Masayoshi Nakano

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4092507/publications.pdf

Version: 2024-02-01

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	Innentitelbild: Dianion and Dication of Tetracyclopentatetraphenylene as Decoupled Annuleneâ€withinâ€anâ€Annulene Models (Angew. Chem. 6/2022). Angewandte Chemie, 2022, 134, .	1.6	0
2	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
3	Dianion and Dication of Tetracyclopentatetraphenylene as Decoupled Annuleneâ€withinâ€anâ€Annulene Models. Angewandte Chemie, 2022, 134, .	1.6	0
4	Dianion and Dication of Tetracyclopentatetraphenylene as Decoupled Annuleneâ€withinâ€anâ€Annulene Models. Angewandte Chemie - International Edition, 2022, 61, .	7.2	7
5	Theoretical study on the effect of applying an external static electric field on the singlet fission dynamics of pentacene dimer models. Physical Chemistry Chemical Physics, 2021, 23, 11624-11634.	1.3	0
6	Theoretical Study on Third-Order Nonlinear Optical Properties for One-Hole-Doped Diradicaloids. ACS Omega, 2021, 6, 3046-3059.	1.6	3
7	Stabilization of Charge-Transfer States in Pentacene Crystals and Its Role in Singlet Fission. Journal of Physical Chemistry C, 2021, 125, 2264-2275.	1.5	7
8	Theoretical Study on Singlet Fission in Aromatic Diaza s-Indacene Dimers. Journal of Physical Chemistry A, 2021, 125, 3257-3267.	1.1	3
9	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
10	Theoretical Study on Singlet Fission Dynamics in Slip-Stack-like Pentacene Ring-Shaped Aggregate Models. Journal of Physical Chemistry A, 2021, 125, 5585-5600.	1.1	2
11	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
12	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
13	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
14	Theoretical Study on Redox Potential Control of Iron-Sulfur Cluster by Hydrogen Bonds: A Possibility of Redox Potential Programming. Molecules, 2021, 26, 6129.	1.7	6
15	Molecule Isomerism Modulates the Diradical Properties of Stable Singlet Diradicaloids. Journal of the American Chemical Society, 2020, 142, 1548-1555.	6.6	65
16	Vibronic coupling density analysis and quantum dynamics simulation for singlet fission in pentacene and its halogenated derivatives. Journal of Chemical Physics, 2020, 153, 134302.	1.2	8
17	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
18	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

#	Article	IF	Citations
19	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
20	Theoretical Study on Singlet Fission Dynamics in Sumanene-Fused Acene Dimers. Journal of Physical Chemistry C, 2020, 124, 19499-19507.	1.5	5
21	Theoretical Molecular Design of Phenanthrenes for Singlet Fission by Diazadibora-Substitution. Journal of Physical Chemistry A, 2020, 124, 6778-6789.	1.1	8
22	Quantum design for singlet-fission-induced nonlinear optical systems: Effects of Ï€-conjugation length and molecular packing of butterfly-shaped acenes. Journal of Chemical Physics, 2020, 153, 084304.	1.2	8
23	Theoretical Study on Singlet Fission Dynamics in Pentacene Ringâ€Shaped Aggregate Models with Different Configurations. ChemPhotoChem, 2020, 4, 5234-5234.	1.5	0
24	Theoretical Study of Non-Markov Effects on Singlet Fission Dynamics of Model Pentacene Dimers Using the Second-Order Time-Convolutionless Quantum Master Equation Method. Journal of Physical Chemistry C, 2020, 124, 12220-12229.	1.5	1
25	Molecular Design Principle for Efficient Singlet Fission Based on Diradical Characters and Exchange Integrals: Multiple Heteroatom Substitution Effect on Anthracenes. Journal of Physical Chemistry C, 2020, 124, 11800-11809.	1.5	14
26	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
27	Diindenoanthracene Diradicaloids Enable Rational, Incremental Tuning of Their Singlet-Triplet Energy Gaps. CheM, 2020, 6, 1353-1368.	5.8	46
28	Theoretical Study on Magnetic Interaction in Pyrazole-Bridged Dinuclear Metal Complex: Possibility of Intramolecular Ferromagnetic Interaction by Orbital Counter-Complementarity. Magnetochemistry, 2020, 6, 10.	1.0	5
29	Theoretical Study on Singlet Fission Dynamics in Pentacene Ringâ€Shaped Aggregate Models with Different Configurations. ChemPhotoChem, 2020, 4, 5249-5263.	1.5	2
30	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
31	Synthesis and properties of hypervalent electron-rich pentacoordinate nitrogen compounds. Chemical Science, 2020, 11, 5082-5088.	3.7	5
32	Singlet-Fission-Induced Enhancement of Third-Order Nonlinear Optical Properties of Pentacene Dimers. ACS Omega, 2019, 4, 16181-16190.	1.6	14
33	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
34	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
35	Quantum master equation approach to singlet fission dynamics in pentacene ring-shaped aggregate models. Journal of Chemical Physics, 2019, 150, 234305.	1.2	13
36	Breakdown of the Perturbative Approach to Molecular Packing Dependence of Singlet Fission Rates in Pentacene Dimer Models: A Systematic Comparison with the Quantum Master Equation Approach. Journal of Physical Chemistry C, 2019, 123, 15403-15411.	1.5	8

#	Article	IF	Citations
37	Theoretical Study on the Difference in Electron Conductivity of a One-Dimensional Penta-Nickel(II) Complex between Anti-Ferromagnetic and Ferromagnetic Statesâ€"Possibility of Molecular Switch with Open-Shell Molecules. Molecules, 2019, 24, 1956.	1.7	8
38	Correlation between Slow Magnetic Relaxations and Molecular Structures of Dy(III) Complexes with N5O4 Nona-Coordination. Magnetochemistry, 2019, 5, 27.	1.0	3
39	Theoretical Study on Second Hyperpolarizabilities of Intramolecular Pancake-Bonded Diradicaloids with Helical Scaffolds. ACS Omega, 2019, 4, 2741-2749.	1.6	4
40	Monte Carlo Wavefunction Approach to Singlet Fission Dynamics of Molecular Aggregates. Molecules, 2019, 24, 541.	1.7	11
41	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
42	Near-infrared absorption by intramolecular charge-transfer transition in 5,10,15,20-tetra(N-carbazolyl)porphyrin through protonation. Chemical Communications, 2019, 55, 2992-2995.	2.2	7
43	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
44	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
45	Theoretical Study on the Effects of Environment around the Active Site on Ionization Potential in [2Fe-2S] Ferredoxin. Journal of Computer Chemistry Japan, 2019, 18, 239-240.	0.0	0
46	Molecular design for efficient singlet fission. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2018, 34, 85-120.	5.6	99
47	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
48	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
49	Theoretical Study on Third-Order Nonlinear Optical Property of One-Dimensional Cyclic Thiazyl Radical Aggregates: Intermolecular Distance, Open-Shell Nature, and Spin State Dependences. Journal of Physical Chemistry C, 2018, 122, 6779-6785.	1.5	11
50	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
51	Synthesis and Functionalization of a 1,4-Bis(trimethylsilyl)tetrasila-1,3-diene through the Selective Cleavage of Si(sp²)â€"Si(sp³) Bonds under Mild Reaction Conditions. Organometallics, 2018, 37, 172-175.	1.1	12
52	Diradical Character and Second Hyperpolarizability of Alkaline Earth Metal Inverse Sandwich Complexes Involving Cyclopentadienyl and Cyclooctatetraene Ligands. European Journal of Inorganic Chemistry, 2018, 2018, 2894-2899.	1.0	3
53	Open-Shell Character Dependences of the Second Hyperpolarizability in Two-Dimensional Tetraradicaloids. Journal of Physical Chemistry A, 2018, 122, 3680-3687.	1.1	4
54	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

