Ryohei Kishi

List of Publications by Year in Descending Order

142 papers	4,554 citations	36 h-index	63 g-index
167 ext. papers	5,009 ext. citations	5 avg, IF	5.01 L-index

#	Paper	IF	Citations
142	Bis-periazulene (Cyclohepta[]fluorene) as a Nonalternant Isomer of Pyrene: Synthesis and Characterization of Its Triaryl Derivatives.. *Journal of the American Chemical Society*, **2022**,	16.4	6
141	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. *Chemistry - an Asian Journal*, **2021**, 16, 1553-1561	4.5	3
140	Theoretical Study on Third-Order Nonlinear Optical Properties for One-Hole-Doped Diradicaloids. *ACS Omega*, **2021**, 6, 3046-3059	3.9	
139	Long Carbon-Carbon Bonding beyond 2 Å in Tris(9-fluorenylidene)methane. *Journal of the American Chemical Society*, **2021**, 143, 14360-14366	16.4	1
138	A Tale of Two Isomers: Enhanced Antiaromaticity/Diradical Character versus Deleterious Ring-Opening of Benzofuran-fused s-Indacenes and Dicyclopenta[b,g]naphthalenes. *Angewandte Chemie*, **2021**, 133, 22559-22566	3.6	0
137	A Tale of Two Isomers: Enhanced Antiaromaticity/Diradical Character versus Deleterious Ring-Opening of Benzofuran-fused s-Indacenes and Dicyclopenta[b,g]naphthalenes. *Angewandte Chemie - International Edition*, **2021**, 60, 22385-22392	16.4	3
136	Dianion and Dication of Tetracyclopentatetraphenylene as Decoupled Annulene-within-an-Annulene Models. *Angewandte Chemie - International Edition*, **2021**,	16.4	1
135	Ultrafast Exciton Self-Trapping and Delocalization in Cycloparaphenylenes: The Role of Excited-State Symmetry in Electron-Vibrational Coupling. *Angewandte Chemie - International Edition*, **2020**, 59, 16989-16996	16.4	4
134	Diindenoanthracene Diradicaloids Enable Rational, Incremental Tuning of Their Singlet-Triplet Energy Gaps. *CheM*, **2020**, 6, 1353-1368	16.2	19
133	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.. *RSC Advances*, **2020**, 10, 25736-25745	3.7	2
132	Molecule Isomerism Modulates the Diradical Properties of Stable Singlet Diradicaloids. *Journal of the American Chemical Society*, **2020**, 142, 1548-1555	16.4	37
131	Late-Stage Modification of Electronic Properties of Antiaromatic and Diradicaloid Indeno[1,2-]fluorene Analogues via Sulfur Oxidation. *Journal of Organic Chemistry*, **2020**, 85, 10846-10857	4.2	12
130	Monoradicals and Diradicals of Dibenzofluoreno[3,2-]fluorene Isomers: Mechanisms of Electronic Delocalization. *Journal of the American Chemical Society*, **2020**,	16.4	10
129	Ultrafast Exciton Self-Trapping and Delocalization in Cycloparaphenylenes: The Role of Excited-State Symmetry in Electron-Vibrational Coupling. *Angewandte Chemie*, **2020**, 132, 17137-17144	3.6	3
128	Synthesis and properties of hypervalent electron-rich pentacoordinate nitrogen compounds. *Chemical Science*, **2020**, 11, 5082-5088	9.4	1
127	A Tetrasilicon Analogue of Bicyclo[1.1.0]but-1(3)-ene Containing a Si=Si Double Bond with an Inverted Geometry. *Angewandte Chemie - International Edition*, **2019**, 58, 4371-4375	16.4	14
126	A Phosphorus Analogue of p-Quinodimethane with a Planar P Ring: A Metal-Free Diphosphorus Source. *Chemistry - A European Journal*, **2019**, 25, 3244-3247	4.8	10

125	Monte Carlo Wavefunction Approach to Singlet Fission Dynamics of Molecular Aggregates. *Molecules*, **2019**, 24,	4.8	11
124	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	3.5	19
123	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	16.4	31
122	Benzonorcorrole NiII Complexes: Enhancement of Paratropic Ring Current and Singlet Diradical Character by Benzo-Fusion. *Angewandte Chemie*, **2018**, 130, 2231-2235	3.6	12
