BenoÃ®t Ãt Champagne

List of Publications by Year
in descending order

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424	14,113	22153	40979
papers	citations	59 h-index	93 g-index

436	436	436	7530
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of Pushâ˜'Pull Ï€-Conjugated Systemsâ€. Journal of Physical Chemistry A, 2000, 104, 4755-4763.	2.5	501
2	Design and Characterization of Molecular Nonlinear Optical Switches. Accounts of Chemical Research, 2013, 46, 2656-2665.	15.6	325
3	Second Hyperpolarizability (Î³) of Singlet Diradical System:Â Dependence of Î³ on the Diradical Character. Journal of Physical Chemistry A, 2005, 109, 885-891.	2.5	296
4	Synthesis and Characterization of Teranthene: A Singlet Biradical Polycyclic Aromatic Hydrocarbon Having KekulÃ© Structures. Journal of the American Chemical Society, 2010, 132, 11021-11023.	13.7	285
5	Nonlinear Optical Molecular Switches as Selective Cation Sensors. Journal of the American Chemical Society, 2012, 134, 8101-8103.	13.7	267
6	Relationship between Third-Order Nonlinear Optical Properties and Magnetic Interactions in Open-Shell Systems: A New Paradigm for Nonlinear Optics. Physical Review Letters, 2007, 99, 033001.	7.8	258
7	Singlet Diradical Character from Experiment. Journal of Physical Chemistry Letters, 2010, 1, 937-940.	4.6	181
8	Electron correlation effects on the first hyperpolarizability of pushâ€“pull Ï€-conjugated systems. Journal of Chemical Physics, 2011, 134, 074113.	3.0	174
9	In silico optimization of merocyanine-spiropyran compounds as second-order nonlinear optical molecular switches. Physical Chemistry Chemical Physics, 2008, 10, 6223.	2.8	153
10	Reference molecules for nonlinear optics: A joint experimental and theoretical investigation. Journal of Chemical Physics, 2012, 136, 024506.	3.0	144
11	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. Journal of Physical Chemistry Letters, 2015, 6, 3236-3256.	4.6	142
12	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.	3.0	141
13	Nonlinear optical properties of quasilinear conjugated oligomers, polymers and organic molecules. International Reviews in Physical Chemistry, 1997, 16, 389-420.	2.3	133
14	Twoâ€Way Molecular Switches with Large Nonlinear Optical Contrast. Chemistry - A European Journal, 2009, 15, 2560-2571.	3.3	132
15	Electric Field Simulation of Substituents in Donorâ˜'Acceptor Polyenes:Â A Comparison with Ab Initio Predictions for Dipole Moments, Polarizabilities, and Hyperpolarizabilities. Journal of the American Chemical Society, 2000, 122, 8007-8012.	13.7	131
16	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. Theoretical Chemistry Accounts, 2011, 130, 711-724.	1.4	125
17	Acido- and Phototriggered NLO Properties Enhancement. Journal of Physical Chemistry B, 2005, 109, 11139-11150.	2.6	120
18	Density-functional theory (hyper)polarizabilities of push-pull Ï€-conjugated systems: Treatment of exact exchange and role of correlation. Journal of Chemical Physics, 2005, 123, 014319.	3.0	120

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19	Three-Wave Mixing in Chiral Liquids. Physical Review Letters, 2000, 85, 4253-4256.	7.8	115
20	Calculation of electric dipole (hyper)polarizabilities by long-range-correction scheme in density functional theory: A systematic assessment for polydiacetylene and polybutatriene oligomers. Journal of Chemical Physics, 2008, 128, 114108.	3.0	114
21	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.	4.6	111
22	Large Off-Diagonal Contribution to the Second-Order Optical Nonlinearities of Î›-Shaped Molecules. Journal of Physical Chemistry A, 2003, 107, 3942-3951.	2.5	105
23	Theoretical and Experimental Investigation of Electric Field Induced Second Harmonic Generation in Tetrathia[7]helicenes. Journal of Physical Chemistry C, 2008, 112, 7900-7907.	3.1	104
