

Ryohei Kishi

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142
papers

4,554
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36
h-index

63
g-index

167
ext. papers

5,009
ext. citations

5
avg, IF

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L-index

#	Paper	IF	Citations
142	Second hyperpolarizability (γ) of singlet diradical system: dependence of γ on the diradical character. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 885-91	2.8	269
141	Relationship between third-order nonlinear optical properties and magnetic interactions in open-shell systems: a new paradigm for nonlinear optics. <i>Physical Review Letters</i> , 2007 , 99, 033001	7.4	246
140	Strong two-photon absorption of singlet diradical hydrocarbons. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 3544-6	16.4	241
139	Synthesis and characterization of quarteranthenes: elucidating the characteristics of the edge state of graphene nanoribbons at the molecular level. <i>Journal of the American Chemical Society</i> , 2013 , 135, 1430-7	16.4	201
138	Indeno[2,1-b]fluorene: a 20- π -electron hydrocarbon with very low-energy light absorption. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 6076-9	16.4	189
137	Singlet Diradical Character from Experiment. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 937-940	6.4	154
136	Second hyperpolarizabilities of polycyclic aromatic hydrocarbons involving phenalenyl radical units. <i>Chemical Physics Letters</i> , 2006 , 418, 142-147	2.5	132
135	Impact of diradical character on two-photon absorption: bis(acridine) dimers synthesized from an allenic precursor. <i>Journal of the American Chemical Society</i> , 2013 , 135, 232-41	16.4	124
134	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. <i>Theoretical Chemistry Accounts</i> , 2011 , 130, 711-724	1.9	114
133	Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Polyaromatic Diphenalenyl Diradicaloids by an External Electric Field and Donor/Acceptor Substitution. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 1094-1098	6.4	104
132	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. <i>Chemical Physics Letters</i> , 2008 , 467, 120-125	2.5	93
131	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. <i>Chemical Physics Letters</i> , 2010 , 489, 212-218	2.5	88
130	Second hyperpolarizabilities (γ) of bisimidazole and bistriazole benzenes: diradical character, charged state, and spin state dependences. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 4238-43	2.8	85
129	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. <i>Journal of Chemical Physics</i> , 2006 , 125, 074113	3.9	84
128	Theoretical study on the second hyperpolarizabilities of phenalenyl radical systems involving acetylene and vinylene linkers: diradical character and spin multiplicity dependences. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 3633-41	2.8	80
127	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. <i>Journal of Chemical Physics</i> , 2010 , 132, 094107	3.9	74
126	A new type of organic-inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. <i>Dalton Transactions</i> , 2013 , 42, 15053-62	4.3	72

125	Indeno[2,1-b]fluorene: A 20- π -Electron Hydrocarbon with Very Low-Energy Light Absorption. <i>Angewandte Chemie</i> , 2013 , 125, 6192-6195	3.6	71
124	Thiophene and its sulfur inhibit indenoindenodibenzothiophene diradicals from low-energy lying thermal triplets. <i>Nature Chemistry</i> , 2018 , 10, 1134-1140	17.6	71
123	Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. <i>Chemical Physics Letters</i> , 2009 , 477, 355-359	2.5	68
122	Tuned CAM-B3LYP functional in the time-dependent density functional theory scheme for excitation energies and properties of diarylethene derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2012 , 235, 29-34	4.7	65
121	Second Hyperpolarizability of Zethrenes. <i>Computing Letters</i> , 2007 , 3, 333-338		57
120	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. <i>Chemical Physics Letters</i> , 2010 , 493, 195-199	2.5	56
119	Halide ion complexes of decaborane (B ₁₀ H ₁₄) and their derivatives: noncovalent charge transfer effect on second-order nonlinear optical properties. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 1417-24	2.8	54
118	Synthesis of the Unknown Indeno[1,2-a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 15363-15367	16.4	50
117	Role of a singlet diradical character in carbon nanomaterials: a novel hot spot for efficient nonlinear optical materials. <i>Nanoscale</i> , 2016 , 8, 17998-18020	7.7	49
116	Remarkable two-photon absorption in open-shell singlet systems. <i>Journal of Chemical Physics</i> , 2009 , 131, 114316	3.9	49
115	Third-order nonlinear optical properties of trigonal, rhombic and bow-tie graphene nanoflakes with strong structural dependence of diradical character. <i>Chemical Physics Letters</i> , 2009 , 480, 278-283	2.5	47
114	Theoretical study on second hyperpolarizabilities of singlet diradical square planar nickel complexes involving o-semiquinonato type ligands. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 8423-9	2.8	47
113	Strong Two-Photon Absorption of Singlet Diradical Hydrocarbons. <i>Angewandte Chemie</i> , 2007 , 119, 3614-3616	3.6	46
112	Photochromic Switching of Diradical Character: Design of Efficient Nonlinear Optical Switches. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 2418-2422	6.4	42
111	Fluoreno[2,3-b]fluorene vs Indeno[2,1-b]fluorene: Unusual Relationship between the Number of π Electrons and Excitation Energy in m-Quinodimethane-Type Singlet Diradicaloids. <i>Journal of Organic Chemistry</i> , 2017 , 82, 1380-1388	4.2	39
110	Finite-Field Spin-Flip Configuration Interaction Calculation of the Second Hyperpolarizabilities of Singlet Diradical Systems. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1699-707	6.4	38
109	First and second hyperpolarizabilities of donor-acceptor disubstituted diphenalenyl radical systems. <i>Chemical Physics Letters</i> , 2007 , 443, 95-101	2.5	38
108	Molecule Isomerism Modulates the Diradical Properties of Stable Singlet Diradicaloids. <i>Journal of the American Chemical Society</i> , 2020 , 142, 1548-1555	16.4	37