#	Article	IF	Citations
55	Diradical Character and Second Hyperpolarizability of Alkaline Earth Metal Inverse Sandwich Complexes Involving Cyclopentadienyl and Cyclooctatetraene Ligands. European Journal of Inorganic Chemistry, 2018, 2018, 4747-4747.	1.0	0
56	Frontispiece: Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on a Magnetically Induced Current. Chemistry - A European Journal, 2018, 24, .	1.7	0
57	Thiophene and its sulfur inhibit indenoindenodibenzothiophene diradicals from low-energy lying thermal triplets. Nature Chemistry, 2018, 10, 1134-1140.	6.6	119
58	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
59	Diradical Character Enhancement by Spacing: Nâ€Heterocyclic Carbene Analogues of MÃ¼ller's Hydrocarbon. Chemistry - A European Journal, 2018, 24, 16537-16542.	1.7	31
60	Quantum Chemical Design Guidelines for Absorption and Emission Color Tuning of fac-Ir(ppy)3 Complexes. Molecules, 2018, 23, 577.	1.7	7
61	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
62	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
63	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
64	Diradical Character and Second Hyperpolarizability of Alkaline Earth Metal Inverse Sandwich Complexes Involving Cyclopentadienyl and Cyclooctatetraene Ligands. European Journal of Inorganic Chemistry, 2018, 2018, 2882-2882.	1.0	0
65	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
66	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
67	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
68	Impact of Diradical/Ionic Character on Thirdâ€Order Nonlinear Optical Property in Asymmetric Phenalenyl Dimers. ChemistrySelect, 2017, 2, 2084-2087.	0.7	9
69	Origin of Solvent-independent Optical Property of Unsubstituted BODIPY Revisited. Chemistry Letters, 2017, 46, 536-538.	0.7	4
70	A theoretical study on quasi-one-dimensional open-shell singlet ladder oligomers: multi-radical nature, aromaticity and second hyperpolarizability. Organic Chemistry Frontiers, 2017, 4, 779-789.	2.3	20
71	Theoretical study on S1 and T1 states of homoleptic bis(dipyrrinato)zinc(II) model complex. Polyhedron, 2017, 136, 113-116.	1.0	5
72	Intramolecular Pancake Bonding in Helical Structures. Chemistry - A European Journal, 2017, 23, 7381-7381.	1.7	0

#	Article	IF	Citations
73	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
74	Intramolecular Pancake Bonding in Helical Structures. Chemistry - A European Journal, 2017, 23, 7474-7482.	1.7	20
75	Electronic Structure of Open-Shell Singlet Molecules: Diradical Character Viewpoint. Topics in Current Chemistry, 2017, 375, 47.	3.0	55
76	Theoretical study of magnetic interaction in pyrazole-bridged dinuclear Cu(II) complex. Polyhedron, 2017, 136, 132-135.	1.0	2
77	Theoretical study on relationship between spin structure and electron conductivity of one-dimensional tri-nickel(II) complex. Polyhedron, 2017, 136, 125-131.	1.0	8
78	Generation of Aromatic (Dehydro)benzoannulene Dications Stabilized by Platinum Catecholate Complexes. ChemPlusChem, 2017, 82, 1052-1056.	1.3	5
79	Diradical and Ionic Characters of Open-Shell Singlet Molecular Systems. Journal of Physical Chemistry A, 2017, 121, 861-873.	1.1	17
80	Singlet fission in pancake-bonded systems. Physical Chemistry Chemical Physics, 2017, 19, 5737-5745.	1.3	25
81	Triaminotriborane(3): A Homocatenated Boron Chain Connected by Bâ‹¯B Multiple Bonds. Angewandte Chemie - International Edition, 2017, 56, 15234-15240.	7.2	21
82	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
83	Synthesis of the Unknown Indeno[1,2â€•a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. Angewandte Chemie, 2017, 129, 15565-15569.	1.6	29
84	Intermolecular Packing Effects on Singlet Fission in Oligorylene Dimers. ACS Omega, 2017, 2, 5095-5103.	1.6	27
85	Rational design of doubly-bridged chromophores for singlet fission and tripletâ€“triplet annihilation. RSC Advances, 2017, 7, 34830-34845.	1.7	15
86	Thirdâ€‹Order Nonlinear Optical Properties of Oneâ€‹Dimensional Quinoidal Oligothiophene Derivatives Involving Phenoxyl Groups. ChemistryOpen, 2017, 6, 506-513.	0.9	4
87	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.	4.2	124
88	Tuning Nonlinear Optical Properties by Altering the Diradical and Chargeâ€‹Transfer Characteristics of Chichibabin's Hydrocarbon Derivatives. ChemPhysChem, 2017, 18, 142-148.	1.0	11
89	Open-Shell-Character-Based Molecular Design Principles: Applications to Nonlinear Optics and Singlet Fission. Chemical Record, 2017, 17, 27-62.	2.9	124
90	Theoretical Study on the Second Hyperpolarizailities of Oligomeric Systems Composed of Carbon and Silicon Ï€-Structures. Molecules, 2016, 21, 1540.	1.7	2