24	Oxazines: A New Class of Second-Order Nonlinear Optical Switches. Journal of the American Chemical Society, 2016, 138, 5052-5062.	13.7	104
25	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.	2.5	100
26	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. Chemical Physics Letters, 2008, 467, 120-125.	2.6	96
27	TDDFT investigation of the optical properties of cyanine dyes. Chemical Physics Letters, 2006, 425, 105-109.	2.6	93
28	Time dependent density functional theory investigation of the resonance Raman properties of the julolidinemalononitrile push-pull chromophore in various solvents. Journal of Chemical Physics, 2007, 127, 164507.	3.0	93
29	Acido-Triggered Nonlinear Optical Switches:â€‰ Benzazolo-oxazolidines. Journal of Physical Chemistry B, 2007, 111, 9795-9802.	2.6	92
30	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. Chemical Physics Letters, 2010, 489, 212-218.	2.6	90
31	Ab Initio Coupled Hartreeâ€“Fock Investigation of the Static First Hyperpolarizability of Model all-trans-Polymethineimine Oligomers of Increasing Size. Journal of Physical Chemistry A, 1997, 101, 3158-3165.	2.5	88
32	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. Journal of Chemical Physics, 2006, 125, 074113.	3.0	88
33	Resonance Raman Scattering of Rhodamine 6G as Calculated by Time-Dependent Density Functional Theory:â€‰ Vibronic and Solvent Effects. Journal of Physical Chemistry A, 2008, 112, 3215-3223.	2.5	87
34	Assessment of time-dependent density functional schemes for computing the oscillator strengths of benzene, phenol, aniline, and fluorobenzene. Journal of Chemical Physics, 2007, 127, 084103.	3.0	85
35	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.	2.5	84
36	Theoretical study of the second-order nonlinear optical properties of [N]helicenes and [N]phenylenes. Journal of Chemical Physics, 2004, 120, 2042-2048.	3.0	82

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37	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. Journal of Chemical Physics, 2010, 132, 094107.	3.0	82
38	Investigation on the Second-Order Nonlinear Optical Responses in the Ketoâ˜Enol Equilibrium of Anil Derivatives. Journal of Physical Chemistry C, 2008, 112, 5638-5645.	3.1	81
39	Spin Multiplicity Effects on the Second Hyperpolarizability of an Open-Shell Neutral Ï€-Conjugated System. Journal of Physical Chemistry A, 2004, 108, 4105-4111.	2.5	80
40	Vibrational polarizability and hyperpolarizability of p-nitroaniline. Chemical Physics Letters, 1996, 261, 57-65.	2.6	79
41	An analytical derivative procedure for the calculation of vibrational Raman optical activity spectra. Journal of Chemical Physics, 2007, 127, 204105.	3.0	79
42	Evaluation of alternative sum-over-states expressions for the first hyperpolarizability of push-pull Ï€-conjugated systems. Journal of Chemical Physics, 2006, 125, 024101.	3.0	78
43	Multichromophoric Dendrimers as Single-Photon Sources:Â A Single-Molecule Study. Journal of Physical Chemistry B, 2004, 108, 16686-16696.	2.6	76
44	Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. Chemical Physics Letters, 2009, 477, 355-359.	2.6	74
45	Assessing long-range corrected functionals with physically-adjusted range-separated parameters for calculating the polarizability and the second hyperpolarizability of polydiacetylene and polybutatriene chains. Physical Chemistry Chemical Physics, 2014, 16, 7083.	2.8	74
46	Investigation of the UV/Visible Absorption Spectra of Merocyanine Dyes Using Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2006, 110, 13007-13013.	2.5	70
47	Calculations of Nonlinear Optical Properties for the Solid State. Advances in Chemical Physics, 2003, , 41-92.	0.3	69