107	Interplay between the diradical character and third-order nonlinear optical properties in fullerene systems. <i>Chemistry - A European Journal</i> , 2013 , 19, 1677-85	4.8	34
106	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. <i>Chemical Physics Letters</i> , 2008 , 454, 97-104	2.5	34
105	Exciton migration dynamics in a dendritic molecule: quantum master equation approach using ab initio molecular orbital configuration interaction method. <i>Journal of Chemical Physics</i> , 2004 , 120, 2359-67	3.9	33
104	Second hyperpolarizabilities ($\chi^{(3)}$) of open-shell singlet one-dimensional systems: Intersite interaction effects on the average diradical character and size dependences of $\chi^{(3)}$. <i>Chemical Physics Letters</i> , 2006 , 432, 473-479	2.5	32
103	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. <i>Journal of Chemical Physics</i> , 2008 , 129, 205103	3.9	31
102	Second hyperpolarizability of phenalenyl radical system involving acetylene π -conjugated bridge. <i>Chemical Physics Letters</i> , 2006 , 420, 432-437	2.5	31
101	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. <i>Journal of the American Chemical Society</i> , 2019 , 141, 560-571	16.4	31
100	Third-order nonlinear optical properties of open-shell supermolecular systems composed of acetylene linked phenalenyl radicals. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 8767-77	2.8	30
99	Approximate spin-projected spin-unrestricted density functional theory method: Application to the diradical character dependences of the (hyper)polarizabilities in p-quinodimethane models. <i>Chemical Physics Letters</i> , 2010 , 501, 140-145	2.5	30
98	Challenging compounds for calculating hyperpolarizabilities: p-quinodimethane derivatives. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 4709-15	2.8	28
97	Isolation of Hypervalent Group-16 Radicals and Their Application in Organic-Radical Batteries. <i>Journal of the American Chemical Society</i> , 2016 , 138, 479-82	16.4	26
96	Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. <i>Nanoscale</i> , 2018 , 10, 16499-16507	7.7	26
95	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. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 5501-9	2.8	24
94	Second hyperpolarizabilities of singlet polycyclic diphenalenyl radicals: effects of the nature of the central heterocyclic ring and substitution to diphenalenyl rings. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 9102-10	2.8	24
93	Benzenorcorrole Ni Complexes: Enhancement of Paratropic Ring Current and Singlet Diradical Character by Benzo-Fusion. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 2209-2213	16.4	23
92	Theoretical Study on the Electronic Structure and Third-Order Nonlinear Optical Properties of Open-Shell Quinoidal Oligothiophenes. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 21498-21508	3.8	23
91	Non-empirical tuning of CAM-B3LYP functional in time-dependent density functional theory for excitation energies of diarylethene derivatives. <i>Chemical Physics Letters</i> , 2013 , 585, 201-206	2.5	22
90	Structure-property relation in two-photon absorption for symmetric molecules involving diacetylene π -conjugated bridge. <i>Chemical Physics Letters</i> , 2004 , 393, 437-441	2.5	22

