BenoÃ®t Ãt Champagne

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8942358/publications.pdf

Version: 2024-02-01

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	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
2	Tuning Electronic and Morphological Properties for Highâ€Performance Wavelengthâ€Selective Organic Nearâ€Infrared Cavity Photodetectors. Advanced Functional Materials, 2022, 32, 2108146.	14.9	21
3	Unraveling the Symmetry Effects on the Second-Order Nonlinear Optical Responses of Molecular Switches: The Case of Ruthenium Complexes. Inorganic Chemistry, 2022, 61, 1928-1940.	4.0	8
4	Bridge control of photophysical properties in benzothiazole-phenoxazine emitters â€“ from thermally activated delayed fluorescence to room temperature phosphorescence. Journal of Materials Chemistry C, 2022, 10, 4775-4784.	5.5	9
5	Unveiling the relationship between structural and polarization effects on the first hyperpolarizability of a merocyanine dye. Journal of Chemical Physics, 2022, 156, 014305.	3.0	7
6	Dominant dimer emission provides colour stability for red thermally activated delayed fluorescence emitter. Journal of Materials Chemistry C, 2022, 10, 5840-5848.	5.5	4
7	Lewis acid-catalyzed Dielsâ€“Alder cycloaddition of 2,5-dimethylfuran and ethylene: a density functional theory investigation. Theoretical Chemistry Accounts, 2022, 141, 1.	1.4	0
8	A molecular loaded dice: When the Ï€ conjugation breaks the statistical addressability of an octastate multimodal molecular switch. Dyes and Pigments, 2022, 202, 110270.	3.7	3
9	Multi-State Second-Order Nonlinear Optical Switches Incorporating One to Three Benzazolo-Oxazolidine Units: A Quantum Chemistry Investigation. Molecules, 2022, 27, 2770.	3.8	3
10	TDDFT Investigation of the Raman and Resonant Raman Spectra of Fluorescent Protein Chromophore Models. Journal of Physical Chemistry B, 2022, 126, 3414-3424.	2.6	4
11	9-Phosphatriptycene Derivatives: From Their Weak Basicity to Their Application in Frustrated Lewis Pair Chemistry. Journal of Physical Chemistry A, 2022, 126, 2794-2801.	2.5	4
12	Frustrated Lewis pairâ€catalyzed hydrogenation of unactivated alkenes with sterically hindered 9â€phosphatriptycenes. ChemCatChem, 2022, 14, .	3.7	4
13	Balancing fluorescence and singlet oxygen formation in pushâ€“pull type near-infrared BODIPY photosensitizers. Journal of Materials Chemistry C, 2022, 10, 9344-9355.	5.5	11
14	Second-order nonlinear optical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mtext>I</mml:mtext></mml:math>-shaped pyrazine derivatives. Dyes and Pigments, 2021, 184, 108850.	3.7	8
15	Benzo[1,2-b:4,5-b']dithiophene as a weak donor component for push-pull materials displaying thermally activated delayed fluorescence or room temperature phosphorescence. Dyes and Pigments, 2021, 186, 109022.	3.7	11
16	Methylene Bridging Effect on the Structures, Lewis Acidities and Optical Properties of Semiâ€planar Triarylboranes. Chemistry - A European Journal, 2021, 27, 1736-1743.	3.3	1
17	Self-assembling, structure and nonlinear optical properties of fluorescent organic nanoparticles in water. Physical Chemistry Chemical Physics, 2021, 23, 23643-23654.	2.8	9
18	Polar and Helical Isomorphous Crystals of Proline Derivatives: Influence of a Fluorine Atom on the Electric Susceptibility. Chemistry Africa, 2021, 4, 553-562.	2.4	1

#	Article	IF	Citations
19	Second Harmonic Generation Responses of Ion Pairs Forming Dimeric Aggregates. Journal of Physical Chemistry B, 2021, 125, 3386-3397.	2.6	13
20	Combining Benzazolo-Oxazolidine Twins toward Multi-state Nonlinear Optical Switches. Journal of Physical Chemistry B, 2021, 125, 3918-3931.	2.6	19
21	Heavyâ€Atomâ€Free Bayâ€Substituted Perylene Diimide Donorâ€Acceptor Photosensitizers. ChemPhysChem, 2021, 22, 1488-1496.	2.1	11
