

Masayoshi Nakano

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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	Theoretical study on second hyperpolarizabilities of phenylacetylene dendrimer: toward an understanding of structure-property relation in NLO responses of fractal antenna dendrimers. <i>Journal of the American Chemical Society</i> , 2002 , 124, 9648-55	16.4	333
400	Synthesis, intermolecular interaction, and semiconductive behavior of a delocalized singlet biradical hydrocarbon. <i>Angewandte Chemie - International Edition</i> , 2005 , 44, 6564-8	16.4	276
399	Second hyperpolarizability (gamma) of singlet diradical system: dependence of gamma on the diradical character. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 885-91	2.8	269
398	Synthesis and characterization of teranthene: a singlet biradical polycyclic aromatic hydrocarbon having Kekulé structures. <i>Journal of the American Chemical Society</i> , 2010 , 132, 11021-3	16.4	249
397	Relationship between third-order nonlinear optical properties and magnetic interactions in open-shell systems: a new paradigm for nonlinear optics. <i>Physical Review Letters</i> , 2007 , 99, 033001	7.4	246
396	Strong two-photon absorption of singlet diradical hydrocarbons. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 3544-6	16.4	241
395	Size-consistent approach and density analysis of hyperpolarizability: Second hyperpolarizabilities of polymeric systems with and without defects. <i>Journal of Chemical Physics</i> , 1995 , 103, 4175-4191	3.9	234
394	Diindeno-fusion of an anthracene as a design strategy for stable organic biradicals. <i>Nature Chemistry</i> , 2016 , 8, 753-9	17.6	217
393	Synthesis and characterization of quarteranthene: elucidating the characteristics of the edge state of graphene nanoribbons at the molecular level. <i>Journal of the American Chemical Society</i> , 2013 , 135, 1430-7	16.4	201
392	Diradical Character View of Singlet Fission. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 145-150	6.4	200
391	Indeno[2,1-b]fluorene: a 20- π -electron hydrocarbon with very low-energy light absorption. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 6076-9	16.4	189
390	Singlet Diradical Character from Experiment. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 937-940	6.4	154
389	Alternating covalent bonding interactions in a one-dimensional chain of a phenalenyl-based singlet biradical molecule having Kekulé structures. <i>Journal of the American Chemical Society</i> , 2010 , 132, 14421-8	16.4	142
388	Singlet biradical character of phenalenyl-based Kekulé hydrocarbon with naphthoquinoid structure. <i>Organic Letters</i> , 2007 , 9, 81-4	6.2	138
387	Second hyperpolarizabilities of polycyclic aromatic hydrocarbons involving phenalenyl radical units. <i>Chemical Physics Letters</i> , 2006 , 418, 142-147	2.5	132
386	Resonance balance shift in stacks of delocalized singlet biradicals. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 5482-6	16.4	131
385	Basis set and electron correlation effects on the polarizability and second hyperpolarizability of model open-shell pi-conjugated systems. <i>Journal of Chemical Physics</i> , 2005 , 122, 114315	3.9	129

384	Impact of diradical character on two-photon absorption: bis(acridine) dimers synthesized from an allenic precursor. <i>Journal of the American Chemical Society</i> , 2013 , 135, 232-41	16.4	124
383	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 3236-3256	6.4	116
382	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. <i>Theoretical Chemistry Accounts</i> , 2011 , 130, 711-724	1.9	114
381	A proposal of new organic third-order nonlinear optical compounds. Centrosymmetric systems with large negative third-order hyperpolarizabilities. <i>Chemical Physics Letters</i> , 1993 , 206, 285-292	2.5	112
380	Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Polyaromatic Diphenalenyl Diradicaloids by an External Electric Field and Donor-Acceptor Substitution. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 1094-1098	6.4	104
379	Open-Shell-Character-Based Molecular Design Principles: Applications to Nonlinear Optics and Singlet Fission. <i>Chemical Record</i> , 2017 , 17, 27-62	6.6	100
378	Fundamental of Diradical-Character-Based Molecular Design for Singlet Fission. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 2133-2137	6.4	95
377	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. <i>Chemical Physics Letters</i> , 2008 , 467, 120-125	2.5	93
376	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. <i>Chemical Physics Letters</i> , 2010 , 489, 212-218	2.5	88
375	Second hyperpolarizabilities (γ) of bisimidazole and bistriazole benzenes: diradical character, charged state, and spin state dependences. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 4238-43	2.8	85
374	Synthesis, Intermolecular Interaction, and Semiconductive Behavior of a Delocalized Singlet Biradical Hydrocarbon. <i>Angewandte Chemie</i> , 2005 , 117, 6722-6726	3.6	85
373	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. <i>Journal of Chemical Physics</i> , 2006 , 125, 074113	3.9	84
372	Theoretical study on the second hyperpolarizabilities of phenalenyl radical systems involving acetylene and vinylene linkers: diradical character and spin multiplicity dependences. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 3633-41	2.8	80
371	Tetracyclopenta[def,jkl,pqr,vwx]tetraphenylene: a potential tetradicaloid hydrocarbon. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 2090-4	16.4	77
370	Push-Pull Type Oligo(N-annulated perylene)quinodimethanes: Chain Length and Solvent-Dependent Ground States and Physical Properties. <i>Journal of the American Chemical Society</i> , 2015 , 137, 8572-83	16.4	76
369	Spin Multiplicity Effects on the Second Hyperpolarizability of an Open-Shell Neutral π -Conjugated System. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 4105-4111	2.8	76
368	Diradical Character Based Design for Singlet Fission of Condensed-Ring Systems with $4n+2$ Electrons. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 19729-19736	3.8	75
367	Many-electron hyperpolarizability density analysis: Application to the dissociation process of one-dimensional H ₂ s. <i>Physical Review A</i> , 1997 , 55, 1503-1513	2.6	75