121	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. *Materials Chemistry Frontiers*, **2018**, 2, 785-790	7.8	5
120	Benzonorcorrole Ni Complexes: Enhancement of Paratropic Ring Current and Singlet Diradical Character by Benzo-Fusion. *Angewandte Chemie - International Edition*, **2018**, 57, 2209-2213	16.4	23
119	Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on a Magnetically Induced Current. *Chemistry - A European Journal*, **2018**, 24, 13457-13466	4.8	10
118	Theoretical Study on Open-Shell Singlet Character and Second Hyperpolarizabilities in Cofacial Stacked Dimers Composed of Weak Open-Shell Antiaromatic Porphyrins. *ChemPhysChem*, **2018**, 19, 2863-2871	3.2	4
117	Exploring the novel donor-nanotube archetype as an efficient third-order nonlinear optical material: asymmetric open-shell carbon nanotubes. *Nanoscale*, **2018**, 10, 16499-16507	7.7	26
116	Tunability of Open-Shell Character, Charge Asymmetry, and Third-Order Nonlinear Optical Properties of Covalently Linked (Hetero)Phenalenyl Dimers. *Chemistry - A European Journal*, **2018**, 24, 1913-1921	4.8	3
115	Thiophene and its sulfur inhibit indenoindenodibenzothiophene diradicals from low-energy lying thermal triplets. *Nature Chemistry*, **2018**, 10, 1134-1140	17.6	71
114	Open-Shell Characters, Aromaticities and Third-Order Nonlinear Optical Properties of Carbon Nanobelts Composed of Five- and Six-Membered Rings. *Asian Journal of Organic Chemistry*, **2018**, 7, 2320-2329	3	2
113	Diradical Character Enhancement by Spacing: N-Heterocyclic Carbene Analogues of Müller's Hydrocarbon. *Chemistry - A European Journal*, **2018**, 24, 16537-16542	4.8	19
112	Theoretical investigation of curved conjugated fullerene flakes: open-shell character, aromaticity, and third-order nonlinear optical property. *Journal of Physical Organic Chemistry*, **2017**, 30, e3581	2.1	4
111	Fluoreno[2,3-b]fluorene vs Indeno[2,1-b]fluorene: Unusual Relationship between the Number of Electrons and Excitation Energy in m-Quinodimethane-Type Singlet Diradicaloids. *Journal of Organic Chemistry*, **2017**, 82, 1380-1388	4.2	39
110	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	2.8	3
109	Generation of Aromatic (Dehydro)benzoannulene Dications Stabilized by Platinum Catecholate Complexes. *ChemPlusChem*, **2017**, 82, 1052-1056	2.8	4
108	Synthesis of the Unknown Indeno[1,2-a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. *Angewandte Chemie - International Edition*, **2017**, 56, 15363-15367	16.4	50

107	Synthesis of the Unknown Indeno[1,2-a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. *Angewandte Chemie*, **2017**, 129, 15565-15569	3.6	19
106	Third-Order Nonlinear Optical Properties of One-Dimensional Quinoidal Oligothiophene Derivatives Involving Phenoxyl Groups. *ChemistryOpen*, **2017**, 6, 506-513	2.3	4
105	Role of a singlet diradical character in carbon nanomaterials: a novel hot spot for efficient nonlinear optical materials. *Nanoscale*, **2016**, 8, 17998-18020	7.7	49
104	Isolation of Hypervalent Group-16 Radicals and Their Application in Organic-Radical Batteries. *Journal of the American Chemical Society*, **2016**, 138, 479-82	16.4	26
103	Diradical Character Tuning for the Third-Order Nonlinear Optical Properties of Quinoidal Oligothiophenes by Introducing Thiophene-S,S-dioxide Rings. *Chemistry - A European Journal*, **2016**, 22, 1493-500	4.8	18
102	A Puckered Singlet Cyclopentane-1,3-diyl: Detection of the Third Isomer in Homolysis. *Chemistry - A European Journal*, **2016**, 22, 2299-306	4.8	10
101	Diradical character and nonlinear optical properties of buckyferrocenes: focusing on the use of suitably modified fullerene fragments. *Physical Chemistry Chemical Physics*, **2015**, 17, 5805-16	3.6	16