22	Difluorodithieno[3,2-a:2â€²,3â€²-c]phenazine as a strong acceptor for materials displaying thermally activated delayed fluorescence or room temperature phosphorescence. Dyes and Pigments, 2021, 190, 109301.	3.7	7
23	Rational Development of a Metalâ€Free Bifunctional System for the Câˆ’H Activation of Methane: A Density Functional Theory Investigation. ChemPhysChem, 2021, 22, 1958-1966.	2.1	7
24	Density Functional Theory Study of Substitution Effects on the Second-Order Nonlinear Optical Properties of Lindquist-Type Organo-Imido Polyoxometalates. Symmetry, 2021, 13, 1636.	2.2	5
25	All-Atom Quantum Mechanical Calculation of the Second-Harmonic Generation of Fluorescent Proteins. Journal of Physical Chemistry Letters, 2021, 12, 9684-9690.	4.6	5
26	Unravelling the Effects of Cholesterol on the Second-Order Nonlinear Optical Responses of Di-8-ANEPPS Dye Embedded in Phosphatidylcholine Lipid Bilayers. Journal of Physical Chemistry B, 2021, 125, 10195-10212.	2.6	13
27	Density functional theory investigation of the electronic and optical properties of metallo-phthalocyanine derivatives. Optical Materials, 2021, 120, 111315.	3.6	10
28	Concerted versus ionic mechanisms of the Î± and Î³ extensions in uncatalyzed Mukaiyama reaction between Î²,Î³-unsaturated bis silyl ketene acetal and benzaldehyde: A DFT study. Computational and Theoretical Chemistry, 2021, 1204, 113395.	2.5	0
29	Computational prediction of the supramolecular self-assembling properties of organic molecules: the role of conformational flexibility of amide moieties. Physical Chemistry Chemical Physics, 2021, 23, 20453-20465.	2.8	2
30	Topological investigation of the reaction mechanism of glycerol carbonate decomposition by bond evolution theory. RSC Advances, 2021, 11, 10083-10093.	3.6	12
31	Simulation of absorption and scattering spectra of crystalline organic nanoparticles with the discrete dipole approximation: Effects of crystal shape, crystal size, and refractive indexÂof the medium. Journal of Chemical Physics, 2021, 155, 164703.	3.0	0
32	Self-aggregation of stilbazolium ion pairs in liquid chloroform. A molecular dynamics study. Journal of Molecular Liquids, 2021, 344, 117735.	4.9	1
33	Nonlinear Optical Switches: from Molecules in Solution to Functionalized Surfaces and Solids â€“ A Quantum Chemistry Perspective. , 2021, , .		0
34	Merocyanines in a Halogen-Bonded Network Involving Inorganic Building Blocks. Crystal Growth and Design, 2020, 20, 608-616.	3.0	10
35	Unraveling the Effects of Co-Crystallization on the UV/Vis Absorption Spectra of an N-Salicylideneaniline Derivative. A Computational RI-CC2 Investigation. Molecules, 2020, 25, 4512.	3.8	1
36	Salicylideneaniline-Based Covalent Organic Frameworks: A New Family of Multistate Second-Order Nonlinear Optical Switches. Journal of Physical Chemistry C, 2020, 124, 24451-24459.	3.1	13

#	Article	IF	Citations
37	Innentitelbild: Controlled Generation of 9â€Boratriptycene by Lewis Adduct Dissociation: Accessing a Nonâ€Planar Triarylborane (Angew. Chem. 30/2020). Angewandte Chemie, 2020, 132, 12322-12322.	2.0	0
38	Unraveling the Electric Field-Induced Second Harmonic Generation Responses of Stilbazolium Ion Pairs Complexes in Solution Using a Multiscale Simulation Method. Journal of Chemical Information and Modeling, 2020, 60, 4817-4826.	5.4	14
39	The effect of halogenation on PBDTT-TQxT based non-fullerene polymer solar cells â€“ Chlorination vs fluorination. Dyes and Pigments, 2020, 181, 108577.	3.7	10
40	Dynamic Structural Effects on the Second-Harmonic Generation of Tryptophane-Rich Peptides and Gramicidin A. Journal of Physical Chemistry B, 2020, 124, 2568-2578.	2.6	13
41	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
42	Nearâ€Infrared BODIPYâ€Acridine Dyads Acting as Heavyâ€Atomâ€Free Dualâ€Functioning Photosensitizers. Chemistry - A European Journal, 2020, 26, 15212-15225.	3.3	14