#	Article	IF	Citations
91	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
92	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
93	Diindeno-fusion of an anthracene as a design strategy for stable organic biradicals. Nature Chemistry, 2016, 8, 753-759.	6.6	302
94	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
95	Origin of the Enhancement of the Second Hyperpolarizabilities of Metalâ€“Carbon Bonds. Journal of Physical Chemistry A, 2016, 120, 6838-6845.	1.1	0
96	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
97	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
98	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
99	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
100	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
101	Nonlinear optical properties in openâ€shell molecular systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 198-210.	6.2	63
102	Theoretical study on the spin state and open-shell character dependences of the second hyperpolarizability in hydrogen chain models. Physical Review A, 2016, 94, .	1.0	5
103	Cover Image, Volume 6, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, i-i.	6.2	0
104	Open-Shell Singlet Nature and Ïƒ-/Ï€-Conjugation Effects on the Third-Order Nonlinear Optical Properties of Si Chains: Polysilane and Poly(disilene-1,2-diyl). Journal of Physical Chemistry A, 2016, 120, 948-955.	1.1	4
105	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
106	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
107	Challenging compounds for calculating molecular second hyperpolarizabilities: the triplet state of the trimethylenemethane diradical and two derivatives. Physical Chemistry Chemical Physics, 2016, 18, 6420-6429.	1.3	5
108	Innentitelbild: Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: A Potential Tetraradicaloid Hydrocarbon (Angew. Chem. 7/2015). Angewandte Chemie, 2015, 127, 2000-2000.	1.6	0

#	Article	IF	Citations
109	Theoretical study on electromagnetically induced transparency in molecular aggregate models using quantum Liouville equation method. , 2015, , .		0
110	Approximate spin projected spin-unrestricted density functional theory method: Application to diradical character dependences of second hyperpolarizabilities. , 2015, , .		1
111	Ab initio molecular orbital-configuration interaction based quantum master equation (MOQME) approach to the dynamic first hyperpolarizabilities of asymmetric Ï€-conjugated systems. , 2015, , .		0
112	Theoretical study on the second hyperpolarizabilities of one-dimensional heteronuclear transition-metalâ€“metal bonded systems: Metal alignment effects. Chemical Physics Letters, 2015, 640, 165-171.	1.2	0
113	Relationship between second hyperpolarizability and diradical character in open-shell singlet metalâ€“metal multiply bonded systems. , 2015, , .		0
114	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
115	Diradical character dependence of third-harmonic generation spectra in open-shell singlet systems. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	9
116	Theoretical Study on the Enhancement of the Second Hyperpolarizabilities of Si-, Ge-Disubstituted Quinodimethanes: Synergy Effects of Open-Shell Nature and Intramolecular Charge Transfer. Journal of Physical Chemistry C, 2015, 119, 1188-1193.	1.5	10
117	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
118	Hydration effects on enzymeâ€“substrate complex of nylon oligomer hydrolase: inter-fragment interaction energy study by the fragment molecular orbital method. Molecular Physics, 2015, 113, 319-326.	0.8	6
119	Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: A Potential Tetraradicaloid Hydrocarbon. Angewandte Chemie - International Edition, 2015, 54, 2090-2094.	7.2	87
120	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
121	DFT and TD-DFT studies of electronic structures and one-electron excitation states of a cyanide-bridged molecular square complex. Inorganic Chemistry Frontiers, 2015, 2, 771-779.	3.0	18
122	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. Journal of Physical Chemistry Letters, 2015, 6, 3236-3256.	2.1	142
123	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
124	Interplay between Open-Shell Character, Aromaticity, and Second Hyperpolarizabilities in Indenofluorenes. Journal of Physical Chemistry A, 2015, 119, 10620-10627.	1.1	42
125	Unraveling the degradation of artificial amide bonds in nylon oligomer hydrolase: from induced-fit to acylation processes. Physical Chemistry Chemical Physics, 2015, 17, 4492-4504.	1.3	12
126	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

#	Article	IF	Citations
127	Theoretical Study on the Relationship between Diradical Character and Second Hyperpolarizabilities of Fourâ€Membered–Ring Diradicals Involving Heavy Mainâ€Group Elements. Chemistry - A European Journal, 2015, 21, 2157-2164.	1.7	17
128	Substitution effects on optical properties of iminonitroxide- substituted iminonitroxide diradical. Molecular Physics, 2015, 113, 267-273.	0.8	1
129	Static electric field effect on third-order nonlinear optical (NLO) properties of singlet diradical molecules: Toward the realization of an electric field induced open-shell NLO switch. , 2015, , .		0
130	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
131	A density functional study on the pK_a of small polyprotic molecules. International Journal of Quantum Chemistry, 2014, 114, 1128-1134.	1.0	30
132	Natural orbital functional calculations of molecular polarizabilities and second hyperpolarizabilities. The hydrogen molecule as a test case. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 015101.	0.6	8
133	Intramolecular Charge Transfer Effects on the Diradical Character and Second Hyperpolarizabilities of Open-Shell Singlet Xâ¯Ïâ€“X (X = Donor/Acceptor) Systems. Journal of Physical Chemistry A, 2014, 118, 3463-3471.	1.1	26
134	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
135	Excitation Energies and Properties of Open-Shell Singlet Molecules. Springer Briefs in Molecular Science, 2014, , .	0.1	101
136	Diradical Character View of Singlet Fission. Springer Briefs in Molecular Science, 2014, , 79-112.	0.1	0
137	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
138	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
139	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
140	Anthenes: Model systems for understanding the edge state of graphene nanoribbons. Pure and Applied Chemistry, 2014, 86, 497-505.	0.9	24
141	Axial ligand effects on the diradical characters and second hyperpolarizabilities of open-shell singlet transition-metal dinuclear complexes. Chemical Physics Letters, 2014, 608, 68-73.	1.2	7
142	Electronic Structures of Symmetric Diradical Systems. Springer Briefs in Molecular Science, 2014, , 9-26.	0.1	3
143	Summary and Future Prospects. Springer Briefs in Molecular Science, 2014, , 113-116.	0.1	0
144	Electronic Structures of Asymmetric Diradical Systems. Springer Briefs in Molecular Science, 2014, , 27-41.	0.1	0

#	Article	IF	Citations
145	Diradical Character View of (Non)Linear Optical Properties. Springer Briefs in Molecular Science, 2014, , 43-77.	0.1	0
146	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
147	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
148	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
149	Quantal cumulant mechanics and dynamics for multidimensional quantum manyâ€body clusters. International Journal of Quantum Chemistry, 2013, 113, 348-355.	1.0	9
150	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
151	Photochromic Switching of Diradical Character: Design of Efficient Nonlinear Optical Switches. Journal of Physical Chemistry Letters, 2013, 4, 2418-2422.	2.1	48
152	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
153	Theoretical study on the diradical characters and third-order nonlinear optical properties of transition-metal heterodinuclear systems. Chemical Physics Letters, 2013, 579, 73-77.	1.2	6
154	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
155	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
156	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
157	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
158	Theoretical study on the diradical characters and third-order nonlinear optical properties of cyclic thiazyl diradical compounds. Chemical Physics Letters, 2013, 585, 112-116.	1.2	14
159	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
160	Equatorial ligand effects on the diradical character dependence of the second hyperpolarizabilities of open-shell singlet transition-metal dinuclear complexes. Chemical Physics Letters, 2013, 570, 75-79.	1.2	10
161	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
162	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

