metals. Japanese Journal of Applied Physics, 1988, 27, L1835-L1838.	0.8	40
87	A theoretical explanation of the organic ferromagnetism in the Î²-phase of para-nitrophenyl nitronyl nitroxide. Chemical Physics Letters, 1993, 207, 1-8.	1.2	39
88	Electronic structures of poly-cations and -anions of C60. Possible mechanisms of organic ferromagnetism. Chemical Physics Letters, 1994, 226, 372-380.	1.2	39
89	Energetic Origin of Proton Affinity to the Air/Water Interface. Journal of Physical Chemistry B, 2011, 115, 4745-4751.	1.2	39
90	Giant electric field effect on the second hyperpolarizability of symmetric singlet diradical molecules. Journal of Chemical Physics, 2010, 133, 154302.	1.2	38

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91	Origin of the Enhancement of the Second Hyperpolarizabilities in Open-Shell Singlet Transition-Metal Systems with Metalâ€“Metal Multiple Bonds. Journal of Physical Chemistry Letters, 2011, 2, 2063-2066.	2.1	37
92	Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. Nanoscale, 2018, 10, 16499-16507.	2.8	37
93	and semiempirical MO calculations of intermolecular effective exchange integrals between organic radicals. Designing of organic ferromagnet, ferrimagnet and ferromagnetic conductors. Synthetic Metals, 1987, 19, 87-92.	2.1	36
94	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. Chemical Physics Letters, 2008, 454, 97-104.	1.2	36
95	Interplay between the Diradical Character and Thirdâ€Order Nonlinear Optical Properties in Fullerene Systems. Chemistry - A European Journal, 2013, 19, 1677-1685.	1.7	36
96	Diradical Character-Based Design for Singlet Fission of Bisanthene Derivatives: Aromatic-Ring Attachment and Ï€-Plane Twisting. Journal of Physical Chemistry Letters, 2016, 7, 3925-3930.	2.1	36
97	NIR Emission and Acid-Induced Intramolecular Electron Transfer Derived from a SOMOâ€“HOMO Converted Non-Aufbau Electronic Structure. Journal of Physical Chemistry C, 2019, 123, 4417-4423.	1.5	36
98	Signature of Singlet Open-Shell Character on the Optically Allowed Singlet Excitation Energy and Singletâ€“Triplet Energy Gap. Journal of Physical Chemistry A, 2013, 117, 2000-2006.	1.1	35
99	Isolation of Hypervalent Group-16 Radicals and Their Application in Organic-Radical Batteries. Journal of the American Chemical Society, 2016, 138, 479-482.	6.6	35
100	Exciton migration dynamics in a dendritic molecule: Quantum master equation approach usingab initiomolecular orbital configuration interaction method. Journal of Chemical Physics, 2004, 120, 2359-2367.	1.2	34
101	Second hyperpolarizabilities (Î³) of open-shell singlet one-dimensional systems: Intersite interaction effects on the average diradical character and size dependences of Î³. Chemical Physics Letters, 2006, 432, 473-479.	1.2	34
102	Third-Order Nonlinear Optical Properties of Asymmetric Non-Alternant Open-Shell Condensed-Ring Hydrocarbons: Effects of Diradical Character, Asymmetricity, and Exchange Interaction. Journal of Physical Chemistry C, 2016, 120, 1193-1207.	1.5	34
103	Intense electron correlation dependence of the first hyperpolarizabilities Î² of a nitroxide radical and formaldehyde. Chemical Physics Letters, 1997, 267, 445-451.	1.2	33
104	Negative Second Hyperpolarizability of the Nitronyl Nitroxide Radical. Bulletin of the Chemical Society of Japan, 1998, 71, 845-850.	2.0	33
105	Second hyperpolarizability of phenalenyl radical system involving acetylene Ï€-conjugated bridge. Chemical Physics Letters, 2006, 420, 432-437.	1.2	33
106	Mechano-, thermo-, solvato-, and vapochromism in bis(acetato-Îº¹O)[4â€²-(4-(diphenylamino)phenyl)](2,2â€²:6â€²,2â€²â€²-terpyridine-Îº³N,Nâ€²,Nâ€²â€²)zinc and its polymer. Chemical Communications, 2017, 53, 9805-9808.	6.1	33
107	Benzonorcorrole Ni^{II} Complexes: Enhancement of Paratropic Ring Current and Singlet Diradical Character by Benzoâ€Fusion. Angewandte Chemie - International Edition, 2018, 57, 2209-2213.	7.2	33
