Ryohei Kishi

List of Publications by Year
in descending order

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155	5,332	87723	91712
papers	citations	38 h-index	69 g-index

167	167	167	2783
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Strong Two-Photon Absorption of Singlet Diradical Hydrocarbons. Angewandte Chemie - International Edition, 2007, 46, 3544-3546.	7.2	261
3	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
4	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
5	Indeno[2,1â€‹b‹/i›]fluorene: A 20â€‹â€‹Electron Hydrocarbon with Very Lowâ€‹Energy Light Absorption. Angewandte Chemie - International Edition, 2013, 52, 6076-6079.	7.2	228
6	Singlet Diradical Character from Experiment. Journal of Physical Chemistry Letters, 2010, 1, 937-940.	2.1	181
7	Second hyperpolarizabilities of polycyclic aromatic hydrocarbons involving phenalenyl radical units. Chemical Physics Letters, 2006, 418, 142-147.	1.2	139
8	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
9	(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
10	Thiophene and its sulfur inhibit indenoindenodibenzothiophene diradicals from low-energy lying thermal triplets. Nature Chemistry, 2018, 10, 1134-1140.	6.6	119
11	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
12	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
13	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
14	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
15	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. Chemical Physics Letters, 2010, 489, 212-218.	1.2	90
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	Molecule Isomerism Modulates the Diradical Properties of Stable Singlet Diradicaloids. Journal of the American Chemical Society, 2020, 142, 1548-1555.	6.6	65
24	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
25	Second Hyperpolarizability of Zethrenes. Computing Letters, 2007, 3, 333-338.	0.5	60
26	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
27	Remarkable two-photon absorption in open-shell singlet systems. Journal of Chemical Physics, 2009, 131, 114316.	1.2	54
28	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
29	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
30	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
31	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
32	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
33	Photochromic Switching of Diradical Character: Design of Efficient Nonlinear Optical Switches. Journal of Physical Chemistry Letters, 2013, 4, 2418-2422.	2.1	48
34	Diindenoanthracene Diradicaloids Enable Rational, Incremental Tuning of Their Singlet-Triplet Energy Gaps. CheM, 2020, 6, 1353-1368.	5.8	46
35	First and second hyperpolarizabilities of donorâ€“acceptor disubstituted diphenalenyl radical systems. Chemical Physics Letters, 2007, 443, 95-101.	1.2	43
36	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

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37	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
38	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
39	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. Chemical Physics Letters, 2008, 454, 97-104.	1.2	36
40	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
41	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
42	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
43	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
44	Second hyperpolarizability of phenalenyl radical system involving acetylene Ï€-conjugated bridge. Chemical Physics Letters, 2006, 420, 432-437.	1.2	33
45	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
46	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
47	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
48	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
49	Diradical Character Enhancement by Spacing: Nâ€Heterocyclic Carbene Analogues of MÃ¼ller's Hydrocarbon. Chemistry - A European Journal, 2018, 24, 16537-16542.	1.7	31
50	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
51	Challenging Compounds for Calculating Hyperpolarizabilities: p-Quinodimethane Derivatives. Journal of Physical Chemistry A, 2013, 117, 4709-4715.	1.1	29
52	Synthesis of the Unknown Indeno[1,2â€•a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. Angewandte Chemie, 2017, 129, 15565-15569.	1.6	29
53	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
54	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

