Masayoshi Nakano

List of Publications by Year in Descending Order

401 papers	10,906 citations	54 h-index	89 g-index
454 ext. papers	11,800 ext. citations	4.2 avg, IF	6.39 L-index

#	Paper	IF	Citations
401	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
400	Theoretical Study on Singlet Fission in Aromatic Diaza -Indacene Dimers. *Journal of Physical Chemistry A*, **2021**, 125, 3257-3267	2.8	1
399	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
398	Theoretical Study on Singlet Fission Dynamics in Slip-Stack-like Pentacene Ring-Shaped Aggregate Models. *Journal of Physical Chemistry A*, **2021**, 125, 5585-5600	2.8	1
397	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	3.6	
396	Theoretical Study on Third-Order Nonlinear Optical Properties for One-Hole-Doped Diradicaloids. *ACS Omega*, **2021**, 6, 3046-3059	3.9	
395	Stabilization of Charge-Transfer States in Pentacene Crystals and Its Role in Singlet Fission. *Journal of Physical Chemistry C*, **2021**, 125, 2264-2275	3.8	2
394	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
393	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
392	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
391	Dianion and Dication of Tetracyclopentatetraphenylene as Decoupled Annulene-within-an-Annulene Models. *Angewandte Chemie - International Edition*, **2021**,	16.4	1
390	Theoretical Study on Singlet Fission Dynamics in Pentacene Ring-Shaped Aggregate Models with Different Configurations. *ChemPhotoChem*, **2020**, 4, 5234-5234	3.3	
389	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	3.8	1
388	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	3.8	10
387	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
386	Diindenoanthracene Diradicaloids Enable Rational, Incremental Tuning of Their Singlet-Triplet Energy Gaps. *CheM*, **2020**, 6, 1353-1368	16.2	19
385	Theoretical Study on Magnetic Interaction in Pyrazole-Bridged Dinuclear Metal Complex: Possibility of Intramolecular Ferromagnetic Interaction by Orbital Counter-Complementarity. *Magnetochemistry*, **2020**, 6, 10	3.1	3

384	Theoretical Study on Singlet Fission Dynamics in Pentacene Ring-Shaped Aggregate Models with Different Configurations. *ChemPhotoChem*, **2020**, 4, 5249-5263	3.3	2
383	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
382	Molecule Isomerism Modulates the Diradical Properties of Stable Singlet Diradicaloids. *Journal of the American Chemical Society*, **2020**, 142, 1548-1555	16.4	37
381	Vibronic coupling density analysis and quantum dynamics simulation for singlet fission in pentacene and its halogenated derivatives. *Journal of Chemical Physics*, **2020**, 153, 134302	3.9	5
380	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
379	Monoradicals and Diradicals of Dibenzofluoreno[3,2-]fluorene Isomers: Mechanisms of Electronic Delocalization. *Journal of the American Chemical Society*, **2020**,	16.4	10
378	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
377	Theoretical Study on Singlet Fission Dynamics in Sumanene-Fused Acene Dimers. *Journal of Physical Chemistry C*, **2020**, 124, 19499-19507	3.8	2
376	Theoretical Molecular Design of Phenanthrenes for Singlet Fission by Diazadibora-Substitution. *Journal of Physical Chemistry A*, **2020**, 124, 6778-6789	2.8	4
375	Quantum design for singlet-fission-induced nonlinear optical systems: Effects of π-conjugation length and molecular packing of butterfly-shaped acenes. *Journal of Chemical Physics*, **2020**, 153, 084304	3.9	2
374	Synthesis and properties of hypervalent electron-rich pentacoordinate nitrogen compounds. *Chemical Science*, **2020**, 11, 5082-5088	9.4	1
373	Singlet-Fission-Induced Enhancement of Third-Order Nonlinear Optical Properties of Pentacene Dimers. *ACS Omega*, **2019**, 4, 16181-16190	3.9	9
372	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
371	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
370	Quantum master equation approach to singlet fission dynamics in pentacene ring-shaped aggregate models. *Journal of Chemical Physics*, **2019**, 150, 234305	3.9	10
369	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	3.8	7
368	Theoretical Study on the Difference in Electron Conductivity of a One-Dimensional Penta-Nickel(II) Complex between Anti-Ferromagnetic and Ferromagnetic States-Possibility of Molecular Switch with Open-Shell Molecules. *Molecules*, **2019**, 24,	4.8	2
367	Correlation between Slow Magnetic Relaxations and Molecular Structures of Dy(III) Complexes with N5O4 Nona-Coordination. *Magnetochemistry*, **2019**, 5, 27	3.1	0