#	Article	IF	Citations
163	Fundamental of Diradical-Character-Based Molecular Design for Singlet Fission. Journal of Physical Chemistry Letters, 2013, 4, 2133-2137.	2.1	110
164	Challenging Compounds for Calculating Hyperpolarizabilities: p-Quinodimethane Derivatives. Journal of Physical Chemistry A, 2013, 117, 4709-4715.	1.1	29
165	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
166	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
167	RÃ¼cktitelbild: Indeno[2,1-b]fluorene: A 20-Ï€-Electron Hydrocarbon with Very Low-Energy Light Absorption (Angew. Chem. 23/2013). Angewandte Chemie, 2013, 125, 6228-6228.	1.6	0
168	Electron donor solvent effects on the (Hyper) polarizabilities of a solute presenting singlet diradical character. AIP Conference Proceedings, 2012, , .	0.3	2
169	Spin polarization and third-order nonlinear optical properties of open-shell singlet graphene nanoflakes. , 2012, , .		0
170	Second hyperpolarizabilities of singlet diradical compounds and their radical ions. , 2012, , .		0
171	Broken-symmetry MO-CI quantum master equation approach to exciton dynamics in open-shell singlet systems. , 2012, , .		0
172	Long-range-corrected UDFT study on second hyperpolarizabilities of open-shell singlet systems. , 2012, , .		0
173	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
174	One- and two-photon absorptions in open-shell singlet systems. AIP Conference Proceedings, 2012, , .	0.3	13
175	Theoretical aspects on the evaluation and interpretation of the third-order nonlinear optical properties of diradical compounds. , 2012, , .		0
176	Singlet open-shell character of conjugated Kekulèmolecules. , 2012, , .		0
177	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
178	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
179	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
180	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

#	Article	IF	Citations
181	Quantum Master Equation Study of Electromagnetically Induced Transparency in Dipole-Coupled Dimer Models. Progress in Theoretical Chemistry and Physics, 2012, , 109-120.	0.2	0
182	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
183	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
184	Theoretical Study of Singlet Fission in Oligorylenes. Journal of Physical Chemistry Letters, 2012, 3, 2719-2723.	2.1	81
185	Oscillatory and rotatory exciton recurrence motions in double-ring molecular aggregates controlled by two-mode circular-polarized laser field. , 2012, , .		0
186	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
187	Diradical Character View of Singlet Fission. Journal of Physical Chemistry Letters, 2012, 3, 145-150.	2.1	252
188	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
189	Enhancement of the second hyperpolarizability by dÏƒ electrons in one-dimensional tetrametallic transition-metal systems. Chemical Physics Letters, 2012, 527, 11-15.	1.2	8
190	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
191	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
192	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
193	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
194	Energetic Origin of Proton Affinity to the Air/Water Interface. Journal of Physical Chemistry B, 2011, 115, 4745-4751.	1.2	39
195	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
196	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
197	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
198	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

#	Article	IF	Citations
199	(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
200	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
201	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
202	Openâ€Shell Characters and Second Hyperpolarizabilities of Oneâ€Dimensional Graphene Nanoflakes Composed of Trigonal Graphene Units. ChemPhysChem, 2011, 12, 1697-1707.	1.0	46
203	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
204	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. Chemical Physics Letters, 2010, 489, 212-218.	1.2	90
205	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
206	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
207	Development of a Quantum Chemical Method Combined with a Theory of Solutionsâ€”Free-Energy Calculation for Chemical Reactions by Condensed Phase Simulations. Advances in Quantum Chemistry, 2010, 59, 283-351.	0.4	2
208	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
209	Singlet Diradical Character from Experiment. Journal of Physical Chemistry Letters, 2010, 1, 937-940.	2.1	181
210	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
211	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
212	Giant electric field effect on the second hyperpolarizability of symmetric singlet diradical molecules. Journal of Chemical Physics, 2010, 133, 154302.	1.2	38
213	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.	1.5	0
214	Chemistry of Phenalenyl-based Delocalized Singlet Biradicals. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 2010, 68, 64-74.	0.0	6
215	A Novel Quantum Chemical Approach to the Computation of the Solvation Free Energy of a Biological Molecule with Structural Flexibility. , 2009, , .		0
216	Third-Order Nonlinear Optical Properties of Open-Shell Systems: Diradical Character and Spin State Dependences. , 2009, , .		0

#	Article	IF	Citations
217	Theoretical Study on Exciton Dynamics in Dendritic Systems: Exciton Recurrence and Migration. Molecules, 2009, 14, 3700-3718.	1.7	11
218	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
219	Resonance Balance Shift in Stacks of Delocalized Singlet Biradicals. Angewandte Chemie - International Edition, 2009, 48, 5482-5486.	7.2	140
220	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
221	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
222	Quantum dynamic simulations for single molecular magnets using anisotropic spin models. Polyhedron, 2009, 28, 2092-2096.	1.0	5
223	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
224	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
225	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
226	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
227	Third-order nonlinear optical properties of open-shell singlet molecular aggregates composed of diphenalenyl diradicals. Synthetic Metals, 2009, 159, 2413-2415.	2.1	3
228	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
229	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
230	Remarkable two-photon absorption in open-shell singlet systems. Journal of Chemical Physics, 2009, 131, 114316.	1.2	54
231	Quantum Master Equation Approach to Exciton Recurrence Motion in a Ring-Shaped Aggregate Complex Induced by Circular-Polarized Laser Field. , 2009, , .		0
232	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
233	Cooperative effects in static polarizabilities and second hyperpolarizabilities of hydrogen-bonded 4-pyridones. Chemical Physics Letters, 2008, 454, 91-96.	1.2	15
234	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. Chemical Physics Letters, 2008, 454, 97-104.	1.2	36

#	Article	IF	Citations
235	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
236	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
237	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
238	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
239	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
240	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
241	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
242	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
243	Spin State Dependence of Second Hyperpolarizabilities of Zethrenes. AIP Conference Proceedings, 2008, , .	0.3	0
244	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
245	A Quantum Chemical Approach to Free Energy Calculation for Chemical Reactions in Condensed System: Combination of a Quantum Chemical Method with a Theory of Statistical Mechanics. Challenges and Advances in Computational Chemistry and Physics, 2008, , 455-505.	0.6	3
246	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
247	Multi-scale simulations for materials and life sciences. AIP Conference Proceedings, 2007, , .	0.3	0
248	Static Polarizabilities (Î±) and Second Hyperpolarizabilities (Î³) of One-Dimensional Hydrogen-Bonded Formamides. Computing Letters, 2007, 3, 251-256.	0.5	2
249	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
250	Second Hyperpolarizability of Zethrenes. Computing Letters, 2007, 3, 333-338.	0.5	60
251	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
252	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