108	Computation of the free energy change associated with one-electron reduction of coenzyme immersed in water: A novel approach within the framework of the quantum mechanical/molecular mechanical method combined with the theory of energy representation. Journal of Chemical Physics, 2008, 129, 205103.	1.2	32

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109	Approximate spin-projected spin-unrestricted density functional theory method: Application to the diradical character dependences of the (hyper)polarizabilities in p-quinodimethane models. Chemical Physics Letters, 2010, 501, 140-145.	1.2	32
110	Non-empirical tuning of CAM-B3LYP functional in time-dependent density functional theory for excitation energies of diarylethene derivatives. Chemical Physics Letters, 2013, 585, 201-206.	1.2	31
111	Diradical Character Enhancement by Spacing: Nâ€Heterocyclic Carbene Analogues of MÃ¼ller's Hydrocarbon. Chemistry - A European Journal, 2018, 24, 16537-16542.	1.7	31
112	Third-Order Nonlinear Optical Properties of Open-Shell Supermolecular Systems Composed of Acetylene Linked Phenalenyl Radicals. Journal of Physical Chemistry A, 2011, 115, 8767-8777.	1.1	30
113	A density functional study on the pK_a of small polyprotic molecules. International Journal of Quantum Chemistry, 2014, 114, 1128-1134.	1.0	30
114	Challenging Compounds for Calculating Hyperpolarizabilities: p-Quinodimethane Derivatives. Journal of Physical Chemistry A, 2013, 117, 4709-4715.	1.1	29
115	Synthesis of the Unknown Indeno[1,2â€•a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. Angewandte Chemie, 2017, 129, 15565-15569.	1.6	29
116	Intermolecular Packing Effects on Singlet Fission in Oligorylene Dimers. ACS Omega, 2017, 2, 5095-5103.	1.6	27
117	Theoretical studies on second hyperpolarizabilities for cation radical states of tetrathiafulvalene and tetrathiapentalene. Chemical Physics Letters, 1999, 311, 221-230.	1.2	26
118	Intramolecular Charge Transfer Effects on the Diradical Character and Second Hyperpolarizabilities of Open-Shell Singlet Xâ^Ï€â€“X (X = Donor/Acceptor) Systems. Journal of Physical Chemistry A, 2014, 118, 3463-3471.	1.1	26
119	Dynamic (hyper)polarizability density analysis based on virtual excitation processes: visualization of the dynamic electron fluctuatability of systems under time-dependent external electric fields. Chemical Physics Letters, 1996, 250, 247-254.	1.2	25
120	Analysis of Spatial Contribution to the Second Hyperpolarizabilities ofÏ€-Conjugated Systems Involving Sulfur Atoms. Journal of Physical Chemistry A, 1999, 103, 3103-3109.	1.1	25
121	Structureâ^'Property Correlation on Second Hyperpolarizabilities of Symmetric One-Center and Three-Center Radicals. Journal of Physical Chemistry A, 1999, 103, 7105-7115.	1.1	25
122	Structureâ€“property relation in two-photon absorption for symmetric molecules involving diacetylene Ï€-conjugated bridge. Chemical Physics Letters, 2004, 393, 437-441.	1.2	25
123	A QM/MM study combined with the theory of energy representation: Solvation free energies for anti/syn acetic acids in aqueous solution. Chemical Physics Letters, 2006, 419, 240-244.	1.2	25
124	Second Hyperpolarizabilities of Singlet Polycyclic Diphenalenyl Radicals:â€‰ Effects of the Nature of the Central Heterocyclic Ring and Substitution to Diphenalenyl Rings. Journal of Physical Chemistry A, 2007, 111, 9102-9110.	1.1	25
125	Experimental consideration of covalentâ€bonding interactions in stacks of singlet biradicals having KekulÃ© structures. Journal of Physical Organic Chemistry, 2011, 24, 876-882.	0.9	25
126	Enhancement of the Third-Order Nonlinear Optical Properties in Open-Shell Singlet Transition-Metal Dinuclear Systems: Effects of the Group, of the Period, and of the Charge of the Metal Atom. Journal of Physical Chemistry A, 2012, 116, 5501-5509.	1.1	25