366	Theoretical Study on Second Hyperpolarizabilities of Intramolecular Pancake-Bonded Diradicaloids with Helical Scaffolds. *ACS Omega*, **2019**, 4, 2741-2749	3.9	2
365	Monte Carlo Wavefunction Approach to Singlet Fission Dynamics of Molecular Aggregates. *Molecules*, **2019**, 24,	4.8	11
364	NIR Emission and Acid-Induced Intramolecular Electron Transfer Derived from a SOMO–HOMO Converted Non-Aufbau Electronic Structure. *Journal of Physical Chemistry C*, **2019**, 123, 4417-4423	3.8	19
363	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	0.2	
362	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	5.8	4
361	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
360	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
359	Molecular design for efficient singlet fission. *Journal of Photochemistry and Photobiology C: Photochemistry Reviews*, **2018**, 34, 85-120	16.4	74
358	Benzonorcorrole NiII Complexes: Enhancement of Paratropic Ring Current and Singlet Diradical Character by Benzo-Fusion. *Angewandte Chemie*, **2018**, 130, 2231-2235	3.6	12
357	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
356	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	3.8	10
355	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
354	Synthesis and Functionalization of a 1,4-Bis(trimethylsilyl)tetrasila-1,3-diene through the Selective Cleavage of Si(sp2)–Si(sp3) Bonds under Mild Reaction Conditions. *Organometallics*, **2018**, 37, 172-175	3.8	9
353	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	2.3	3
352	Open-Shell Character Dependences of the Second Hyperpolarizability in Two-Dimensional Tetraradicaloids. *Journal of Physical Chemistry A*, **2018**, 122, 3680-3687	2.8	1
351	Quantum Chemical Design Guidelines for Absorption and Emission Color Tuning of fac-Ir(ppy) Complexes. *Molecules*, **2018**, 23,	4.8	4
350	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
349	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

348	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
347	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	2.3	
346	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
345	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	2.3	
344	Thiophene and its sulfur inhibit indenoindenodibenzothiophene diradicals from low-energy lying thermal triplets. *Nature Chemistry*, **2018**, 10, 1134-1140	17.6	71
343	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
342	Diradical Character Enhancement by Spacing: N-Heterocyclic Carbene Analogues of Müller's Hydrocarbon. *Chemistry - A European Journal*, **2018**, 24, 16537-16542	4.8	19
341	Theoretical investigation of curved π-conjugated fullerene flakes: open-shell character, aromaticity, and third-order nonlinear optical property. *Journal of Physical Organic Chemistry*, **2017**, 30, e3581	2.1	4
340	Fluoreno[2,3-b]fluorene vs Indeno[2,1-b]fluorene: Unusual Relationship between the Number of π Electrons and Excitation Energy in m-Quinodimethane-Type Singlet Diradicaloids. *Journal of Organic Chemistry*, **2017**, 82, 1380-1388	4.2	39
339	A simple zinc(ii) complex that features multi-functional luminochromism induced by reversible ligand dissociation. *Chemical Communications*, **2017**, 53, 3657-3660	5.8	22
338	Impact of Diradical/Ionic Character on Third-Order Nonlinear Optical Property in Asymmetric Phenalenyl Dimers. *ChemistrySelect*, **2017**, 2, 2084-2087	1.8	8
337	Origin of Solvent-independent Optical Property of Unsubstituted BODIPY Revisited. *Chemistry Letters*, **2017**, 46, 536-538	1.7	3
336	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	5.2	16
335	Theoretical study on S 1 and T 1 states of homoleptic bis(dipyrrinato)zinc(II) model complex. *Polyhedron*, **2017**, 136, 113-116	2.7	5
334	Intramolecular Pancake Bonding in Helical Structures. *Chemistry - A European Journal*, **2017**, 23, 7381-7381	4.8	
333	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
332	Intramolecular Pancake Bonding in Helical Structures. *Chemistry - A European Journal*, **2017**, 23, 7474-7482	4.8	16
331	Electronic Structure of Open-Shell Singlet Molecules: Diradical Character Viewpoint. *Topics in Current Chemistry*, **2017**, 375, 47	7.2	40