48	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.	2.8	69
49	Second-Harmonic Generation in GFP-like Proteins. Journal of the American Chemical Society, 2008, 130, 15713-15719.	13.7	66
50	Pushing the Lewis Acidity Boundaries of Boron Compounds With Nonâ€Planar Triarylboranes Derived from Triptycenes. Angewandte Chemie - International Edition, 2019, 58, 16889-16893.	13.8	66
51	Role of collective modes in vibrational polarizabilities and hyperpolarizabilities of polyacetylene and other quasilinear polymers. Journal of Chemical Physics, 1996, 104, 4125-4136.	3.0	65
52	Theoretical approach to the design of organic molecular and polymeric nonlinear optical materials. , 2001, , 63-126.		64
53	Naphthidine di(radical cation)s-stabilized palladium nanoparticles for efficient catalytic Suzukiâ€“Miyaura cross-coupling reactions. Tetrahedron, 2008, 64, 372-381.	1.9	63
54	Solvent Effects on the Second-Order Nonlinear Optical Responses in the Ketoâ˜Enol Equilibrium of a 2-Hydroxy-1-naphthaldehyde Derivative. Journal of Physical Chemistry C, 2010, 114, 12760-12768.	3.1	63

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55	Nonlinear optical properties in openâ€shell molecular systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 198-210.	14.6	63
56	Simple Scheme To Evaluate Crystal Nonlinear Susceptibilities: Semiempirical AM1 Model Investigation of 3-Methyl-4-nitroaniline Crystal. Journal of Physical Chemistry A, 2001, 105, 1366-1370.	2.5	62
57	Ring Current Model and Anisotropic Magnetic Response of Cyclopropane. Journal of Chemical Theory and Computation, 2010, 6, 2002-2018.	5.3	62
58	Theoretical investigation of the dynamic first hyperpolarizability of DHAâ€“VHF molecular switches. New Journal of Chemistry, 2009, 33, 1349.	2.8	61
59	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.	3.1	61
60	Second Hyperpolarizability of Zethrenes. Computing Letters, 2007, 3, 333-338.	0.5	60
61	Density functional theory investigation of the polarizability and second hyperpolarizability of polydiacetylene and polybutatriene chains: Treatment of exact exchange and role of correlation. Journal of Chemical Physics, 2006, 125, 194114.	3.0	59
62	Theoretical investigation on the second hyperpolarizabilities of open-shell singlet systems by spin-unrestricted density functional theory with long-range correction: Range separating parameter dependence. Chemical Physics Letters, 2010, 493, 195-199.	2.6	59
63	Major intermolecular effects on nonlinear electrical response in a hexatriene model of solid state polyacetylene. Chemical Physics Letters, 1999, 305, 132-138.	2.6	58
64	Theoretical Design of Substituted Tetrathia-[7]-Helicenes with Large Second-Order Nonlinear Optical Responses. ChemPhysChem, 2004, 5, 1438-1442.	2.1	58
65	Performance of DFT functionals for calculating the second-order nonlinear optical properties of dipolar merocyanines. Physical Chemistry Chemical Physics, 2020, 22, 16579-16594.	2.8	58
66	ZIF-8 as Nonlinear Optical Material: Influence of Structure and Synthesis. Chemistry of Materials, 2016, 28, 3203-3209.	6.7	57
67	Vibrational polarizability of polyacetylene chains. Journal of Chemical Physics, 1994, 101, 10796-10807.	3.0	55
68	Electron correlation effects upon the static (hyper)polarizabilities of push-pull conjugated polyenes and polyynes. , 1997, 65, 679-688.		55
69	Acidoswitchable NLO-phores:Â Benzimidazolo[2,3-b]oxazolidines. Journal of Physical Chemistry B, 2006, 110, 10672-10682.	2.6	54
70	Remarkable two-photon absorption in open-shell singlet systems. Journal of Chemical Physics, 2009, 131, 114316.	3.0	54
71	Symmetrical and Nonsymmetrical Chromophores with TrÃ¶gerâ€™s Base Skeleton: Chiroptical, Linear, and Quadratic Nonlinear Optical Propertiesâ€”A Joint Theoretical and Experimental Study. Chemistry - A European Journal, 2010, 16, 8181-8190.	3.3	54