89	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. <i>Journal of Chemical Physics</i> , 2008 , 128, 064507	3.9	21
88	Polarizability and second hyperpolarizability of open-shell π -conjugated compounds from spin projection method calculations. <i>Chemical Physics Letters</i> , 2005 , 407, 372-378	2.5	21
87	Theoretical study on diradical characters and nonlinear optical properties of 1,3-diradical compounds. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 10837-48	2.8	20
86	Synthesis of the Unknown Indeno[1,2-a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. <i>Angewandte Chemie</i> , 2017 , 129, 15565-15569	3.6	19
85	Diindenoanthracene Diradicaloids Enable Rational, Incremental Tuning of Their Singlet-Triplet Energy Gaps. <i>Chem</i> , 2020 , 6, 1353-1368	16.2	19
84	Quantum Master Equation Approach to Singlet Fission Dynamics in Pentacene Linear Aggregate Models: Size Dependences of Excitonic Coupling Effects. <i>Journal of Computational Chemistry</i> , 2019 , 40, 89-104	3.5	19
83	Diradical Character Enhancement by Spacing: N-Heterocyclic Carbene Analogues of M π er π Hydrocarbon. <i>Chemistry - A European Journal</i> , 2018 , 24, 16537-16542	4.8	19
82	Second hyperpolarizabilities of polycyclic diphenalenyl radicals: Effects of para/ortho-quinoid structures and central ring modification. <i>Chemical Physics Letters</i> , 2006 , 429, 174-179	2.5	18
81	Hyperpolarizability density analysis of the enhancement of second hyperpolarizability of π -conjugated oligomers by intermolecular interaction. <i>International Journal of Quantum Chemistry</i> , 2005 , 102, 702-710	2.1	18
80	Diradical Character Tuning for the Third-Order Nonlinear Optical Properties of Quinoidal Oligothiophenes by Introducing Thiophene-S,S-dioxide Rings. <i>Chemistry - A European Journal</i> , 2016 , 22, 1493-500	4.8	18
79	Full configuration interaction calculations of the second hyperpolarizabilities of the H4 model compound: summation-over-states analysis and interplay with diradical characters. <i>Journal of Chemical Physics</i> , 2012 , 136, 024315	3.9	17
78	Diradical character and nonlinear optical properties of buckyferrocenes: focusing on the use of suitably modified fullerene fragments. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 5805-16	3.6	16
77	Quantum master equation method based on the broken-symmetry time-dependent density functional theory: application to dynamic polarizability of open-shell molecular systems. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 3565-75	2.8	16
76	Cooperative effects in static polarizabilities and second hyperpolarizabilities of hydrogen-bonded 4-pyridones. <i>Chemical Physics Letters</i> , 2008 , 454, 91-96	2.5	15
75	Computation of the reduction free energy of coenzyme in aqueous solution by the QM/MM-ER method. <i>Chemical Physics Letters</i> , 2008 , 456, 176-180	2.5	15
74	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. <i>Journal of Chemical Physics</i> , 2007 , 126, 084508	3.9	15
73	A Tetrasilicon Analogue of Bicyclo[1.1.0]but-1(3)-ene Containing a Si=Si Double Bond with an Inverted Geometry. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 4371-4375	16.4	14
72	Quantum master equation approach to the second hyperpolarizability of nanostar dendritic systems. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 7631-6	3.4	13