100	Theoretical design of solvatochromism switching by photochromic reactions using donor-acceptor disubstituted diarylethene derivatives with oxidized thiophene rings. *Physical Chemistry Chemical Physics*, **2015**, 17, 6484-94	3.6	4
99	Theoretical study on diradical characters and nonlinear optical properties of 1,3-diradical compounds. *Journal of Physical Chemistry A*, **2014**, 118, 10837-48	2.8	20
98	Open-shell character and second hyperpolarizabilities of one-dimensional chromium(II) chains: size dependence and bond-length alternation effect. *Inorganic Chemistry*, **2014**, 53, 8700-7	5.1	9
97	Open-shell characters and second hyperpolarizabilities for hexagonal graphene nanoflakes including boron nitride domains. *Chemical Physics Letters*, **2014**, 595-596, 220-225	2.5	9
96	Comparative study of diradical characters and third-order nonlinear optical properties of linear/cyclic acenes versus phenylenes. *International Journal of Quantum Chemistry*, **2013**, 113, 592-598	2.1	11
95	Diradicalology in third-order nonlinear optical systems: Second hyperpolarizabilities of acetylene-linked phenalenyl-based superpolyenes. *International Journal of Quantum Chemistry*, **2013**, 113, 585-591	2.1	3
94	Quantal cumulant mechanics and dynamics for multidimensional quantum many-body clusters. *International Journal of Quantum Chemistry*, **2013**, 113, 348-355	2.1	8
93	Antidot effects on the open-shell characters and second hyperpolarizabilities of rectangular graphene nanoflakes. *International Journal of Quantum Chemistry*, **2013**, 113, 605-611	2.1	3
92	Photochromic Switching of Diradical Character: Design of Efficient Nonlinear Optical Switches. *Journal of Physical Chemistry Letters*, **2013**, 4, 2418-2422	6.4	42
91	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	3.8	23
90	Impact of diradical character on two-photon absorption: bis(acridine) dimers synthesized from an allenic precursor. *Journal of the American Chemical Society*, **2013**, 135, 232-41	16.4	124

89	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, 1430-7	16.4	201
88	Interplay between the diradical character and third-order nonlinear optical properties in fullerene systems. *Chemistry - A European Journal*, **2013**, 19, 1677-85	4.8	34
87	A new type of organic-inorganic hybrid NLO-phore with large off-diagonal first hyperpolarizability tensors: a two-dimensional approach. *Dalton Transactions*, **2013**, 42, 15053-62	4.3	72
86	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	2.5	22
85	Challenging compounds for calculating hyperpolarizabilities: p-quinodimethane derivatives. *Journal of Physical Chemistry A*, **2013**, 117, 4709-15	2.8	28
84	Finite-field method with unbiased polarizable continuum model for evaluation of the second hyperpolarizability of an open-shell singlet molecule in solvents. *Journal of Computational Chemistry*, **2013**, 34, 2345-52	3.5	1
83	Indeno[2,1-b]fluorene: a 20-□electron hydrocarbon with very low-energy light absorption. *Angewandte Chemie - International Edition*, **2013**, 52, 6076-9	16.4	189
82	Indeno[2,1-b]fluorene: A 20-□Electron Hydrocarbon with Very Low-Energy Light Absorption. *Angewandte Chemie*, **2013**, 125, 6192-6195	3.6	71
81	R□cktitelbild: Indeno[2,1-b]fluorene: A 20-□Electron Hydrocarbon with Very Low-Energy Light Absorption (Angew. Chem. 23/2013). *Angewandte Chemie*, **2013**, 125, 6228-6228	3.6	
80	Tuned long-range corrected density functional theory method for evaluating the second hyperpolarizabilities of open-shell singlet metal□metal bonded systems. *Chemical Physics Letters*, **2012**, 523, 60-64	2.5	10
79	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	4.7	65