72	Improving the Second-Order Nonlinear Optical Response of Fluorescent Proteins: The Symmetry Argument. Journal of the American Chemical Society, 2013, 135, 4061-4069.	13.7	54

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73	Hyper-Rayleigh scattering of neutral and charged helicenes. Chemical Physics Letters, 2005, 412, 274-279.	2.6	53
74	From uncoupled to coupled Hartreeâ€“Fock polarizabilities of infinite polymeric chains. Pariserâ€“Parrâ€“Pople applications to the polyacetylene chains. Journal of Chemical Physics, 1992, 96, 8330-8337.	3.0	51
75	On the Aromatic Character of 1,2-Dihydro-1,2-azaborine According to Magnetic Criteria. Journal of Physical Chemistry Letters, 2010, 1, 1563-1568.	4.6	51
76	Diradical character dependences of the first and second hyperpolarizabilities of asymmetric open-shell singlet systems. Journal of Chemical Physics, 2013, 138, 244306.	3.0	51
77	Evaluation of the molecular static and dynamic first hyperpolarizabilities. International Journal of Quantum Chemistry, 2014, 114, 900-910.	2.0	51
78	Evaluation of the Linear and Second-Order NLO Properties of Molecular Crystals within the Local Field Theory: Electron Correlation Effects, Choice of XC Functional, ZPVA Contributions, and Impact of the Geometry in the Case of 2-Methyl-4-nitroaniline. Journal of Chemical Theory and Computation, 2014, 10, 2114-2124.	5.3	51
79	Polymorphic and Isomorphic Cocrystals of a N-Salicylidene-3-aminopyridine with Dicarboxylic Acids: Tuning of Solid-State Photo- and Thermochromism. Journal of Physical Chemistry C, 2016, 120, 10001-10008.	3.1	51
80	Second-Order ab Initio MÃ¸llerâ^'Plesset Study of Optimum Chain Length for Total (Electronic Plus) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 9748-9755.	2.5	50
81	Multimode simulation of dimer absorption spectra from first principles calculations: Application to the 3,4,9,10-perylenetetracarboxylic diimide dimer. Journal of Chemical Physics, 2009, 131, 154302.	3.0	50
82	Second-Order Nonlinear Optical Properties of Multiaddressable Indolinooxazolidine Derivatives: Joint Computational and Hyper-Rayleigh Scattering Investigations. Journal of Physical Chemistry C, 2017, 121, 1851-1860.	3.1	50
83	Mixed electric-magnetic second-order nonlinear optical response of helicenes. Journal of Chemical Physics, 2005, 122, 234713.	3.0	49
84	Ab Initio Investigation on the Second-Order Nonlinear Optical Responses in Ketoâ^'Enol Equilibria of Salicylideneanilines. Journal of Physical Chemistry A, 2007, 111, 9914-9923.	2.5	49
85	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.	2.5	49
86	Third-order nonlinear optical properties of trigonal, rhombic and bow-tie graphene nanoflakes with strong structural dependence of diradical character. Chemical Physics Letters, 2009, 480, 278-283.	2.6	49
87	Determination of ab initio polarizabilities of polymers: Application to polyethylene and polysilane. International Journal of Quantum Chemistry, 1992, 42, 1009-1024.	2.0	48
88	Efficient treatment of the effect of vibrations on electrical, magnetic, and spectroscopic properties. Journal of Computational Chemistry, 2000, 21, 1572-1588.	3.3	48
89	Theoretical investigation of the linear and second-order nonlinear susceptibilities of the 3-methyl-4-nitropyridine-1-oxyde (POM) crystal. Journal of Chemical Physics, 2004, 121, 7390-7400.	3.0	48
90	Effects of the Nature and Length of the Ï€â€Conjugated Bridge on the Secondâ€Order Nonlinear Optical Responses of Pushâ€“Pull Molecules Including 4,5â€Dicyanoimidazole and Their Protonated Forms. ChemPhysChem, 2011, 12, 3245-3252.	2.1	48