43	Finding the optimal exchangeâ€“correlation functional to describe the excited state properties of pushâ€“pull organic dyes designed for thermally activated delayed fluorescence. Physical Chemistry Chemical Physics, 2020, 22, 16387-16399.	2.8	20
44	Second-Order Nonlinear Optical Properties of an Amphiphilic Dye Embedded in a Lipid Bilayer. A Combined Molecular Dynamicsâ€“Quantum Chemistry Study. Journal of Physical Chemistry B, 2020, 124, 2101-2109.	2.6	24
45	Controlled Generation of 9â€Boratriptycene by Lewis Adduct Dissociation: Accessing a Nonâ€Planar Triarylborane. Angewandte Chemie, 2020, 132, 12502-12506.	2.0	25
46	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
47	Density Functional Theory Investigation of the Binding of ThioTEPA to Purine Bases: Thermodynamics and Bond Evolution Theory Analysis. Journal of Physical Chemistry A, 2020, 124, 4068-4080.	2.5	12
48	Acido-triggered switching of the second-order nonlinear optical properties of a ferrocenyl-containing indolino-oxazolidine derivative. Dyes and Pigments, 2019, 160, 641-646.	3.7	19
49	Theoretical Assessment of the Second-Order Nonlinear Optical Responses of Lindqvist-Type Organoimido Polyoxometalates. Inorganic Chemistry, 2019, 58, 11210-11219.	4.0	22
50	Coupled cluster investigation of the vibrational and electronic second and third harmonic scattering hyperpolarizabilities of the water molecule. Journal of Chemical Physics, 2019, 151, 064303.	3.0	7
51	Periodic DFT Study of the Effects of Coâ€Crystallization on a Nâ€Salicylideneaniline Molecular Switch. ChemPhysChem, 2019, 20, 2434-2442.	2.1	3
52	A coloring tool for spiropyrans: solid state metalâ€“organic complexation versus salification. CrystEngComm, 2019, 21, 4925-4933.	2.6	9
53	Synthesis and switching properties of new derivatives of azoresveratrol. Dyes and Pigments, 2019, 171, 107666.	3.7	2
54	Are Fully Conjugated Expanded Indenofluorenes Analogues and Diindeno[n]thiophene Derivatives Diradicals? A Simplified (Spin-Flip) Time-Dependent Density Functional Theory [(SF-)sTD-DFT] Study. Journal of Physical Chemistry A, 2019, 123, 9828-9839.	2.5	5

#	Article	IF	Citations
55	Periodic DFT Study of the Effects of Coâ€Crystallization on a Nâ€Salicylideneaniline Molecular Switch. ChemPhysChem, 2019, 20, 2402-2402.	2.1	0
56	Pushing the Lewis Acidity Boundaries of Boron Compounds With Nonâ€Planar Triarylboranes Derived from Triptycenes. Angewandte Chemie, 2019, 131, 17045-17049.	2.0	25
57	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
58	New Insights into Photochromic Properties of N-Salicylideneaniline Derivatives Using a Cocrystal Engineering Approach. Crystal Growth and Design, 2019, 19, 5544-5556.	3.0	11
59	Magnetically-induced current density investigation in carbohelicenes and azahelicenes. Physical Chemistry Chemical Physics, 2019, 21, 14678-14691.	2.8	11
60	Nonlinear Optical Contrast in Azobenzene-Based Self-Assembled Monolayers. Chemistry of Materials, 2019, 31, 6759-6769.	6.7	25
61	First Principles Investigation of the Polarizability and First Hyperpolarizability of Anhydride Derivatives. Chemistry Africa, 2019, 2, 443-453.	2.4	19
62	All-polymer solar cells based on photostable bis(perylene diimide) acceptor polymers. Solar Energy Materials and Solar Cells, 2019, 196, 178-184.	6.2	10
63	Probing alkylsilane molecular structure on amorphous silica surfaces by sum frequency generation vibrational spectroscopy: First-principles calculations. Journal of Chemical Physics, 2019, 150, 074703.	3.0	2
64	Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. Journal of Physical Chemistry C, 2019, 123, 7318-7335.	3.1	32
65	ONIOM Investigation of the Second-Order Nonlinear Optical Responses of Fluorescent Proteins. Journal of Physical Chemistry B, 2018, 122, 4993-5005.	2.6	18