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55	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
56	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
57	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
58	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
59	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
60	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
61	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
62	Quantum Master Equation Approach to Singlet Fission Dynamics in Pentacene Linear Aggregate Models: Size Dependences of Excitonic Coupling Effects. Journal of Computational Chemistry, 2019, 40, 89-104.	1.5	21
63	Late-Stage Modification of Electronic Properties of Antiaromatic and Diradicaloid Indeno[1,2-b]fluorene Analogues via Sulfur Oxidation. Journal of Organic Chemistry, 2020, 85, 10846-10857.	1.7	21
64	A Tale of Two Isomers: Enhanced Antiaromaticity/Diradical Character versus Deleterious Ringâ€Opening of Benzofuranâ€fused sâ€Indacenes and Dicyclopenta[b,g]naphthalenes. Angewandte Chemie - International Edition, 2021, 60, 22385-22392.	7.2	21
65	Hyperpolarizability density analysis of the enhancement of second hyperpolarizability of ?-conjugated oligomers by intermolecular interaction. International Journal of Quantum Chemistry, 2005, 102, 702-710.	1.0	20
66	Second hyperpolarizabilities of polycyclic diphenalenyl radicals: Effects of para/ortho-quinoid structures and central ring modification. Chemical Physics Letters, 2006, 429, 174-179.	1.2	20
67	Full configuration interaction calculations of the second hyperpolarizabilities of the H4 model compound: Summation-over-states analysis and interplay with diradical characters. Journal of Chemical Physics, 2012, 136, 024315.	1.2	20
68	Diradical character and nonlinear optical properties of buckyferrocenes: focusing on the use of suitably modified fullerene fragments. Physical Chemistry Chemical Physics, 2015, 17, 5805-5816.	1.3	20
69	Long Carbonâ€“Carbon Bonding beyond 2 Ã… in Tris(9-fluorenylidene)methane. Journal of the American Chemical Society, 2021, 143, 14360-14366.	6.6	19
70	A Phosphorus Analogue of pâ€Quinodimethane with a Planar P₄ Ring: A Metalâ€Free Diphosphorus Source. Chemistry - A European Journal, 2019, 25, 3244-3247.	1.7	18
71	Novel quantum mechanical/molecular mechanical method combined with the theory of energy representation: Free energy calculation for the Beckmann rearrangement promoted by proton transfers in the supercritical water. Journal of Chemical Physics, 2007, 126, 084508.	1.2	16
72	Quantum Master Equation Method Based on the Broken-Symmetry Time-Dependent Density Functional Theory: Application to Dynamic Polarizability of Open-Shell Molecular Systems. Journal of Physical Chemistry A, 2011, 115, 3565-3575.	1.1	16

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73	Cooperative effects in static polarizabilities and second hyperpolarizabilities of hydrogen-bonded 4-pyridones. Chemical Physics Letters, 2008, 454, 91-96.	1.2	15
74	Computation of the reduction free energy of coenzyme in aqueous solution by the QM/MM-ER method. Chemical Physics Letters, 2008, 456, 176-180.	1.2	15
75	Comparative study of diradical characters and thirdâ€order nonlinear optical properties of linear/cyclic acenes versus phenylenes. International Journal of Quantum Chemistry, 2013, 113, 592-598.	1.0	15
76	Evaluation of Aromaticity for Openâ€Shell Singlet Dicyclopentaâ€Fused Acenes and Polyacenes Based on a Magnetically Induced Current. Chemistry - A European Journal, 2018, 24, 13457-13466.	1.7	14
77	Quantum Master Equation Approach to the Second Hyperpolarizability of Nanostar Dendritic Systems. Journal of Physical Chemistry B, 2005, 109, 7631-7636.	1.2	13
78	Theoretical study on the second hyperpolarizability of open-shell singlet one-dimensional systems with a charged defect. Chemical Physics Letters, 2008, 451, 111-115.	1.2	13
79	One- and two-photon absorptions in open-shell singlet systems. AIP Conference Proceedings, 2012, , .	0.3	13
80	Benzonorcorrole Ni^{II} Complexes: Enhancement of Paratropic Ring Current and Singlet Diradical Character by Benzoâ€Fusion. Angewandte Chemie, 2018, 130, 2231-2235.	1.6	13
81	Theoretical Study on Exciton Recurrence Motion in Anthracene Dimer Using the Ab Initio MO-CI Based Quantum Master Equation Approach. Journal of Physical Chemistry A, 2009, 113, 5455-5462.	1.1	12
82	Theoretical Study on Exciton Dynamics in Dendritic Systems: Exciton Recurrence and Migration. Molecules, 2009, 14, 3700-3718.	1.7	11
83	A Puckered Singlet Cyclopentaneâ€1,3â€diyl: Detection of the Third Isomer in Homolysis. Chemistry - A European Journal, 2016, 22, 2299-2306.	1.7	11
84	Monte Carlo Wavefunction Approach to Singlet Fission Dynamics of Molecular Aggregates. Molecules, 2019, 24, 541.	1.7	11
85	Core molecule dependence of energy migration in phenylacetylene nanostar dendrimers: Ab initio molecular orbitalâ€“configuration interaction based quantum master equation study. Journal of Chemical Physics, 2008, 128, 244306.	1.2	10
86	Tuned long-range corrected density functional theory method for evaluating the second hyperpolarizabilities of open-shell singlet metalâ€“metal bonded systems. Chemical Physics Letters, 2012, 523, 60-64.	1.2	10
87	Open-Shell Character and Second Hyperpolarizabilities of One-Dimensional Chromium(II) Chains: Size Dependence and Bond-Length Alternation Effect. Inorganic Chemistry, 2014, 53, 8700-8707.	1.9	10
88	Characterization of Benzo[a]naphtho[2,3â€f]pentalene: Interrelation between Openâ€shell and Antiaromatic Characters Governed by Mode of the Quinoidal Subunit and Molecular Symmetry. Chemistry - an Asian Journal, 2021, 16, 1553-1561.	1.7	10
89	Exciton recurrence motion in aggregate systems in the presence of quantized optical fields. Journal of Chemical Physics, 2006, 125, 234707.	1.2	9
90	Electron donor solvent effects on the (hyper)polarizabilities of a singlet diradical molecule involving a boron atom. Chemical Physics Letters, 2009, 477, 309-314.	1.2	9