78	Development of calculation and analysis methods for the dynamic first hyperpolarizability based on the ab initio molecular orbital-quantum master equation method. *Journal of Physical Chemistry A*, **2012**, 116, 4371-80	2.8	4
77	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, 1417-24	2.8	54
76	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, 5501-9	2.8	24
75	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	3.9	17
74	Electron donor solvent effects on the (Hyper) polarizabilities of a solute presenting singlet diradical character **2012**,		2
73	One- and two-photon absorptions in open-shell singlet systems **2012**,		11
72	Third-order nonlinear optical properties of open-shell supermolecular systems composed of acetylene linked phenalenyl radicals. *Journal of Physical Chemistry A*, **2011**, 115, 8767-77	2.8	30

71	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. *Theoretical Chemistry Accounts*, **2011**, 130, 711-724	1.9	114
70	The QM/MM-ER studies for the origin of the antioxidative properties of MCI-186 in aqueous solutions. *International Journal of Quantum Chemistry*, **2011**, 111, 1748-1762	2.1	5
69	Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Polyaromatic Diphenalenyl Diradicaloids by an External Electric Field and Donor–Acceptor Substitution. *Journal of Physical Chemistry Letters*, **2011**, 2, 1094-1098	6.4	104
68	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, 3565-75	2.8	16
67	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. *Journal of Chemical Physics*, **2010**, 132, 094107	3.9	74
66	Singlet Diradical Character from Experiment. *Journal of Physical Chemistry Letters*, **2010**, 1, 937-940	6.4	154
65	The Exchange-Energy Density Functional Based on the Modified Becke-Roussel Model. *Journal of Chemical Theory and Computation*, **2010**, 6, 647-61	6.4	6
64	Exciton Recurrence Motion in Double-Ring Molecular Aggregates Induced by Two-Mode Circular-Polarized Laser Field. *Journal of Physical Chemistry C*, **2010**, 114, 6067-6076	3.8	
63	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. *Chemical Physics Letters*, **2010**, 489, 212-218	2.5	88
62	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	2.5	30
61	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	2.5	56
60	Theoretical study on exciton dynamics in dendritic systems: exciton recurrence and migration. *Molecules*, **2009**, 14, 3700-18	4.8	10
59	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	0.6	1
58	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	2.5	47
57	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	2.1	8
56	Electron donor solvent effects on the (hyper)polarizabilities of a singlet diradical molecule involving a boron atom. *Chemical Physics Letters*, **2009**, 477, 309-314	2.5	9
55	Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. *Chemical Physics Letters*, **2009**, 477, 355-359	2.5	68
54	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	3.8	5

53	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, 5455-62	2.8	12
52	Third-order nonlinear optical properties of open-shell singlet molecular aggregates composed of diphenalenyl diradicals. *Synthetic Metals*, **2009**, 159, 2413-2415	3.6	3
51	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	3.6	7
50	Ab initio MO□CI based quantum master equation approach: Exciton dynamics of weakly and strongly coupled J-type aggregates. *Synthetic Metals*, **2009**, 159, 2194-2197	3.6	2
49	Remarkable two-photon absorption in open-shell singlet systems. *Journal of Chemical Physics*, **2009** , 131, 114316	3.9	49
48	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	3.8	4