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91	Assessment of DFT Exchangeâ€“Correlation Functionals for Evaluating the Multipolar Contributions to the Quadratic Nonlinear Optical Responses of Small Reference Molecules. Journal of Chemical Theory and Computation, 2012, 8, 2044-2052.	5.3	47
92	Electron-correlation effects on the static longitudinal polarizability of polymeric chains. Physical Review A, 1995, 52, 178-188.	2.5	46
93	Time-dependent density functional theory investigation of the absorption and emission spectra of a cyanine dye. Chemical Physics Letters, 2007, 446, 165-169.	2.6	46
94	Openâ€Shell Characters and Second Hyperpolarizabilities of Oneâ€Dimensional Graphene Nanoflakes Composed of Trigonal Graphene Units. ChemPhysChem, 2011, 12, 1697-1707.	2.1	46
95	Thirdâ€Order Nonlinear Optical Properties of Oneâ€Dimensional Openâ€Shell Molecular Aggregates Composed of Phenalenyl Radicals. Chemistry - A European Journal, 2014, 20, 11129-11136.	3.3	46
96	Controlled Generation of 9â€Boratriptycene by Lewis Adduct Dissociation: Accessing a Nonâ€Planar Triarylborane. Angewandte Chemie - International Edition, 2020, 59, 12402-12406.	13.8	46
97	TDHF Evaluation of the Dipoleâ^'Quadrupole Polarizability and Its Geometrical Derivatives. Journal of Chemical Theory and Computation, 2005, 1, 444-452.	5.3	45
98	First and second hyperpolarizabilities of donorâ€“acceptor disubstituted diphenalenyl radical systems. Chemical Physics Letters, 2007, 443, 95-101.	2.6	43
99	Linear, cyclic, and MÃ¶bius strip polyacenes: The influence of the topology on the size-dependent HOMO-LUMO energy gap. International Journal of Quantum Chemistry, 2001, 84, 607-616.	2.0	42
100	Identification of free radicals trapped in solid methacrylated resins. Journal of Polymer Science Part A, 2003, 41, 1691-1699.	2.3	42
101	Strong Two-Photon Circular Dichroism in Helicenes:â€‰ A Theoretical Investigation. Journal of Chemical Theory and Computation, 2008, 4, 457-467.	5.3	42
102	Second-order nonlinear optical properties of fluorescent proteins for second-harmonic imaging. Journal of Materials Chemistry, 2009, 19, 7514.	6.7	42
103	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.	5.3	41
104	Ab initio coupled and uncoupled Hartree-Fock calculations of the polarizabilities of finite and infinite polyacetylene chains. International Journal of Quantum Chemistry, 1993, 48, 667-685.	2.0	40
105	Bond length alternation effects on the static electronic polarizability and second hyperpolarizability of polyacetylene chains. International Journal of Quantum Chemistry, 1999, 75, 441-447.	2.0	40
106	Finding optimal finite field strengths allowing for a maximum of precision in the calculation of polarizabilities and hyperpolarizabilities. Journal of Computational Chemistry, 2013, 34, 1497-1507.	3.3	40
107	Experimental and theoretical investigation of the Raman and hyper-Raman spectra of acetonitrile and its derivatives. Journal of Chemical Physics, 2006, 124, 244312.	3.0	39
108	Linear and second-order nonlinear optical properties of ionic organic crystals. Journal of Chemical Physics, 2014, 141, 104109.	3.0	39

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109	All-Conjugated ABC-block-copolymer Formation with a Varying Sequence via an Unassociated Catalyst. Macromolecules, 2014, 47, 4668-4675.	4.8	39
110	Polarization effects on the hyper-Raman spectra of carbon tetrachloride: A joint experimental-theoretical study. Journal of Chemical Physics, 2004, 121, 4705-4710.	3.0	38
111	Theoretical Investigation of the Second-Order Nonlinear Optical Properties of Helical Pyridineâ€“Pyrimidine Oligomers. Chemistry - A European Journal, 2006, 12, 8687-8695.	3.3	38
112	Orientational Analysis of Dodecanethiol and pâ€Nitrothiophenol SAMs on Metals with Polarisationâ€Dependent SFG Spectroscopy. ChemPhysChem, 2010, 11, 607-615.	2.1	38