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91	Quantal cumulant mechanics and dynamics for multidimensional quantum manyâ€body clusters. International Journal of Quantum Chemistry, 2013, 113, 348-355.	1.0	9
92	Open-shell characters and second hyperpolarizabilities for hexagonal graphene nanoflakes including boron nitride domains. Chemical Physics Letters, 2014, 595-596, 220-225.	1.2	9
93	A novel dynamic exciton expression based on the ab initio MO CI based quantum master equation approach. Chemical Physics Letters, 2008, 460, 370-374.	1.2	8
94	Hydration effects on the reaction with an open-shell transition state: QM/MM-ER study for the dehydration reaction of alcohol in hot water. Journal of Mathematical Chemistry, 2009, 46, 781-794.	0.7	8
95	Theoretical Study on Openâ€Shell Singlet Character and Second Hyperpolarizabilities in Cofacial Ï€â€Stacked Dimers Composed of Weak Openâ€Shell Antiaromatic Porphyrins. ChemPhysChem, 2018, 19, 2863-2871.	1.0	8
96	Exciton dynamics in nanostar dendritic systems using a quantum master equation approach: core monomer effects and possibility of energy transport control. Journal of Luminescence, 2005, 111, 359-366.	1.5	7
97	Control of third-order nonlinear optical properties of singlet diradical square planar metal complexes involving o-semiquinonato type ligands. Synthetic Metals, 2009, 159, 2416-2418.	2.1	7
98	Openâ€Shell Characters, Aromaticities and Thirdâ€Order Nonlinear Optical Properties of Carbon Nanobelts Composed of Fiveâ€and Sixâ€Membered Rings. Asian Journal of Organic Chemistry, 2018, 7, 2320-2329.	1.3	7
99	Ultrafast Exciton Selfâ€Trapping and Delocalization in Cycloparaphenylenes: The Role of Excitedâ€State Symmetry in Electronâ€Vibrational Coupling. Angewandte Chemie - International Edition, 2020, 59, 16989-16996.	7.2	7
100	Dianion and Dication of Tetracyclopentatetraphenylene as Decoupled Annuleneâ€within‐anâ€Annulene Models. Angewandte Chemie - International Edition, 2022, 61, .	7.2	7
101	Second-order Monte Carlo wave-function approach to the relaxation effects on ringing revivals in a molecular system interacting with a strongly squeezed coherent field. Physical Review A, 2004, 70, .	1.0	6
102	Theoretical Study on Static Second Hyperpolarizabilities for Several Ï€-Conjugated Systems Including Nitrogen Atoms:Â Effects of Charged Defects and Extension of Ï€-Conjugation. Journal of Physical Chemistry A, 2004, 108, 4151-4155.	1.1	6
103	Monte Carlo wavefunction approach to the exciton dynamics of molecular aggregates with excitonâ€“phonon coupling. Chemical Physics Letters, 2006, 419, 70-74.	1.2	6
104	The Exchange-Energy Density Functional Based on the Modified Becke-Roussel Model. Journal of Chemical Theory and Computation, 2010, 6, 647-661.	2.3	6
105	Theoretical study on the gigantic effect of external static electric field application on the nonlinear optical properties of 1,2,3,5-dithiadiazolyl Ï€-radical dimers. Materials Chemistry Frontiers, 2018, 2, 785-790.	3.2	6
106	Theoretical study on aromatic and open-shell characteristics of carbon nanobelts composed of indeno[1,2-b]fluorene units: dependence on the number of units and charge states. RSC Advances, 2020, 10, 25736-25745.	1.7	6
107	Monte Carlo wave-function approach to the quantum-phase dynamics of a dissipative molecular system interacting with a single-mode amplitude-squeezed field. Journal of Chemical Physics, 2003, 119, 12106-12118.	1.2	5
108	Molecular orientation effects on two-photon absorption spectra of dimer systems. Chemical Physics Letters, 2007, 448, 99-105.	1.2	5