#	Article	IF	Citations
253	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
254	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
255	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
256	Singlet Biradical Character of Phenalenyl-Based KekulÃ© Hydrocarbon with Naphthoquinoid Structure. Organic Letters, 2007, 9, 81-84.	2.4	148
257	Second Hyperpolarizabilities (Î³) of 1,3-Dipole Systems: Diradical Character Dependence of Î³. AIP Conference Proceedings, 2007, , .	0.3	0
258	Multi-Scale Simulations For Materials and Life Sciences. AIP Conference Proceedings, 2007, , .	0.3	0
259	Strong Two-Photon Absorption of Singlet Diradical Hydrocarbons. Angewandte Chemie - International Edition, 2007, 46, 3544-3546.	7.2	261
260	First and second hyperpolarizabilities of donorâ€“acceptor disubstituted diphenalenyl radical systems. Chemical Physics Letters, 2007, 443, 95-101.	1.2	43
261	Molecular orientation effects on two-photon absorption spectra of dimer systems. Chemical Physics Letters, 2007, 448, 99-105.	1.2	5
262	Molecular simulation study on adsorption of methanol/water mixtures in mesoporous silicas modified pore surface silylation. Fluid Phase Equilibria, 2007, 257, 212-216.	1.4	15
263	Synthesis and Characterization of Acetyleneâ€Linked Bisphenalenyl and Metallicâ€Like Behavior in Its Chargeâ€Transfer Complex. Chemistry - an Asian Journal, 2007, 2, 1370-1379.	1.7	20
264	Non-equilibrium molecular dynamics simulation study on permeation phenomena of LJ particles in slit-shaped membranes with periodic belt-like heterogeneous surfaces. Fluid Phase Equilibria, 2007, 257, 190-194.	1.4	2
265	Exciton recurrence motion in aggregate systems in the presence of quantized optical fields. Journal of Chemical Physics, 2006, 125, 234707.	1.2	9
266	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
267	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
268	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
269	THIRD-ORDER NONLINEAR OPTICAL PROPERTIES OF OPEN-SHELL AND/OR CHARGED MOLECULAR SYSTEMS. , 2006, , 337-404.		3
270	N-band Hubbard models. III. Boson-fermion and interaction-boson models for high-Tcsuperconductivity. International Journal of Quantum Chemistry, 2006, 106, 1052-1075.	1.0	4

#	Article	IF	Citations
271	Second hyperpolarizabilities of polycyclic aromatic hydrocarbons involving phenalenyl radical units. Chemical Physics Letters, 2006, 418, 142-147.	1.2	139
272	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
273	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
274	Second hyperpolarizability of phenalenyl radical system involving acetylene Ï€-conjugated bridge. Chemical Physics Letters, 2006, 420, 432-437.	1.2	33
275	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
276	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
277	Quantum dynamics of exciton recurrence motion in dendritic molecular aggregates. Journal of Photochemistry and Photobiology A: Chemistry, 2006, 178, 264-270.	2.0	9
278	Monte Carlo wavefunction approach to the dissipative quantum-phase dynamics of two-component Bose-Einstein condensates. European Physical Journal D, 2006, 38, 523-532.	0.6	1
279	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
280	Molecular Simulation Study on Adsorption of Methanol/Water Mixed Gases in Mesoporous Silicas with Surface Modification. Kagaku Kogaku Ronbunshu, 2006, 32, 18-24.	0.1	0
281	Theoretical Study on the Second Hyperpolarizabilities of Diphenalenyl Radical Systems. , 2006, , 231-240.		0
282	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
283	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
284	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
285	Formulation of master equation approach involving spinâ€“phonon coupling: Toward an understanding of spin dynamics in magnetic dendrimers. Polyhedron, 2005, 24, 2653-2657.	1.0	7
286	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
287	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
288	Synthesis, Intermolecular Interaction, and Semiconductive Behavior of a Delocalized Singlet Biradical Hydrocarbon. Angewandte Chemie - International Edition, 2005, 44, 6564-6568.	7.2	312

#	Article	IF	Citations
289	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
290	Quantum dynamics in high-spin molecules, spin dendrimers, and spin lattices. International Journal of Quantum Chemistry, 2005, 105, 615-627.	1.0	11
291	Quantum Master Equation Approach to the Second Hyperpolarizability of Nanostar Dendritic Systems. Journal of Physical Chemistry B, 2005, 109, 7631-7636.	1.2	13
292	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
293	A proposal of spin-and charge-modulated open-shell nonlinear optical systems. Synthetic Metals, 2005, 154, 309-312.	2.1	1
294	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
295	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
296	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
297	Theoretical Study on Open-Shell Nonlinear Optical Systems. Materials Research Society Symposia Proceedings, 2004, 846, DD1.4.1.	0.1	2
298	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
299	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
300	Quantum-phase dynamics of molecular systems interacting with a two-mode squeezed vacuum field: Detuning effects. International Journal of Quantum Chemistry, 2004, 99, 421-430.	1.0	2
301	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
302	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
303	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
304	One- and two-exciton migration dynamics of a dendritic molecular aggregate. International Journal of Quantum Chemistry, 2003, 95, 472-478.	1.0	4
305	Monte Carlo Wave Function (MCWF) approach to dissipative quantum systems interacting with a single-mode quantized field. International Journal of Quantum Chemistry, 2003, 95, 461-471.	1.0	3
306	Quantum-phase dynamics of an atomic/molecular system interacting with a two-mode squeezed vacuum field: coexistence of quantum and thermal features. Chemical Physics, 2003, 286, 257-266.	0.9	6