113	Giant electric field effect on the second hyperpolarizability of symmetric singlet diradical molecules. Journal of Chemical Physics, 2010, 133, 154302.	3.0	38
114	Investigation of the linear and second-order nonlinear optical properties of molecular crystals within the local field theory. Journal of Chemical Physics, 2013, 139, 114105.	3.0	38
115	Aromaticity as a Guiding Concept for Spectroscopic Features and Nonlinear Optical Properties of Porphyrinoids. Molecules, 2018, 23, 1333.	3.8	38
116	Calculation of static zero-point vibrational averaging corrections and other vibrational curvature contributions to polarizabilities and hyperpolarizabilities using field-induced coordinates. International Journal of Quantum Chemistry, 2000, 80, 471-479.	2.0	37
117	Theoretical investigation on H1 and C13 NMR chemical shifts of small alkanes and chloroalkanes. Journal of Chemical Physics, 2006, 125, 144309.	3.0	37
118	Theoretical Determination of the Vibrational Raman Optical Activity Signatures of Helical Polypropylene Chains. ChemPhysChem, 2006, 7, 2366-2376.	2.1	37
119	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.	4.6	37
120	Linear and nonlinear optical properties of arylvinyldiazine dyes: A theoretical investigation. Dyes and Pigments, 2014, 110, 256-260.	3.7	37
121	Second-order nonlinear optical properties of Stenhouse photoswitches: insights from density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 27658-27667.	2.8	37
122	Modeling the electric field third-order nonlinear responses of an infinite aggregate of hexatriene chains using the electrostatic interaction model. Physical Chemistry Chemical Physics, 2005, 7, 3284.	2.8	36
123	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. Chemical Physics Letters, 2008, 454, 97-104.	2.6	36
124	Theoretical Simulation of Vibrational Sumâ€Frequency Generation Spectra from Density Functional Theory: Application to pâ€Nitrothiophenol and 2,4â€Dinitroaniline. ChemPhysChem, 2009, 10, 2132-2142.	2.1	35
125	Explicit versus Implicit Solvation Effects on the First Hyperpolarizability of an Organic Biphotochrome. Journal of Physical Chemistry A, 2015, 119, 5496-5503.	2.5	35
126	Second-order nonlinear optical coefficient of polyphosphazene-based materials: A theoretical study. Journal of Chemical Physics, 2004, 120, 9401-9409.	3.0	34

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127	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.	2.6	34
128	Circular dichroism of helical structures using semiempirical methods. Journal of Chemical Physics, 2007, 127, 204101.	3.0	34
129	Prediction of Vibronic Coupling and Absorption Spectra of Dimers from Time-Dependent Density Functional Theory: The Case of a Stacked Streptocyanine. Journal of Chemical Theory and Computation, 2008, 4, 2094-2100.	5.3	34
130	Vibrational Raman optical activity of Ï€â€conjugated helical systems: Hexahelicene and heterohelicenes. Journal of Computational Chemistry, 2009, 30, 1261-1278.	3.3	34
131	Secondâ€order Nonlinear Optical Susceptibilities and Refractive Indices of Organic Crystals from a Multiscale Numerical Simulation Approach. Advanced Optical Materials, 2014, 2, 1000-1006.	7.3	34
132	How the Second-Order Nonlinear Optical Response of the Collagen Triple Helix Appears: A Theoretical Investigation. Journal of Physical Chemistry C, 2014, 118, 8595-8602.	3.1	34
133	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.	3.1	34
134	Ab initio determination of polarizabilities per subunit in polymeric systems using the polarization propagator: Application to model hydrogen chains. International Journal of Quantum Chemistry, 1993, 46, 1-17.	2.0	33