71	Benzenorcorrole Nill Complexes: Enhancement of Paratropic Ring Current and Singlet Diradical Character by Benzo-Fusion. <i>Angewandte Chemie</i> , 2018 , 130, 2231-2235	3.6	12
70	Theoretical study on exciton recurrence motion in anthracene dimer using the Ab initio MO-CI based quantum master equation approach. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 5455-62	2.8	12
69	Theoretical study on the second hyperpolarizability of open-shell singlet one-dimensional systems with a charged defect. <i>Chemical Physics Letters</i> , 2008 , 451, 111-115	2.5	12
68	Late-Stage Modification of Electronic Properties of Antiaromatic and Diradicaloid Indeno[1,2-]fluorene Analogues via Sulfur Oxidation. <i>Journal of Organic Chemistry</i> , 2020 , 85, 10846-10857	4.2	12
67	Monte Carlo Wavefunction Approach to Singlet Fission Dynamics of Molecular Aggregates. <i>Molecules</i> , 2019 , 24,	4.8	11
66	Comparative study of diradical characters and third-order nonlinear optical properties of linear/cyclic acenes versus phenylenes. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 592-598	2.1	11
65	One- and two-photon absorptions in open-shell singlet systems 2012 ,		11
64	A Phosphorus Analogue of p-Quinodimethane with a Planar P Ring: A Metal-Free Diphosphorus Source. <i>Chemistry - A European Journal</i> , 2019 , 25, 3244-3247	4.8	10
63	Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on a Magnetically Induced Current. <i>Chemistry - A European Journal</i> , 2018 , 24, 13457-13466	4.8	10
62	Tuned long-range corrected density functional theory method for evaluating the second hyperpolarizabilities of open-shell singlet metalmetal bonded systems. <i>Chemical Physics Letters</i> , 2012 , 523, 60-64	2.5	10
61	Theoretical study on exciton dynamics in dendritic systems: exciton recurrence and migration. <i>Molecules</i> , 2009 , 14, 3700-18	4.8	10
60	Core molecule dependence of energy migration in phenylacetylene nanostar dendrimers: Ab initio molecular orbital-configuration interaction based quantum master equation study. <i>Journal of Chemical Physics</i> , 2008 , 128, 244306	3.9	10
59	Monoradicals and Diradicals of Dibenzofluoreno[3,2-]fluorene Isomers: Mechanisms of Electronic Delocalization. <i>Journal of the American Chemical Society</i> , 2020 ,	16.4	10
58	A Puckered Singlet Cyclopentane-1,3-diyl: Detection of the Third Isomer in Homolysis. <i>Chemistry - A European Journal</i> , 2016 , 22, 2299-306	4.8	10
57	Open-shell character and second hyperpolarizabilities of one-dimensional chromium(II) chains: size dependence and bond-length alternation effect. <i>Inorganic Chemistry</i> , 2014 , 53, 8700-7	5.1	9
56	Open-shell characters and second hyperpolarizabilities for hexagonal graphene nanoflakes including boron nitride domains. <i>Chemical Physics Letters</i> , 2014 , 595-596, 220-225	2.5	9
55	Electron donor solvent effects on the (hyper)polarizabilities of a singlet diradical molecule involving a boron atom. <i>Chemical Physics Letters</i> , 2009 , 477, 309-314	2.5	9
54	Exciton recurrence motion in aggregate systems in the presence of quantized optical fields. <i>Journal of Chemical Physics</i> , 2006 , 125, 234707	3.9	9

53	Quantal cumulant mechanics and dynamics for multidimensional quantum many-body clusters. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 348-355	2.1	8
52	Hydration effects on the reaction with an open-shell transition state: QM/MM-ER study for the dehydration reaction of alcohol in hot water. <i>Journal of Mathematical Chemistry</i> , 2009 , 46, 781-794	2.1	8
51	A novel dynamic exciton expression based on the ab initio MO CI based quantum master equation approach. <i>Chemical Physics Letters</i> , 2008 , 460, 370-374	2.5	8
50	Control of third-order nonlinear optical properties of singlet diradical square planar metal complexes involving o-semiquinonato type ligands. <i>Synthetic Metals</i> , 2009 , 159, 2416-2418	3.6	7
49	Exciton dynamics in nanostar dendritic systems using a quantum master equation approach: core monomer effects and possibility of energy transport control. <i>Journal of Luminescence</i> , 2005 , 111, 359-366	3.8	7
48	The Exchange-Energy Density Functional Based on the Modified Becke-Roussel Model. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 647-61	6.4	6
47	Monte Carlo wavefunction approach to the exciton dynamics of molecular aggregates with exciton-phonon coupling. <i>Chemical Physics Letters</i> , 2006 , 419, 70-74	2.5	6
46	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. <i>Physical Review A</i> , 2004 , 70,	2.6	6
45	Bis-periazulene (Cyclohepta[fluorene) as a Nonalternant Isomer of Pyrene: Synthesis and Characterization of Its Triaryl Derivatives.. <i>Journal of the American Chemical Society</i> , 2022 ,	16.4	6
44	Theoretical study on the gigantic effect of external static electric field application on the nonlinear optical properties of 1,2,3,5-dithiadiazolyl radical dimers. <i>Materials Chemistry Frontiers</i> , 2018 , 2, 785-790	7.8	5
43	The QM/MM-ER studies for the origin of the antioxidative properties of MCI-186 in aqueous solutions. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 1748-1762	2.1	5
42	Quantum Master Equation Approach to Exciton Recurrence Motion in Ring-Shaped Aggregate Complexes Induced by Linear- and Circular-Polarized Laser Fields. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 3332-3338	3.8	5
41	Molecular orientation effects on two-photon absorption spectra of dimer systems. <i>Chemical Physics Letters</i> , 2007 , 448, 99-105	2.5	5
40	Theoretical Study on Static Second Hyperpolarizabilities for Several π -Conjugated Systems Including Nitrogen Atoms: Effects of Charged Defects and Extension of π -Conjugation. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 4151-4155	2.8	5
39	Monte Carlo wave-function approach to the quantum-phase dynamics of a dissipative molecular system interacting with a single-mode amplitude-squeezed field. <i>Journal of Chemical Physics</i> , 2003 , 119, 12106-12118	3.9	5
38	Theoretical investigation of curved π -conjugated fullerene flakes: open-shell character, aromaticity, and third-order nonlinear optical property. <i>Journal of Physical Organic Chemistry</i> , 2017 , 30, e3581	2.1	4
37	Generation of Aromatic (Dehydro)benzoannulene Dications Stabilized by Platinum Catecholate Complexes. <i>ChemPlusChem</i> , 2017 , 82, 1052-1056	2.8	4
36	Ultrafast Exciton Self-Trapping and Delocalization in Cycloparaphenylenes: The Role of Excited-State Symmetry in Electron-Vibrational Coupling. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 16989-16996	16.4	4