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109	Quantum Master Equation Approach to Exciton Recurrence Motion in Ring-Shaped Aggregate Complexes Induced by Linear- and Circular-Polarized Laser Fields. Journal of Physical Chemistry C, 2009, 113, 3332-3338.	1.5	5
110	The QM/MMâ€ER studies for the origin of the antioxidative properties of MCIâ€186 in aqueous solutions. International Journal of Quantum Chemistry, 2011, 111, 1748-1762.	1.0	5
111	Generation of Aromatic (Dehydro)benzoannulene Dications Stabilized by Platinum Catecholate Complexes. ChemPlusChem, 2017, 82, 1052-1056.	1.3	5
112	Synthesis and properties of hypervalent electron-rich pentacoordinate nitrogen compounds. Chemical Science, 2020, 11, 5082-5088.	3.7	5
113	THEORETICAL STUDY ON THE SECOND HYPERPOLARIZABILITY (Î³) OF A HOMOGENEOUS MOLECULE IN THE BOND DISSOCIATION PROCESS: ENHANCEMENT OF Î³ IN THE INTERMEDIATE CORRELATION REGIME. Journal of Nonlinear Optical Physics and Materials, 2004, 13, 411-416.	1.1	4
114	Theoretical study on two-photon absorption for symmetric molecular systems composed of charged groups linked with a Ï€-conjugated bridge. Synthetic Metals, 2005, 154, 181-184.	2.1	4
115	Exciton Dynamics of Molecular Aggregate Systems Composed of Triangular Lattice Units: Structural Dependence of Exciton Migration and Recurrence. Journal of Physical Chemistry C, 2008, 112, 16675-16681.	1.5	4
116	Development of Calculation and Analysis Methods for the Dynamic First Hyperpolarizability Based on the Ab Initio Molecular Orbital â€“ Quantum Master Equation Method. Journal of Physical Chemistry A, 2012, 116, 4371-4380.	1.1	4
117	Diradicalology in thirdâ€order nonlinear optical systems: Second hyperpolarizabilities of acetyleneâ€linked phenalenylâ€based superpolyenes. International Journal of Quantum Chemistry, 2013, 113, 585-591.	1.0	4
118	Theoretical design of solvatochromism switching by photochromic reactions using donorâ€“acceptor disubstituted diarylethene derivatives with oxidized thiophene rings. Physical Chemistry Chemical Physics, 2015, 17, 6484-6494.	1.3	4
119	Theoretical investigation of curved Ï€â€conjugated fullerene flakes: openâ€shell character, aromaticity, and thirdâ€order nonlinear optical property. Journal of Physical Organic Chemistry, 2017, 30, e3581.	0.9	4
120	Thirdâ€Order Nonlinear Optical Properties of Oneâ€Dimensional Quinoidal Oligothiophene Derivatives Involving Phenoxyl Groups. ChemistryOpen, 2017, 6, 506-513.	0.9	4
121	Tunability of Openâ€Shell Character, Charge Asymmetry, and Thirdâ€Order Nonlinear Optical Properties of Covalently Linked (Hetero)Phenalenyl Dimers. Chemistry - A European Journal, 2018, 24, 1913-1921.	1.7	4
122	Ultrafast Exciton Selfâ€Trapping and Delocalization in Cycloparaphenylenes: The Role of Excitedâ€State Symmetry in Electronâ€Vibrational Coupling. Angewandte Chemie, 2020, 132, 17137-17144.	1.6	4
123	Third-order nonlinear optical properties of open-shell singlet molecular aggregates composed of diphenalenyl diradicals. Synthetic Metals, 2009, 159, 2413-2415.	2.1	3
124	Antidot effects on the openâ€shell characters and second hyperpolarizabilities of rectangular graphene nanoflakes. International Journal of Quantum Chemistry, 2013, 113, 605-611.	1.0	3
125	Theoretical Study on the Open-Shell Singlet Nature and the Second Hyperpolarizabilities of Corannulene Derivatives with Two Phenoxyl Radicals. Journal of Physical Chemistry A, 2017, 121, 4171-4179.	1.1	3
126	Theoretical Study on Third-Order Nonlinear Optical Properties for One-Hole-Doped Diradicaloids. ACS Omega, 2021, 6, 3046-3059.	1.6	3