47	Theoretical study on second hyperpolarizabilities of singlet diradical square planar nickel complexes involving o-semiquinonato type ligands. *Journal of Physical Chemistry A*, **2008**, 112, 8423-9	2.8	47
46	Core molecule dependence of energy migration in phenylacetylene nanostar dendrimers: Ab initio molecular orbital-configuration interaction based quantum master equation study. *Journal of Chemical Physics*, **2008**, 128, 244306	3.9	10
45	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	3.9	21
44	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	3.9	31
43	Theoretical study on the second hyperpolarizability of open-shell singlet one-dimensional systems with a charged defect. *Chemical Physics Letters*, **2008**, 451, 111-115	2.5	12
42	Cooperative effects in static polarizabilities and second hyperpolarizabilities of hydrogen-bonded 4-pyridones. *Chemical Physics Letters*, **2008**, 454, 91-96	2.5	15
41	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. *Chemical Physics Letters*, **2008**, 454, 97-104	2.5	34
40	Computation of the reduction free energy of coenzyme in aqueous solution by the QM/MM-ER method. *Chemical Physics Letters*, **2008**, 456, 176-180	2.5	15
39	A novel dynamic exciton expression based on the ab initio MO CI based quantum master equation approach. *Chemical Physics Letters*, **2008**, 460, 370-374	2.5	8
38	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. *Chemical Physics Letters*, **2008**, 467, 120-125	2.5	93
37	Finite-Field Spin-Flip Configuration Interaction Calculation of the Second Hyperpolarizabilities of Singlet Diradical Systems. *Journal of Chemical Theory and Computation*, **2007**, 3, 1699-707	6.4	38
36	Theoretical study on the second hyperpolarizabilities of phenalenyl radical systems involving acetylene and vinylene linkers: diradical character and spin multiplicity dependences. *Journal of Physical Chemistry A*, **2007**, 111, 3633-41	2.8	80

35	Second hyperpolarizabilities of singlet polycyclic diphenalenyl radicals: effects of the nature of the central heterocyclic ring and substitution to diphenalenyl rings. *Journal of Physical Chemistry A*, **2007**, 111, 9102-10	2.8	24
34	Strong two-photon absorption of singlet diradical hydrocarbons. *Angewandte Chemie - International Edition*, **2007**, 46, 3544-6	16.4	241
33	Strong Two-Photon Absorption of Singlet Diradical Hydrocarbons. *Angewandte Chemie*, **2007**, 119, 3614-3616	3.6	46
32	First and second hyperpolarizabilities of donor–acceptor disubstituted diphenalenyl radical systems. *Chemical Physics Letters*, **2007**, 443, 95-101	2.5	38
31	Molecular orientation effects on two-photon absorption spectra of dimer systems. *Chemical Physics Letters*, **2007**, 448, 99-105	2.5	5
30	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	3.9	15
29	Static Polarizabilities (β) and Second Hyperpolarizabilities (γ) of One-Dimensional Hydrogen-Bonded Formamides. *Computing Letters*, **2007**, 3, 251-256		2
28	Second Hyperpolarizability of Zethrenes. *Computing Letters*, **2007**, 3, 333-338		57
27	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	7.4	246
26	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. *Journal of Chemical Physics*, **2006**, 125, 074113	3.9	84
25	Exciton recurrence motion in aggregate systems in the presence of quantized optical fields. *Journal of Chemical Physics*, **2006**, 125, 234707	3.9	9
24	Second hyperpolarizabilities (gamma) of bisimidazole and bistriazole benzenes: diradical character, charged state, and spin state dependences. *Journal of Physical Chemistry A*, **2006**, 110, 4238-43	2.8	85
23	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	3.6	