#	Article	IF	Citations
307	Density Analysis of Intermolecular Orbital-Interaction Effects on the Second Hyperpolarizabilities of Ï€â˜†Ï€ Stacking Dimers. Journal of Physical Chemistry A, 2003, 107, 4157-4164.	1.1	13
308	Theoretical study on the structural dependency of the exciton migration of a denritic molecular aggregate. Synthetic Metals, 2003, 137, 875-876.	2.1	3
309	Intermolecular-interaction effects on the quantum dynamics of dimers interacting with a two-mode squeezed vacuum field. Synthetic Metals, 2003, 137, 1379-1380.	2.1	0
310	Remarkable enhancement of two-photon absorption in cation molecules. Synthetic Metals, 2003, 137, 1391-1392.	2.1	2
311	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
312	EXCITON MIGRATION IN DENDRITIC AGGREGATE SYSTEMS USING THE QUANTUM MASTER EQUATION APPROACH INVOLVING WEAK EXCITON-PHONON COUPLING. Journal of Theoretical and Computational Chemistry, 2003, 02, 459-479.	1.8	16
313	Polarizabilities and Hyperpolarizabilities of Dendritic Systems. Advances in Multi-photon Processes and Spectroscopy, 2003, , 3-146.	0.6	2
314	SECOND HYPERPOLARIZABILITIES OF MOLECULAR AGGREGATES: INTERMOLECULAR ORBITAL-INTERACTION AND SPIN-CONFIGURATION EFFECTS. , 2003, , .		0
315	THEORETICAL STUDY OF EXCITONâ€“EXCITON CORRELATION EFFECT ON EXCITON MIGRATION IN MOLECULAR AGGREGATE. , 2003, , .		0
316	NONLINEAR OPTICAL PROPERTIES OF SEVERAL Ï€-CONJUGATED SYSTEMS INCLUDING NITROGEN ATOMS. , 2003, , .		0
317	Intermolecular-interaction effects on quantum-phase dynamics of dimer systems interacting with a two-mode squeezed vacuum field. Journal of Chemical Physics, 2002, 117, 9671-9687.	1.2	6
318	SECOND HYPERPOLARIZABILITIES OF MOLECULAR AGGREGATES: INTERMOLECULAR ORBITAL-INTERACTION AND SPIN-CONFIGURATION EFFECTS. International Journal of Nanoscience, 2002, 01, 545-549.	0.4	0
319	NONLINEAR OPTICAL PROPERTIES OF SEVERAL Ï€-CONJUGATED SYSTEMS INCLUDING NITROGEN ATOMS. International Journal of Nanoscience, 2002, 01, 651-655.	0.4	0
320	THEORETICAL STUDY OF EXCITONâ€“EXCITON CORRELATION EFFECT ON EXCITON MIGRATION IN MOLECULAR AGGREGATE. International Journal of Nanoscience, 2002, 01, 713-717.	0.4	0
321	Quantum-phase dynamics of dimer systems interacting with a two-mode squeezed coherent field. Journal of Chemical Physics, 2002, 116, 10069-10082.	1.2	11
322	Density analysis of imaginary part of Î³ related to two-photon absorption. Chemical Physics Letters, 2002, 356, 462-468.	1.2	16
323	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
324	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

#	Article	IF	Citations
325	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
326	Quantum-phase and information-entropy dynamics of a molecular system interacting with a two-mode squeezed coherent field. Physical Review A, 2001, 64, .	1.0	13
327	Quantum-phase and information-entropy dynamics of molecular dimers and trimers interacting with quantized fields. Synthetic Metals, 2001, 121, 1473-1474.	2.1	0
328	Theoretical design of organo-magnetic conducting crystal. Synthetic Metals, 2001, 121, 1826-1827.	2.1	0
329	Theoretical study on the off-resonant polarizabilities of linear, square-lattice and dendritic molecular aggregates. Synthetic Metals, 2001, 121, 1263-1264.	2.1	1
330	Theoretical study on the near-resonant second hyperpolarizability (Î³) of a dendritic molecular aggregate: the spatial contribution of intermolecular-interaction and relaxation to Î³. Synthetic Metals, 2001, 121, 1265-1266.	2.1	1
331	Polarizabilities (Î±) of Dendritic Molecular Aggregates:Â Visualization of Intermolecular-Interaction and Damping Effects on Î±. Journal of Physical Chemistry A, 2001, 105, 5473-5478.	1.1	10
332	Theoretical Study on Near-Resonant Third-Order Nonlinear Optical Properties (Î³) of Dendritic Molecular Aggregates: Intermolecular-Interaction and Relaxation Effects on Î³. Molecular Crystals and Liquid Crystals, 2001, 371, 261-264.	0.3	0
333	Theoretical study on quantum dynamics of bose system interacting with photon field. International Journal of Quantum Chemistry, 2001, 84, 401-408.	1.0	0
334	Quantum-phase and information-entropy dynamics of dimers interacting with a single-mode coherent field: The difference between one- and two-exciton models. International Journal of Quantum Chemistry, 2001, 84, 530-545.	1.0	1
335	Third-order nonlinear optical properties of dendritic molecular aggregates: Effects of fractal architecture. International Journal of Quantum Chemistry, 2001, 84, 649-659.	1.0	3
336	Exciton Migration Dynamics of D58-like Dendritic Molecular Aggregate. Molecular Crystals and Liquid Crystals, 2001, 371, 345-348.	0.3	2
337	Theoretical Study on the Polarizabilities of Two-Dimensionally-Grown Dendritic Molecular Aggregates: The Artichitecture- and Size-Dependency. Molecular Crystals and Liquid Crystals, 2001, 371, 215-218.	0.3	0
338	Third-order nonlinear optical properties of fractal- and nonfractal-structured oligomers modeled after dendron parts in Cayley-tree-type dendrimers. Journal of Chemical Physics, 2001, 115, 6780-6784.	1.2	10
339	Size-dependency of polarizabilities of fractal- and nonfractal-structured oligomers modeled after dendron parts in Cayley-tree-type dendrimers. Journal of Chemical Physics, 2001, 115, 1052-1059.	1.2	18
340	Exciton migration dynamics in a dendritic molecular aggregate. Chemical Physics Letters, 2000, 323, 249-256.	1.2	57
341	Intermolecular-interaction effects on quantum-phase and information-entropy dynamics of dimers interacting with a single-mode coherent field. Chemical Physics Letters, 2000, 324, 289-300.	1.2	10
342	Electronâ€"photon field dynamics: numerically exact calculations of multi-state molecule systems interacting with a single-mode coherent photon field. Chemical Physics, 2000, 252, 115-150.	0.9	15