35	Theoretical Study on Open-Shell Singlet Character and Second Hyperpolarizabilities in Cofacial π -Stacked Dimers Composed of Weak Open-Shell Antiaromatic Porphyrins. <i>ChemPhysChem</i> , 2018 , 19, 2863-2871	3.2	4
34	Third-Order Nonlinear Optical Properties of One-Dimensional Quinoidal Oligothiophene Derivatives Involving Phenoxy Groups. <i>ChemistryOpen</i> , 2017 , 6, 506-513	2.3	4
33	Theoretical design of solvatochromism switching by photochromic reactions using donor-acceptor disubstituted diarylethene derivatives with oxidized thiophene rings. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 6484-94	3.6	4
32	Development of calculation and analysis methods for the dynamic first hyperpolarizability based on the ab initio molecular orbital-quantum master equation method. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 4371-80	2.8	4
31	Exciton Dynamics of Molecular Aggregate Systems Composed of Triangular Lattice Units: Structural Dependence of Exciton Migration and Recurrence. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 16675-16681	2.8	4
30	Theoretical study on two-photon absorption for symmetric molecular systems composed of charged groups linked with a π -conjugated bridge. <i>Synthetic Metals</i> , 2005 , 154, 181-184	3.6	4
29	THEORETICAL STUDY ON THE SECOND HYPERPOLARIZABILITY ($\chi^{(2)}$) OF A HOMOGENEOUS MOLECULE IN THE BOND DISSOCIATION PROCESS: ENHANCEMENT OF $\chi^{(2)}$ IN THE INTERMEDIATE CORRELATION REGIME. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2004 , 13, 411-416	0.8	4
28	Theoretical Study on the Open-Shell Singlet Nature and the Second Hyperpolarizabilities of Corannulene Derivatives with Two Phenoxy Radicals. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 4171-4179	2.8	3
27	Diradicalology in third-order nonlinear optical systems: Second hyperpolarizabilities of acetylene-linked phenalenyl-based superpolyenes. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 585-591	2.1	3
26	Antidot effects on the open-shell characters and second hyperpolarizabilities of rectangular graphene nanoflakes. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 605-611	2.1	3
25	Third-order nonlinear optical properties of open-shell singlet molecular aggregates composed of diphenalenyl diradicals. <i>Synthetic Metals</i> , 2009 , 159, 2413-2415	3.6	3
24	Ultrafast Exciton Self-Trapping and Delocalization in Cycloparaphenylenes: The Role of Excited-State Symmetry in Electron-Vibrational Coupling. <i>Angewandte Chemie</i> , 2020 , 132, 17137-17144	3.6	3
23	Characterization of Benzo[a]naphtho[2,3-f]pentalene: Interrelation between Open-shell and Antiaromatic Characters Governed by Mode of the Quinoidal Subunit and Molecular Symmetry. <i>Chemistry - an Asian Journal</i> , 2021 , 16, 1553-1561	4.5	3
22	Tunability of Open-Shell Character, Charge Asymmetry, and Third-Order Nonlinear Optical Properties of Covalently Linked (Hetero)Phenalenyl Dimers. <i>Chemistry - A European Journal</i> , 2018 , 24, 1913-1921	4.8	3
21	A Tale of Two Isomers: Enhanced Antiaromaticity/Diradical Character versus Deleterious Ring-Opening of Benzofuran-fused s-Indacenes and Dicyclopenta[b,g]naphthalenes. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 22385-22392	16.4	3
20	Theoretical study on aromatic and open-shell characteristics of carbon nanobelts composed of indeno[1,2-]fluorene units: dependence on the number of units and charge states.. <i>RSC Advances</i> , 2020 , 10, 25736-25745	3.7	2
19	Ab initio MOCI based quantum master equation approach: Exciton dynamics of weakly and strongly coupled J-type aggregates. <i>Synthetic Metals</i> , 2009 , 159, 2194-2197	3.6	2
18	Electron donor solvent effects on the (Hyper) polarizabilities of a solute presenting singlet diradical character 2012 ,		2