22	Intermolecular interaction effects on second hyperpolarizabilities of clusters including charged species. *Journal of Computational Methods in Sciences and Engineering*, **2006**, 6, 211-222	0.3	
21	Second hyperpolarizabilities of polycyclic aromatic hydrocarbons involving phenalenyl radical units. *Chemical Physics Letters*, **2006**, 418, 142-147	2.5	132
20	Monte Carlo wavefunction approach to the exciton dynamics of molecular aggregates with exciton–phonon coupling. *Chemical Physics Letters*, **2006**, 419, 70-74	2.5	6
19	Second hyperpolarizability of phenalenyl radical system involving acetylene π-conjugated bridge. *Chemical Physics Letters*, **2006**, 420, 432-437	2.5	31
18	Second hyperpolarizabilities of polycyclic diphenalenyl radicals: Effects of para/ortho-quinoid structures and central ring modification. *Chemical Physics Letters*, **2006**, 429, 174-179	2.5	18

17	Second hyperpolarizabilities (γ) of open-shell singlet one-dimensional systems: Intersite interaction effects on the average diradical character and size dependences of γ. *Chemical Physics Letters*, **2006**, 432, 473-479	2.5	32
16	Quantum master equation approach to the second hyperpolarizability of nanostar dendritic systems. *Journal of Physical Chemistry B*, **2005**, 109, 7631-6	3.4	13
15	Theoretical study on two-photon absorption for symmetric molecular systems composed of charged groups linked with a π-conjugated bridge. *Synthetic Metals*, **2005**, 154, 181-184	3.6	4
14	A proposal of spin-and charge-modulated open-shell nonlinear optical systems. *Synthetic Metals*, **2005**, 154, 309-312	3.6	1
13	Second hyperpolarizability (gamma) of singlet diradical system: dependence of gamma on the diradical character. *Journal of Physical Chemistry A*, **2005**, 109, 885-91	2.8	269
12	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	3.8	7
11	Quantum-phase dynamics of two-component Bose-Einstein condensates: Collapse-revival of macroscopic superposition states. *Physica B: Condensed Matter*, **2005**, 370, 110-120	2.8	1
10	Polarizability and second hyperpolarizability of open-shell π-conjugated compounds from spin projection method calculations. *Chemical Physics Letters*, **2005**, 407, 372-378	2.5	21
9	Hyperpolarizability density analysis of the enhancement of second hyperpolarizability of π-conjugated oligomers by intermolecular interaction. *International Journal of Quantum Chemistry*, **2005**, 102, 702-710	2.1	18
8	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,	2.6	6
7	Exciton migration dynamics in a dendritic molecule: quantum master equation approach using ab initio molecular orbital configuration interaction method. *Journal of Chemical Physics*, **2004**, 120, 2359-67	3.9	33
6	Theoretical Study on Open-Shell Nonlinear Optical Systems. *Materials Research Society Symposia Proceedings*, **2004**, 846, DD1.4.1		0
5	AB INITIO STUDY ON NONLINEAR OPTICAL PROPERTIES FOR SMALL DENDRITIC MOLECULES. *Journal of Nonlinear Optical Physics and Materials*, **2004**, 13, 417-422	0.8	
4	THEORETICAL STUDY ON THE SECOND HYPERPOLARIZABILITY (γ) OF A HOMOGENEOUS MOLECULE IN THE BOND DISSOCIATION PROCESS: ENHANCEMENT OF γ IN THE INTERMEDIATE CORRELATION REGIME. *Journal of Nonlinear Optical Physics and Materials*, **2004**, 13, 411-416	0.8	4
3	Structure-property relation in two-photon absorption for symmetric molecules involving diacetylene π-conjugated bridge. *Chemical Physics Letters*, **2004**, 393, 437-441	2.5	22
2	Theoretical Study on Static Second Hyperpolarizabilities for Several π-Conjugated Systems Including Nitrogen Atoms: Effects of Charged Defects and Extension of π-Conjugation. *Journal of Physical Chemistry A*, **2004**, 108, 4151-4155	2.8	5
1	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	3.9	5