#	Article	IF	Citations
343	On the second hyperpolarizabilities Î³ of three charged states of tetrathiapentalene and tetrathiafulvalene: a Î³ density analysis. Chemical Physics Letters, 2000, 321, 491-497.	1.2	16
344	Electron-correlation dynamics of a one-dimensional H2 model in a quantized photon field. Chemical Physics Letters, 2000, 317, 103-108.	1.2	13
345	Polarizabilities of Dendritic Molecular Aggregates: Contribution of Exciton Generation. Molecular Crystals and Liquid Crystals, 2000, 342, 303-308.	0.3	0
346	Exciton Condensate in Model Dendrimers. Molecular Crystals and Liquid Crystals, 2000, 342, 273-278.	0.3	2
347	Exciton Migration Pathways in Dendritic Molecular Aggregates. Molecular Crystals and Liquid Crystals, 2000, 342, 297-302.	0.3	0
348	Quantum-phase and information-entropy dynamics of a two-state molecular system interacting with strongly amplitude- and phase-squeezed fields. Journal of Chemical Physics, 2000, 112, 2769-2780.	1.2	14
349	Theoretical Study on the Second Hyperpolarizabilities for Small Radical Systems. Molecular Crystals and Liquid Crystals, 1999, 337, 393-396.	0.3	0
350	Quantum phase dynamics of an initially one-mode amplitude-squeezed field interacting with a two-state molecular system. Chemical Physics Letters, 1999, 304, 241-252.	1.2	8
351	Second hyperpolarizability density analyses for trithiapentalene and dioxathiapentalene: visualization of unique Ï€-electron contributions. Chemical Physics Letters, 1999, 306, 187-196.	1.2	19
352	Theoretical studies on second hyperpolarizabilities for cation radical states of tetrathiafulvalene and tetrathiapentalene. Chemical Physics Letters, 1999, 311, 221-230.	1.2	26
353	Quantum Phase Dynamics of Interaction between Photon Field and Magnetic System: Effects of Magnetic Quantum Tunnelling. Optical Review, 1999, 6, 227-231.	1.2	2
354	Theoretical Studies on the Second Hyperpolarizabilities of Trithiapentalene and Its Donor and Acceptor Disubstituted Species. Optical Review, 1999, 6, 232-236.	1.2	1
355	Theoretical Study on the Second Hyperpolarizabilities for Small Radical Systems. Optical Review, 1999, 6, 237-241.	1.2	0
356	Electron correlation and structure dependencies of the second hyperpolarizability of ethylene. International Journal of Quantum Chemistry, 1999, 71, 177-183.	1.0	6
357	Numerical coupled Liouville approach: Application to second hyperpolarizability of molecular aggregate. International Journal of Quantum Chemistry, 1999, 71, 295-306.	1.0	3
358	CAS-SCF and density functional calculations of second hyperpolarizabilities for a nitronyl nitroxide radical. International Journal of Quantum Chemistry, 1999, 71, 329-336.	1.0	10
359	Self-consistent-field calculations of molecular magnetic properties using gauge-invariant atomic orbitals. International Journal of Quantum Chemistry, 1999, 75, 637-643.	1.0	6
360	Visualization of two-body electron densities and wave functions of magnetic molecules. International Journal of Quantum Chemistry, 1999, 75, 645-654.	1.0	8

#	Article	IF	Citations
361	Third-Order Nonlinear Optical Properties of Ï€-Conjugated Systems Involving Sulfur Atoms: A Proposal of Multi-Property Materials Combining Conductivity and Unique Third-Order Nonlinearity. Molecular Crystals and Liquid Crystals, 1999, 337, 369-372.	0.3	2
362	Dynamics of Photon Phase and Information Entropy for a Two-State Molecular System Interacting with Amplitude- and Phase-Squeezed Fields. Journal of Physical Chemistry A, 1999, 103, 6036-6048.	1.1	15
363	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
364	Quantum phase dynamics: collapse and revival behavior in a two- and a three-state molecule systems interacting with an initially one-mode coherent field. Synthetic Metals, 1999, 102, 1540-1541.	2.1	0
365	Polarizabilities of molecular clusters: linear dimer models composed of h2no. Synthetic Metals, 1999, 102, 1542.	2.1	2
366	Second hyperpolarizability of trithiapentalene. Synthetic Metals, 1999, 102, 1543.	2.1	1
367	Second hyperpolarizabilities of 1-center radicals. Synthetic Metals, 1999, 102, 1554-1555.	2.1	0
368	Theoretical study on second hyperpolarizability of copper dimer. Synthetic Metals, 1999, 102, 1562.	2.1	2
369	Visualization of two-body electron-densities and wavefuctions for several molecules. Synthetic Metals, 1999, 103, 2002-2003.	2.1	3
370	Theoretical study on polarizability of ethylene by path integral method. Synthetic Metals, 1999, 101, 513.	2.1	1
371	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
372	Numerical coupled Liouville approach: dependence of population differences between excited and ground states on field intensity and size of molecular aggregates. Chemical Physics Letters, 1998, 288, 25-32.	1.2	2
373	Quasiprobability distribution dynamics of an initially one-mode coherent photon field interacting with two- and three-state molecular systems. Chemical Physics Letters, 1998, 295, 317-327.	1.2	19
374	Electronâ€“photon field dynamics: a molecular aggregate interacting with an initially one-mode coherent photon field. Chemical Physics Letters, 1998, 295, 328-336.	1.2	9
375	Numerical coupled Liouville approach: the dependence of the second hyperpolarizability on field intensity and the size of linear molecular aggregates. Chemical Physics Letters, 1998, 290, 216-222.	1.2	1
376	Numerical coupled Liouville approach: Quantum dynamics of linear molecular aggregates under intense electric fields. International Journal of Quantum Chemistry, 1998, 70, 77-87.	1.0	0
377	Hyperpolarizabilities of one-dimensional Hn systems: Second hyperpolarizability density analyses for regular and charged solitonlike linear chains. International Journal of Quantum Chemistry, 1998, 70, 269-282.	1.0	10
378	Third-Order Nonlinear Optical Properties of a Stable Radical Species with Nitronyl Nitroxide Group. Molecular Crystals and Liquid Crystals, 1998, 315, 117-122.	0.3	9

#	Article	IF	Citations
379	Numerical Coupled Liouville Approach:Â Dependence of Polarizability on Field Intensity and the Size of Linear Molecular Aggregates. Journal of Physical Chemistry A, 1998, 102, 6807-6811.	1.1	1
380	Numerical Coupled Liouville Approach: Application to Nonperturbative Second Hyperpolarizability of a Molecular Aggregate. Bulletin of the Chemical Society of Japan, 1998, 71, 1315-1320.	2.0	2
381	Negative Second Hyperpolarizability of the Nitronyl Nitroxide Radical. Bulletin of the Chemical Society of Japan, 1998, 71, 845-850.	2.0	33
382	Hyperpolarizabilities of oneâ€dimensional Hn systems: Second hyperpolarizability density analyses for regular and charged solitonlike linear chains. International Journal of Quantum Chemistry, 1998, 70, 269-282.	1.0	1
383	Many-electron hyperpolarizability density analysis: Application to the dissociation processof one-dimensionalH2s. Physical Review A, 1997, 55, 1503-1513.	1.0	76
384	Theoretical Studies on Hyperpolarizabelities of Nitroxide Species II. Second Hyperpolarizability of p-NPNN. Molecular Crystals and Liquid Crystals, 1997, 294, 251-254.	0.3	0
385	Hyperpolarizabilities of one-dimensional systems I. Synthetic Metals, 1997, 85, 1147-1148.	2.1	1
386	Theoretical studies for second hyperpolarizabilities of alternant and condensed-ring conjugated systems II. Synthetic Metals, 1997, 85, 1163-1164.	2.1	5
387	Theoretical studies on nonlinear optical properties of organometallic conjugated systems III: second hyperpolarizabilities of Mn(I)-carbene systems. Synthetic Metals, 1997, 86, 2241-2242.	2.1	5
388	Theoretical studies of second hyperpolarizability by path integral method: Effects of external magnetic field. International Journal of Quantum Chemistry, 1997, 65, 697-707.	1.0	3
389	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
390	Theoretical study of the third-order nonlinear optical susceptibilities for the Î²-phase crystal of p-NPNN. Chemical Physics Letters, 1997, 267, 438-444.	1.2	11
391	Structure-property correlation in the second hyperpolarizabilities Î³ for phenyl nitronyl nitroxide radicals. Chemical Physics Letters, 1997, 276, 375-380.	1.2	21
392	Theoretical studies of second hyperpolarizability by path integral method: Effects of external magnetic field. , 1997, 65, 697.		1
393	Many-electron-wavepackets method. International Journal of Quantum Chemistry, 1996, 60, 1291-1301.	1.0	3
394	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
395	Theoretical study on the geometry dependence of the second hyperpolarizability of the allyl cation based on a numerical Liouville three-type analysis. Chemical Physics Letters, 1996, 251, 381-386.	1.2	13
396	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