17	Static Polarizabilities (H) and Second Hyperpolarizabilities (H) of One-Dimensional Hydrogen-Bonded Formamides. <i>Computing Letters</i> , 2007 , 3, 251-256		2
16	Open-Shell Characters, Aromaticities and Third-Order Nonlinear Optical Properties of Carbon Nanobelts Composed of Five- and Six-Membered Rings. <i>Asian Journal of Organic Chemistry</i> , 2018 , 7, 2320 ³ -2329 ²		
15	Finite-field method with unbiased polarizable continuum model for evaluation of the second hyperpolarizability of an open-shell singlet molecule in solvents. <i>Journal of Computational Chemistry</i> , 2013 , 34, 2345-52	3.5	1
14	THEORETICAL STUDY ON OPEN-SHELL NONLINEAR OPTICAL MOLECULAR SYSTEMS AND A DEVELOPMENT OF A NOVEL COMPUTATIONAL SCHEME OF EXCITON DYNAMICS. <i>International Journal of Nanoscience</i> , 2009 , 08, 123-129	0.6	1
13	A proposal of spin-and charge-modulated open-shell nonlinear optical systems. <i>Synthetic Metals</i> , 2005 , 154, 309-312	3.6	1
12	Quantum-phase dynamics of two-component Bose-Einstein condensates: Collapse-Revival of macroscopic superposition states. <i>Physica B: Condensed Matter</i> , 2005 , 370, 110-120	2.8	1
11	Synthesis and properties of hypervalent electron-rich pentacoordinate nitrogen compounds. <i>Chemical Science</i> , 2020 , 11, 5082-5088	9.4	1
10	Long Carbon-Carbon Bonding beyond 2 Å in Tris(9-fluorenylidene)methane. <i>Journal of the American Chemical Society</i> , 2021 , 143, 14360-14366	16.4	1
9	Dianion and Dication of Tetracyclopentatetraphenylene as Decoupled Annulene-within-an-Annulene Models. <i>Angewandte Chemie - International Edition</i> , 2021 ,	16.4	1
8	Theoretical Study on Open-Shell Nonlinear Optical Systems. <i>Materials Research Society Symposia Proceedings</i> , 2004 , 846, DD1.4.1		0
7	A Tale of Two Isomers: Enhanced Antiaromaticity/Diradical Character versus Deleterious Ring-Opening of Benzofuran-fused s-Indacenes and Dicyclopenta[b,g]naphthalenes. <i>Angewandte Chemie</i> , 2021 , 133, 22559-22566	3.6	0
6	Räktitelbild: Indeno[2,1-b]fluorene: A 20-EElectron Hydrocarbon with Very Low-Energy Light Absorption (Angew. Chem. 23/2013). <i>Angewandte Chemie</i> , 2013 , 125, 6228-6228	3.6	
5	Exciton Recurrence Motion in Double-Ring Molecular Aggregates Induced by Two-Mode Circular-Polarized Laser Field. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 6067-6076	3.8	
4	Theoretical study on the second hyperpolarizabilities of tetrathiafulvalene (TTF) and tetrathiapentalene (TTP) using highly correlated ab initio MO and the density functional theory methods. <i>Synthetic Metals</i> , 2006 , 156, 375-378	3.6	
3	Intermolecular interaction effects on second hyperpolarizabilities of clusters including charged species. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2006 , 6, 211-222	0.3	
2	AB INITIO STUDY ON NONLINEAR OPTICAL PROPERTIES FOR SMALL DENDRITIC MOLECULES. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2004 , 13, 417-422	0.8	
1	Theoretical Study on Third-Order Nonlinear Optical Properties for One-Hole-Doped Diradicaloids. <i>ACS Omega</i> , 2021 , 6, 3046-3059	3.9	