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- 364 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 3.4 74
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- 358 Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. *Chemical Physics Letters*, **2009**, 477, 355-359 2.5 68
- 357 MO theoretical studies of magnetic interactions in clusters of nitronyl nitroxide and related species. *Chemical Physics Letters*, **1992**, 190, 353-360 2.5 68
- 356 Tuned CAM-B3LYP functional in the time-dependent density functional theory scheme for excitation energies and properties of diarylethene derivatives. *Journal of Photochemistry and Photobiology A: Chemistry*, **2012**, 235, 29-34 4.7 65
- 355 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, 20575-83 3.6 64
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- 353 Second Hyperpolarizability of Zethrenes. *Computing Letters*, **2007**, 3, 333-338 57
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- 351 Exciton migration dynamics in a dendritic molecular aggregate. *Chemical Physics Letters*, **2000**, 323, 249-256 55
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347	Theoretical consideration of singlet open-shell character of polyperiacenes using Clar's aromatic sextet valence bond model and quantum chemical calculations 2012 ,		52
346	Static second hyperpolarizabilities of nitroxide radical and formaldehyde: evaluation of spatial contributions to by a hyperpolarizability density analysis. <i>Chemical Physics Letters</i> , 1996 , 254, 158-164	2.5	51
345	Synthesis of the Unknown Indeno[1,2-a]fluorene Regioisomer: Crystallographic Characterization of Its Dianion. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 15363-15367	16.4	50
344	Role of a singlet diradical character in carbon nanomaterials: a novel hot spot for efficient nonlinear optical materials. <i>Nanoscale</i> , 2016 , 8, 17998-18020	7.7	49
343	Remarkable two-photon absorption in open-shell singlet systems. <i>Journal of Chemical Physics</i> , 2009 , 131, 114316	3.9	49
342	Theoretical Molecular Design of Heteroacenes for Singlet Fission: Tuning the Diradical Character by Modifying Conjugation Length and Aromaticity. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 148-157	3.8	48
341	Nonlinear optical properties in open-shell molecular systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016 , 6, 198-210	7.9	47
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339	Theoretical study on second hyperpolarizabilities of singlet diradical square planar nickel complexes involving o-semiquinonato type ligands. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 8423-9	2.8	47
338	Mechanism of exciton migration of dendritic molecular aggregate: a master equation approach including weak exciton-phonon coupling. <i>Chemical Physics Letters</i> , 2002 , 363, 422-428	2.5	47
337	Biphenalenylidene: Isolation and Characterization of the Reactive Intermediate on the Decomposition Pathway of Phenalenyl Radical. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2399-410	16.4	46
336	Strong Two-Photon Absorption of Singlet Diradical Hydrocarbons. <i>Angewandte Chemie</i> , 2007 , 119, 3614-3616	3.6	46
335	Coupled-Hartree-Fock calculations of the third-order hyperpolarizabilities of substituted polydiacetylenes. <i>Chemical Physics Letters</i> , 1991 , 185, 550-554	2.5	46
334	Open-shell characters and second hyperpolarizabilities of one-dimensional graphene nanoflakes composed of trigonal graphene units. <i>ChemPhysChem</i> , 2011 , 12, 1697-707	3.2	45
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332	Theoretical calculations of effective exchange integrals between nitronyl nitroxides with donor and acceptor groups. <i>Chemical Physics Letters</i> , 1992 , 191, 237-244	2.5	44
331	Diradical character dependences of the first and second hyperpolarizabilities of asymmetric open-shell singlet systems. <i>Journal of Chemical Physics</i> , 2013 , 138, 244306	3.9	43

- 330 Resonance Balance Shift in Stacks of Delocalized Singlet Biradicals. *Angewandte Chemie*, **2009**, 121, 5590-5594 43
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308	Interplay between Open-Shell Character, Aromaticity, and Second Hyperpolarizabilities in Indeno[1,2-b]fluorenes. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 10620-7	2.8	33
307	Signature of singlet open-shell character on the optically allowed singlet excitation energy and singlet-triplet energy gap. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 2000-6	2.8	33
306	Exciton migration dynamics in a dendritic molecule: quantum master equation approach using ab initio molecular orbital configuration interaction method. <i>Journal of Chemical Physics</i> , 2004 , 120, 2359-67	3.9	33
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303	Second hyperpolarizability of phenalenyl radical system involving acetylene π -conjugated bridge. <i>Chemical Physics Letters</i> , 2006 , 420, 432-437	2.5	31
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