#	Article	IF	Citations
397	Damping wave packet approach: a calculation method of nonperturbative nonlinear optical susceptibilities including effects of nuclear motion at finite temperatures. Chemical Physics Letters, 1996, 258, 307-315.	1.2	0
398	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
399	Third-order optical nonlinearity in new Ï€-conjugated polymers: polydiethynylsilane and polysilole. Chemical Physics Letters, 1996, 263, 119-125.	1.2	24
400	Theoretical Studies on Nonlinear Optical Properties of Organometallic Conjugated Systems I: Static Third-Order Hyperpolarizabilities of First- Transition-Metal and Metal-Methylene Cations. Molecular Crystals and Liquid Crystals, 1996, 286, 159-164.	0.3	1
401	Numerical Liouville approach. Third-order nonlinear optical susceptibilities in THG, EFISH and DFWM. Chemical Physics Letters, 1995, 233, 411-419.	1.2	10
402	Numerical Liouville approach: intensity-dependent transient linear and nonlinear optical susceptibilities. Chemical Physics Letters, 1995, 234, 323-329.	1.2	9
403	Theoretical studies of spin density populations on nitroxide and nitronylnitroxide derivatives. Chemical Physics Letters, 1995, 240, 268-277.	1.2	17
404	Numerical Liouville approach: Threeâ€type analysis of virtual excitation processes of thirdâ€order nonlinear optical spectra in thirdâ€harmonic generation. Journal of Chemical Physics, 1995, 102, 2996-3004.	1.2	16
405	Numerical Liouville approach: Formulation of thirdâ€order nonlinear optical susceptibilities. Journal of Chemical Physics, 1995, 102, 2986-2995.	1.2	21
406	Theoretical studies on hyperpolarizabilities of nitroxide species. I. Synthetic Metals, 1995, 71, 1691-1692.	2.1	6
407	Second hyperpolarizabilities of Ï€-conjugated silicon-ring polymers. Synthetic Metals, 1995, 71, 1737-1738.	2.1	8
408	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
409	Theoretical Studies for Third-Order Hyperpolarizabilities of Alternant and Condensed-Ring Conjugated Systems I. Molecular Crystals and Liquid Crystals, 1994, 255, 139-148.	0.3	16
410	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
411	A theoretical study on the electron-exchange mechanism in the CF3H+Ar(3P) â†’CF*3 + H + Ar reaction. Chemical Physics Letters, 1994, 224, 445-450.	1.2	4
412	Electronic structures of poly-cations and -anions of C60. Possible mechanisms of organic ferromagnetism. Chemical Physics Letters, 1994, 226, 372-380.	1.2	39
413	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
414	Numerical Liouville approach: A calculation method for nonlinear optical susceptibilities ofN-state systems. Physical Review A, 1994, 50, 2989-3004.	1.0	44

#	Article	IF	Citations
415	Orientation Dependence of Transition Matrix Elements for Energy Transfer Reaction CF3H + Ar(3P) â†' CF3*+ Ar + H. Chemistry Letters, 1994, 23, 1985-1988.	0.7	1
416	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
417	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
418	Ferromagnetic and Antiferromagnetic Behavior of 4-Methacryloyloxy- and 4-Acryloyloxy-2,2,6,6-Tetramethylpiperideste-1-Oxyl. Molecular Crystals and Liquid Crystals, 1993, 232, 53-60.	0.3	20
419	Ab Initio Calculations of Nonlinear Optical Properties of Silicon Compounds. Molecular Crystals and Liquid Crystals, 1992, 217, 71-76.	0.3	9
420	Theoretical calculations of effective exchange integrals between nitronyl nitroxides with donor and acceptor groups. Chemical Physics Letters, 1992, 191, 237-244.	1.2	48
421	MO theoretical studies of magnetic interactions in clusters of nitronyl nitroxide and related species. Chemical Physics Letters, 1992, 190, 353-360.	1.2	72
422	A new model of the third-order nonlinear optical systems which utilizes both through-bond and through-space charge-transfer effects: Polymeric systems with polar side chains. Synthetic Metals, 1991, 43, 3755-3758.	2.1	10
423	Coupled-Hartreeâ€"Fock calculations of the third-order hyperpolarizabilities of substituted polydiacetylenes. Chemical Physics Letters, 1991, 185, 550-554.	1.2	46
424	A CLASSIFICATION OF THE THIRD-ORDER ORGANIC NONLINEAR OPTICAL SYSTEMS AND PROPOSAL OF NEW-TYPE SYSTEMS. , 1991, , 259-262.		2
425	Theoretical studies of third hyperpolarizabilities for .PI.-conjugated organic systems with intra- and inter-molecular charge-transfer effects.. Kobunshi Ronbunshu, 1990, 47, 779-790.	0.2	2
426	A Two-Band Hubbard Model for Clusters of Doped Copper Oxides and Other Metal Oxides: Populations of Holes and Spin Densities by the Full VB CI Method. Japanese Journal of Applied Physics, 1989, 28, L479-L482.	0.8	12
427	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
428	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
429	Anion-exchange Experiment of Zr, Hf, and Th in HNO₃ and Quantum Chemical Study on the Nitrate Complexes toward Chemical Research on Element 104, Rf. Solvent Extraction and Ion Exchange, 0, , 1-16.	0.8	0
430	Medium Diradical Character, Small Hole and Electron Reorganization Energies and Ambipolar Transistors in Difluorenoheteroles. Angewandte Chemie, 0, , .	1.6	0