330	Theoretical study of magnetic interaction in pyrazole-bridged dinuclear Cu(II) complex. *Polyhedron*, **2017**, 136, 132-135	2.7	2
329	Theoretical study on relationship between spin structure and electron conductivity of one-dimensional tri-nickel(II) complex. *Polyhedron*, **2017**, 136, 125-131	2.7	6
328	Generation of Aromatic (Dehydro)benzoannulene Dications Stabilized by Platinum Catecholate Complexes. *ChemPlusChem*, **2017**, 82, 1052-1056	2.8	4
327	Diradical and Ionic Characters of Open-Shell Singlet Molecular Systems. *Journal of Physical Chemistry A*, **2017**, 121, 861-873	2.8	14
326	Singlet fission in pancake-bonded systems. *Physical Chemistry Chemical Physics*, **2017**, 19, 5737-5745	3.6	20
325	Triaminotriborane(3): A Homocatenated Boron Chain Connected by B-B Multiple Bonds. *Angewandte Chemie - International Edition*, **2017**, 56, 15234-15240	16.4	17
324	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
323	Synthesis of the Unknown Indeno[1,2-a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. *Angewandte Chemie*, **2017**, 129, 15565-15569	3.6	19
322	Intermolecular Packing Effects on Singlet Fission in Oligorylene Dimers. *ACS Omega*, **2017**, 2, 5095-5103	3.9	21
321	Rational design of doubly-bridged chromophores for singlet fission and triplet–triplet annihilation. *RSC Advances*, **2017**, 7, 34830-34845	3.7	12
320	Third-Order Nonlinear Optical Properties of One-Dimensional Quinoidal Oligothiophene Derivatives Involving Phenoxyl Groups. *ChemistryOpen*, **2017**, 6, 506-513	2.3	4
319	Mechano-, thermo-, solvato-, and vapochromism in bis(acetato-O)[4-(4-(diphenylamino)phenyl)]-(2,2′:6′,2″-terpyridine-N,N′,N″)-zinc(ii) and its polymer. *Chemical Communications*, **2017**, 53, 9805-9808	5.8	29
318	Tuning Nonlinear Optical Properties by Altering the Diradical and Charge-Transfer Characteristics of Chichibabin's Hydrocarbon Derivatives. *ChemPhysChem*, **2017**, 18, 142-148	3.2	10
317	Open-Shell-Character-Based Molecular Design Principles: Applications to Nonlinear Optics and Singlet Fission. *Chemical Record*, **2017**, 17, 27-62	6.6	100
316	Electronic Structure of Open-Shell Singlet Molecules: Diradical Character Viewpoint. *Topics in Current Chemistry Collections*, **2017**, 1-67	1.8	2
315	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, 12648-54	16.4	39
314	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
313	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	3.8	35

312	Diradical Character-Based Design for Singlet Fission of Bisanthene Derivatives: Aromatic-Ring Attachment and Plane Twisting. *Journal of Physical Chemistry Letters*, **2016**, 7, 3925-3930	6.4	30
311	Nonlinear optical properties in open-shell molecular systems. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 198-210	7.9	47
310	Theoretical study on the spin state and open-shell character dependences of the second hyperpolarizability in hydrogen chain models. *Physical Review A*, **2016**, 94,	2.6	5
309	Open-Shell Singlet Nature and /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, 948-55	2.8	4
308	Biphenalenylidene: Isolation and Characterization of the Reactive Intermediate on the Decomposition Pathway of Phenalenyl Radical. *Journal of the American Chemical Society*, **2016**, 138, 2399-410	16.4	46
307	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
306	Challenging compounds for calculating molecular second hyperpolarizabilities: the triplet state of the trimethylenemethane diradical and two derivatives. *Physical Chemistry Chemical Physics*, **2016**, 18, 6420-9	3.6	5
305	Theoretical Study on the Second Hyperpolarizailities of Oligomeric Systems Composed of Carbon and Silicon Structures. *Molecules*, **2016**, 21,	4.8	2
304	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
303	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
302	Diindeno-fusion of an anthracene as a design strategy for stable organic biradicals. *Nature Chemistry*, **2016**, 8, 753-9	17.6	217
301	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	3.8	31
300	Origin of the Enhancement of the Second Hyperpolarizabilities of Metal-Carbon Bonds. *Journal of Physical Chemistry A*, **2016**, 120, 6838-45	2.8	
299	Design Principles of Electronic Couplings for Intramolecular Singlet Fission in Covalently-Linked Systems. *Journal of Physical Chemistry A*, **2016**, 120, 6236-41	2.8	39
298	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
297	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	6.8	14
296	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. *Journal of Physical Chemistry Letters*, **2015**, 6, 3236-3256	6.4	116
295	Push-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, 8572-83	16.4	76