135	Large effect of dopant level on second hyperpolarizability of alkali-doped polyacetylene chains. Chemical Physics Letters, 2005, 412, 217-222.	2.6	33
136	Second hyperpolarizability of phenalenyl radical system involving acetylene Ï€-conjugated bridge. Chemical Physics Letters, 2006, 420, 432-437.	2.6	33
137	Resonance Raman Spectra and Raman Excitation Profiles of Rhodamine 6G from Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2008, 9, 1667-1669.	2.1	33
138	A Joined Theoreticalâ^'Experimental Investigation on the 1H and 13C NMR Signatures of Defects in Poly(vinyl chloride). Journal of Physical Chemistry B, 2008, 112, 14804-14818.	2.6	33
139	Theoretical investigation on the polarizability and second hyperpolarizability of polysilole. Chemical Physics Letters, 2009, 471, 111-115.	2.6	33
140	Enhanced open-circuit voltage in polymer solar cells by dithieno[3,2-b:2â€²,3â€²-d]pyrrole N-acylation. Journal of Materials Chemistry A, 2014, 2, 7535-7545.	10.3	33
141	Taming the Lewis Superacidity of Nonâ€Planar Boranes: Câ^'H Bond Activation and Nonâ€Classical Binding Modes at Boron. Angewandte Chemie - International Edition, 2022, 61, .	13.8	33
142	Electrostatic interaction schemes for evaluating the polarizability of silicon clusters. Journal of Chemical Physics, 2009, 130, 134715.	3.0	32
143	Approximate spin-projected spin-unrestricted density functional theory method: Application to the diradical character dependences of the (hyper)polarizabilities in p-quinodimethane models. Chemical Physics Letters, 2010, 501, 140-145.	2.6	32
144	Fluorination as an effective tool to increase the open-circuit voltage and charge carrier mobility of organic solar cells based on poly(cyclopenta[2,1-b:3,4-bâ€²]dithiophene-alt-quinoxaline) copolymers. Journal of Materials Chemistry A, 2015, 3, 2960-2970.	10.3	32

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145	Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. Journal of Physical Chemistry C, 2019, 123, 7318-7335.	3.1	32
146	First hyperpolarizability of Hâ€“(BN)Nâ€“H oligomers: analysis of geometry, asymmetry and delocalization effectsElectronic Supplementary Information available. See http://www.rsc.org/suppdata/cp/b1/b108044j/. Physical Chemistry Chemical Physics, 2002, 4, 432-440.	2.8	31
147	Structural properties of doped polyacetylene chains: a comparative theoretical investigation using Hartreeâ€“Fock, MÃ¸llerâ€“Plesset second-order perturbation theory, and density functional theory approaches. Physical Chemistry Chemical Physics, 2004, 6, 3167-3174.	2.8	30
148	Theoretical Calculations and Experimental Measurements of the Vibrational Response of p-NTP SAMs: An Orientational Analysis. Journal of Physical Chemistry C, 2010, 114, 4106-4113.	3.1	30
149	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.	2.5	30
150	Secondâ€Order Nonlinear Optical Properties of a Dithienylethene–Indolinooxazolidine Hybrid: A Joint Experimental and Theoretical Investigation. Chemistry - A European Journal, 2015, 21, 18749-18757.	3.3	30
151	The first hyperpolarizability of nitrobenzene in benzene solutions: investigation of the effects of electron correlation within the sequential QM/MM approach. Physical Chemistry Chemical Physics, 2015, 17, 23634-23642.	2.8	30
152	QTAIM-Based Scheme for Describing the Linear and Nonlinear Optical Susceptibilities of Molecular Crystals Composed of Molecules with Complex Shapes. Journal of Physical Chemistry C, 2016, 120, 4481-4494.	3.1	30
153	Abinitioinvestigation of the electronic properties of planar and twisted polyparaphenylenes. Physical Review B, 1996, 54, 2381-2389.	3.2	29
154	Analysis of the vibrational static and dynamic second hyperpolarizabilities of polyacetylene chains. Synthetic Metals, 1997, 85, 1047-1050.	3.9	29
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