66	The Impact of Acceptorâ€“Acceptor Homocoupling on the Optoelectronic Properties and Photovoltaic Performance of PDTSQx_{ff} Low Bandgap Polymers. Macromolecular Rapid Communications, 2018, 39, e1800086.	3.9	11
67	Acidochromic spiropyranâ€“merocyanine stabilisation in the solid state. CrystEngComm, 2018, 20, 3318-3327.	2.6	17
68	DFT Investigation of the Diastereoselectivity of the MX2 and MX3 Lewis-Acid-Catalyzed Mukaiyama Aldol Reaction between C,O,O-Tris(trimethylsilyl)ketene Acetal and Aldehydes. Journal of Physical Chemistry A, 2018, 122, 1938-1947.	2.5	3
69	Assessing the Structure of Octastate Molecular Switches Using ¹H NMR Density Functional Theory Calculations. Journal of Physical Chemistry C, 2018, 122, 1800-1808.	3.1	3
70	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.	3.1	11
71	Tetraphenylborate Anion Induces Photochromism in N-Salicylideneamino-1-alkylpyridinium Derivatives Through Formation of Tetra-Aryl Boxes. Journal of Physical Chemistry C, 2018, 122, 10999-11007.	3.1	13
72	Coupled cluster evaluation of the second and third harmonic scattering responses of small molecules. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	8

#	Article	IF	Citations
73	Investigation of the Electronic Excited-State Equilibrium Geometries of Three Molecules Undergoing ESIPT: A RI-CC2 and TDDFT Study. Journal of Physical Chemistry A, 2018, 122, 972-984.	2.5	20
74	Quantum Chemical Methods for Predicting and Interpreting Second-Order Nonlinear Optical Properties: From Small to Extended Ï€-Conjugated Molecules. , 2018, , 117-138.		18
75	Second-order nonlinear optical properties of Stenhouse photoswitches: insights from density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 27658-27667.	2.8	37
76	Dynamical Behavior and Second Harmonic Generation Responses in Acido-Triggered Molecular Switches. Journal of Physical Chemistry C, 2018, 122, 26160-26168.	3.1	24
77	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, .	3.3	0
78	Aromaticity as a Guiding Concept for Spectroscopic Features and Nonlinear Optical Properties of Porphyrinoids. Molecules, 2018, 23, 1333.	3.8	38
79	Predicting Ketoâ€“Enol Equilibrium from Combining UV/Visible Absorption Spectroscopy with Quantum Chemical Calculations of Vibronic Structures for Many Excited States. A Case Study on Salicylideneanilines. Journal of Physical Chemistry A, 2018, 122, 5370-5374.	2.5	19
80	Nonlinear optical responses of self-assembled monolayers functionalized with indolinoâ€“oxazolidine photoswitches. Physical Chemistry Chemical Physics, 2018, 20, 21590-21597.	2.8	14
81	Effects of Empirical Dispersion Energy on the Geometrical Parameters and Relative Energy of a Salicylideneaniline Molecular Switch in the Solid State. Crystals, 2018, 8, 125.	2.2	6
82	Intramolecular [3 + 2] Cycloaddition Reactions of Unsaturated Nitrile Oxides. A Study from the Perspective of Bond Evolution Theory (BET). Journal of Physical Chemistry A, 2018, 122, 7472-7481.	2.5	17
83	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.	3.3	14
84	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.	1.9	4
85	Assessing Density Functional Theory Approaches for Predicting the Structure and Relative Energy of Salicylideneaniline Molecular Switches in the Solid State. Journal of Physical Chemistry C, 2017, 121, 6898-6908.	3.1	25
86	Simulation of the UV/Visible Absorption Spectra of Fluorescent Protein Chromophore Models. ChemPhotoChem, 2017, 1, 281-296.	3.0	22
87	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.	4.5	20
88	Assigning the stereochemistry of syn and anti Î²-trimethylsiloxy-Î±-trimethylsilyl alkanoic acid silyl esters using GIAO 1 H NMR chemical shift calculations. Journal of Molecular Structure, 2017, 1141, 436-440.	3.6	2