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127	Theoretical Study on Open-Shell Nonlinear Optical Systems. Materials Research Society Symposia Proceedings, 2004, 846, DD1.4.1.	0.1	2
128	Static Polarizabilities (Î±) and Second Hyperpolarizabilities (Î³) of One-Dimensional Hydrogen-Bonded Formamides. Computing Letters, 2007, 3, 251-256.	0.5	2
129	Ab initio MOâ€“CI based quantum master equation approach: Exciton dynamics of weakly and strongly coupled J-type aggregates. Synthetic Metals, 2009, 159, 2194-2197.	2.1	2
130	Electron donor solvent effects on the (Hyper) polarizabilities of a solute presenting singlet diradical character. AIP Conference Proceedings, 2012, , .	0.3	2
131	Quantum-phase dynamics of two-component Boseâ€“Einstein condensates: Collapseâ€“revival of macroscopic superposition states. Physica B: Condensed Matter, 2005, 370, 110-120.	1.3	1
132	A proposal of spin-and charge-modulated open-shell nonlinear optical systems. Synthetic Metals, 2005, 154, 309-312.	2.1	1
133	Theoretical Study on the Polarizabilities of Molecules in Solution by the Quantum Mechanical/Molecular Mechanical Approach: Comparison with the Polarizable Continuum Model. Computing Letters, 2007, 3, 441-448.	0.5	1
134	THEORETICAL STUDY ON OPEN-SHELL NONLINEAR OPTICAL MOLECULAR SYSTEMS AND A DEVELOPMENT OF A NOVEL COMPUTATIONAL SCHEME OF EXCITON DYNAMICS. International Journal of Nanoscience, 2009, 08, 123-129.	0.4	1
135	Finiteâ€field method with unbiased polarizable continuum model for evaluation of the second hyperpolarizability of an openâ€shell singlet molecule in solvents. Journal of Computational Chemistry, 2013, 34, 2345-2352.	1.5	1
136	A Tale of Two Isomers: Enhanced Antiaromaticity/Diradical Character versus Deleterious Ringâ€Opening of Benzofuranâ€fused s â€Indacenes and Dicyclopenta[b , g]naphthalenes. Angewandte Chemie, 2021, 133, 22559-22566.	1.6	1
137	AB INITIO STUDY ON NONLINEAR OPTICAL PROPERTIES FOR SMALL DENDRITIC MOLECULES. Journal of Nonlinear Optical Physics and Materials, 2004, 13, 417-422.	1.1	0
138	Theoretical study on the second hyperpolarizabilities of tetrathiafulvalene (TTF) and tetrathiapentalene (TTP) using highly correlated ab initio MO and the density functional theory methods. Synthetic Metals, 2006, 156, 375-378.	2.1	0
139	Intermolecular interaction effects on second hyperpolarizabilities of clusters including charged species. Journal of Computational Methods in Sciences and Engineering, 2006, 6, 211-222.	0.1	0
140	Second Hyperpolarizabilities (Î³) of 1,3-Dipole Systems: Diradical Character Dependence of Î³. AIP Conference Proceedings, 2007, , .	0.3	0
141	Spin State Dependence of Second Hyperpolarizabilities of Zethrenes. AIP Conference Proceedings, 2008, , .	0.3	0
142	Computation of the Reduction Free Energy of Coenzyme in Water: A Novel Approach within the Framework of the QMÂ•MM-ER Method. AIP Conference Proceedings, 2008, , .	0.3	0
143	A Novel Quantum Chemical Approach to the Computation of the Solvation Free Energy of a Biological Molecule with Structural Flexibility. , 2009, , .		0
144	Third-Order Nonlinear Optical Properties of Open-Shell Systems: Diradical Character and Spin State Dependences. , 2009, , .		0

#	Article	IF	Citations
145	Quantum Master Equation Approach to Exciton Recurrence Motion in a Ring-Shaped Aggregate Complex Induced by Circular-Polarized Laser Field. , 2009, , .		0
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