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127	Functional dependence of excitation energy for pentacene/C₆₀ model complex in the nonempirically tuned longâ€range corrected density functional theory. International Journal of Quantum Chemistry, 2013, 113, 252-256.	1.0	25
128	Singlet fission in pancake-bonded systems. Physical Chemistry Chemical Physics, 2017, 19, 5737-5745.	1.3	25
129	A Tetrasilicon Analogue of Bicyclo[1.1.0]butâ€1(3)â€ene Containing a Si=Si Double Bond with an Inverted Geometry. Angewandte Chemie - International Edition, 2019, 58, 4371-4375.	7.2	25
130	Third-order optical nonlinearity in new Ï€-conjugated polymers: polydiethynylsilane and polysilole. Chemical Physics Letters, 1996, 263, 119-125.	1.2	24
131	A Molecular Simulation Study on Adsorption of Acetone/Water in Mesoporous Silicas Modified by Pore Surface Silylation. Journal of Chemical Engineering of Japan, 2005, 38, 999-1007.	0.3	24
132	Computational Study on the Relative Acidity of Acetic Acid by the QM/MM Method Combined with the Theory of Energy Representation. Journal of Physical Chemistry B, 2007, 111, 581-588.	1.2	24
133	Theoretical Study on the Electronic Structure and Third-Order Nonlinear Optical Properties of Open-Shell Quinoidal Oligothiophenes. Journal of Physical Chemistry C, 2013, 117, 21498-21508.	1.5	24
134	Anthenes: Model systems for understanding the edge state of graphene nanoribbons. Pure and Applied Chemistry, 2014, 86, 497-505.	0.9	24
135	The Odd Electron Density Is the Guide toward Achieving Organic Molecules with Gigantic Third-Order Nonlinear Optical Responses. Journal of Physical Chemistry Letters, 2012, 3, 3338-3342.	2.1	23
136	On the inducedâ€fit mechanism of substrateâ€enzyme binding structures of nylonâ€oligomer hydrolase. Journal of Computational Chemistry, 2014, 35, 1240-1247.	1.5	23
137	Diradical Character Tuning for the Thirdâ€Order Nonlinear Optical Properties of Quinoidal Oligothiophenes by Introducing Thiopheneâ€S,Sâ€dioxide Rings. Chemistry - A European Journal, 2016, 22, 1493-1500.	1.7	23
138	A simple zinc(<scp>ii</scp>) complex that features multi-functional luminochromism induced by reversible ligand dissociation. Chemical Communications, 2017, 53, 3657-3660.	2.2	23
139	Numerical Liouville approach: Formulation of thirdâ€order nonlinear optical susceptibilities. Journal of Chemical Physics, 1995, 102, 2986-2995.	1.2	21
140	Structure-property correlation in the second hyperpolarizabilities Î³ for phenyl nitronyl nitroxide radicals. Chemical Physics Letters, 1997, 276, 375-380.	1.2	21
141	A new strategy of enhancing two-photon absorption in conjugated molecules: introduction of charged defects. Chemical Physics Letters, 2002, 358, 435-441.	1.2	21
142	Polarizability and second hyperpolarizability of open-shell Ï€-conjugated compounds from spin projection method calculations. Chemical Physics Letters, 2005, 407, 372-378.	1.2	21
143	Investigation of the dominant hydration structures among the ionic species in aqueous solution: Novel quantum mechanics/molecular mechanics simulations combined with the theory of energy representation. Journal of Chemical Physics, 2008, 128, 064507.	1.2	21
144	Enhancement of Second Hyperpolarizabilities in Open-Shell Singlet Slipped-Stack Dimers Composed of Square Planar Nickel Complexes Involving o-Semiquinonato Type Ligands. Journal of Physical Chemistry A, 2011, 115, 1117-1124.	1.1	21

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145	Theoretical Study on Diradical Characters and Nonlinear Optical Properties of 1,3-Diradical Compounds. Journal of Physical Chemistry A, 2014, 118, 10837-10848.	1.1	21
146	Triaminotriborane(3): A Homocatenated Boron Chain Connected by Bâ‹¯B Multiple Bonds. Angewandte Chemie - International Edition, 2017, 56, 15234-15240.	7.2	21
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