89	Faraday Effect in Stacks of Aromatic Molecules. Journal of Physical Chemistry C, 2017, 121, 15348-15352.	3.1	13
90	Diradical and Ionic Characters of Open-Shell Singlet Molecular Systems. Journal of Physical Chemistry A, 2017, 121, 861-873.	2.5	17

#	Article	IF	Citations
91	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
92	How Dimerization Through a Spiro Junction Modifies the Nonlinear Optical Properties of a Pushâ€“Pull Organic Dye: Insights from Theory and Hyperâ€Rayleigh Scattering. ChemPhotoChem, 2017, 1, 93-101.	3.0	2
93	Electronic Band Structure of Helical Polyisocyanides. Journal of Physical Chemistry A, 2017, 121, 7993-8002.	2.5	1
94	Emergence of Nonlinear Optical Activity by Incorporation of a Linker Carrying the p-Nitroaniline Motif in MIL-53 Frameworks. Journal of Physical Chemistry C, 2017, 121, 25509-25519.	3.1	20
95	Coupled-cluster sum-frequency generation nonlinear susceptibilities of methyl (CH₃) and methylene (CH₂) groups. Physical Chemistry Chemical Physics, 2017, 19, 29822-29832.	2.8	5
96	Tuning Nonlinear Optical Properties by Altering the Diradical and Chargeâ€Transfer Characteristics of Chichibabin's Hydrocarbon Derivatives. ChemPhysChem, 2017, 18, 142-148.	2.1	11
97	A Structural Analysis of Spiropyran and Spirooxazine Compounds and Their Polymorphs. Crystals, 2017, 7, 84.	2.2	18
98	Coupled cluster evaluation of the frequency dispersion of the first and second hyperpolarizabilities of water, methanol, and dimethyl ether. Journal of Chemical Physics, 2016, 145, 044311.	3.0	11
99	Elucidating Batch-to-Batch Variation Caused by Homocoupled Side Products in Solution-Processable Organic Solar Cells. Chemistry of Materials, 2016, 28, 9088-9098.	6.7	25
100	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
101	ZIF-8 as Nonlinear Optical Material: Influence of Structure and Synthesis. Chemistry of Materials, 2016, 28, 3203-3209.	6.7	57
102	Synthetic, Optical and Theoretical Study of Alternating Ethylenedioxythiopheneâ€“Pyridine Oligomers: Evolution from Planar Conjugated to Helicoidal Structure towards a Chiral Configuration. ChemPhysChem, 2016, 17, 4090-4101.	2.1	6
103	Investigating the first hyperpolarizability of liquid carbon tetrachloride. RSC Advances, 2016, 6, 99558-99563.	3.6	4
104	Origin of the Enhancement of the Second Hyperpolarizabilities of Metalâ€“Carbon Bonds. Journal of Physical Chemistry A, 2016, 120, 6838-6845.	2.5	0
105	Nonlinear optical properties in openâ€shell molecular systems. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 198-210.	14.6	63
106	Theoretical study on the spin state and open-shell character dependences of the second hyperpolarizability in hydrogen chain models. Physical Review A, 2016, 94, .	2.5	5
107	Unraveling the Concerted Reaction Mechanism of the Noncatalyzed Mukaiyama Reaction between C,O,O-Tris(trimethylsilyl)ketene Acetal and Aldehydes Using Density Functional Theory. Journal of Physical Chemistry A, 2016, 120, 5649-5657.	2.5	3
108	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

#	Article	IF	Citations
109	Second-order nonlinear optical responses of heptahelicene and heptathiahelicene derivatives. Chemical Physics Letters, 2016, 644, 195-200.	2.6	11
110	Oxazines: A New Class of Second-Order Nonlinear Optical Switches. Journal of the American Chemical Society, 2016, 138, 5052-5062.	13.7	104
111	Second-Order Nonlinear Optical Susceptibilities of Metalâ€“Organic Frameworks Using a Combined Local Field Theory/Charge Embedding Electrostatic Scheme. Journal of Physical Chemistry C, 2016, 120, 6741-6749.	3.1	19
112	Cover Image, Volume 6, Issue 2. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, i-i.	14.6	0
113	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
114	Fourier Space Uncoupled Hartreeâ€“Fock Polarizabilities of One-Dimensionally Periodic Systems. Polyethylene and Polysilane Revisited. Zeitschrift Fur Physikalische Chemie, 2016, 230, 589-632.	2.8	1