294	Interplay between Open-Shell Character, Aromaticity, and Second Hyperpolarizabilities in Indenofluorenes. *Journal of Physical Chemistry A*, **2015**, 119, 10620-7	2.8	33
293	Unraveling the degradation of artificial amide bonds in nylon oligomer hydrolase: from induced-fit to acylation processes. *Physical Chemistry Chemical Physics*, **2015**, 17, 4492-504	3.6	10
292	Density Analysis of Intra- and Intermolecular Vibronic Couplings toward Bath Engineering for Singlet Fission. *Journal of Physical Chemistry Letters*, **2015**, 6, 4972-7	6.4	44
291	Theoretical study on the relationship between diradical character and second hyperpolarizabilities of four-membered-ring diradicals involving heavy main-group elements. *Chemistry - A European Journal*, **2015**, 21, 2157-64	4.8	15
290	Substitution effects on optical properties of iminonitroxide- substituted iminonitroxide diradical. *Molecular Physics*, **2015**, 113, 267-273	1.7	1
289	Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: A Potential Tetraradicaloid Hydrocarbon. *Angewandte Chemie*, **2015**, 127, 2118-2122	3.6	26
288	Innentitelbild: Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: A Potential Tetraradicaloid Hydrocarbon (Angew. Chem. 7/2015). *Angewandte Chemie*, **2015**, 127, 2000-2000	3.6	
287	Theoretical study on the second hyperpolarizabilities of one-dimensional heteronuclear transition-metal–metal bonded systems: Metal alignment effects. *Chemical Physics Letters*, **2015**, 640, 165-171	2.5	
286	Theoretical Molecular Design of Heteroacenes for Singlet Fission: Tuning the Diradical Character by Modifying π-Conjugation Length and Aromaticity. *Journal of Physical Chemistry C*, **2015**, 119, 148-157	3.8	48
285	Diradical character dependence of third-harmonic generation spectra in open-shell singlet systems. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	9
284	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	3.8	9
283	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
282	Hydration effects on enzyme–substrate complex of nylon oligomer hydrolase: inter-fragment interaction energy study by the fragment molecular orbital method. *Molecular Physics*, **2015**, 113, 319-326	1.7	6
281	Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: a potential tetraradicaloid hydrocarbon. *Angewandte Chemie - International Edition*, **2015**, 54, 2090-4	16.4	77
280	On the induced-fit mechanism of substrate-enzyme binding structures of nylon-oligomer hydrolase. *Journal of Computational Chemistry*, **2014**, 35, 1240-7	3.5	16
279	A density functional study on the pKa of small polyprotic molecules. *International Journal of Quantum Chemistry*, **2014**, 114, 1128-1134	2.1	26
278	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	1.3	8
277	Intramolecular charge transfer effects on the diradical character and second hyperpolarizabilities of open-shell singlet X–X (X = donor/acceptor) systems. *Journal of Physical Chemistry A*, **2014**, 118, 3463-71	2.8	22

276	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
275	Excitation Energies and Properties of Open-Shell Singlet Molecules. *Springer Briefs in Molecular Science*, **2014**,	0.6	71
274	Diradical Character View of Singlet Fission. *Springer Briefs in Molecular Science*, **2014**, 79-112	0.6	
273	Third-order nonlinear optical properties of one-dimensional open-shell molecular aggregates composed of phenalenyl radicals. *Chemistry - A European Journal*, **2014**, 20, 11129-36	4.8	42
272	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
271	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
270	Anthenes: Model systems for understanding the edge state of graphene nanoribbons. *Pure and Applied Chemistry*, **2014**, 86, 497-505	2.1	17
269	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	2.5	7
268	Electronic Structures of Symmetric Diradical Systems. *Springer Briefs in Molecular Science*, **2014**, 9-26	0.6	
267	Summary and Future Prospects. *Springer Briefs in Molecular Science*, **2014**, 113-116	0.6	
266	Electronic Structures of Asymmetric Diradical Systems. *Springer Briefs in Molecular Science*, **2014**, 27-41	0.6	
265	Diradical Character View of (Non)Linear Optical Properties. *Springer Briefs in Molecular Science*, **2014**, 43-77	0.6	
264	Functional dependence of excitation energy for pentacene/C60 model complex in the nonempirically tuned long-range corrected density functional theory. *International Journal of Quantum Chemistry*, **2013**, 113, 252-256	2.1	22
263	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
262	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
261	Quantal cumulant mechanics and dynamics for multidimensional quantum many-body clusters. *International Journal of Quantum Chemistry*, **2013**, 113, 348-355	2.1	8
260	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
259	Photochromic Switching of Diradical Character: Design of Efficient Nonlinear Optical Switches. *Journal of Physical Chemistry Letters*, **2013**, 4, 2418-2422	6.4	42

258	Diradical character dependences of the first and second hyperpolarizabilities of asymmetric open-shell singlet systems. *Journal of Chemical Physics*, **2013**, 138, 244306	3.9	43
257	Theoretical study on the diradical characters and third-order nonlinear optical properties of transition-metal heterodinuclear systems. *Chemical Physics Letters*, **2013**, 579, 73-77	2.5	6
256	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
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