115	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.	2.8	5
116	Secondâ€Order Nonlinear Optical Properties of a Dithienyletheneâ€“Indolinooxazolidine Hybrid: A Joint Experimental and Theoretical Investigation. Chemistry - A European Journal, 2015, 21, 18749-18757.	3.3	30
117	PPV Polymerization through the Gilch Route: Diradical Character of Monomers. Chemistry - A European Journal, 2015, 21, 19176-19185.	3.3	9
118	The Fourier Space Restricted Hartreeâ€“Fock Method for the Electronic Structure Calculation of One-Dimensionally Periodic Systems. Advances in Quantum Chemistry, 2015, 71, 153-194.	0.8	0
119	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
120	Frequency dispersion of the first hyperpolarizabilities of reference molecules for nonlinear optics. Journal of Chemical Physics, 2015, 142, 194102.	3.0	22
121	Numerical differentiation method to calculate molecular properties at ground and excited states â€“ Application to Julolidinemalononitrile. Chemical Physics Letters, 2015, 634, 249-254.	2.6	3
122	Diradical character dependence of third-harmonic generation spectra in open-shell singlet systems. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	9
123	Theoretical Investigation of Vibrational Sum-Frequency Generation Signatures of Functionalized Hâ€”Si(111). Journal of Physical Chemistry C, 2015, 119, 3180-3191.	3.1	9
124	N-acyl-dithieno[3,2-b:2â€™,3â€™-d]pyrrole-based low bandgap copolymers affording improved open-circuit voltages and efficiencies in polymer solar cells. Solar Energy Materials and Solar Cells, 2015, 136, 70-77.	6.2	13
125	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. Journal of Physical Chemistry Letters, 2015, 6, 3236-3256.	4.6	142
126	Spectroscopic and second-order nonlinear optical properties of Ruthenium(<scp>ii</scp>) complexes: a DFT/MRCI and ADC(2) study. Physical Chemistry Chemical Physics, 2015, 17, 18908-18912.	2.8	12

#	Article	IF	Citations
127	Which charge definition for describing the crystal polarizing field and the Ï‡⁽¹⁾ and Ï‡⁽²⁾ of organic crystals?. Physical Chemistry Chemical Physics, 2015, 17, 19546-19556.	2.8	21
128	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
129	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
130	Inelastic Electron Tunneling of C₆₀ on Gold Surfaces from First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 803-818.	3.1	3
131	Pigment violet 19 â€" a test case to define a simple method to simulate the vibronic structure of absorption spectra of organic pigments and dyes in solution. Photochemical and Photobiological Sciences, 2015, 14, 444-456.	2.9	14
132	Modeling of Structural, Energetic, and Dynamic Properties of Fewâ€Atom Silver Clusters Embedded in Polynucleotide Strands by Using Molecular Dynamics. ChemPhysChem, 2015, 16, 360-369.	2.1	2
133	Nonlinear Optical Molecular Switches for Alkali Ion Identification. Molecules, 2014, 19, 10574-10586.	3.8	14
134	Ab initio simulation of the sum-frequency generation response of optically active liquids in the presence of a dc electric fieldâ€"determination of the absolute molecular configuration. Science China Chemistry, 2014, 57, 1405-1408.	8.2	0
135	Feature issue introduction: chirality in optics. Optical Materials Express, 2014, 4, 2663.	3.0	6
136	QM/MM investigation of the concentration effects on the second-order nonlinear optical responses of solutions. Journal of Chemical Physics, 2014, 141, 234104.	3.0	20
137	Linear and nonlinear optical properties of arylvinyldiazine dyes: A theoretical investigation. Dyes and Pigments, 2014, 110, 256-260.	3.7	37
138	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
139	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
140	Evaluation of the molecular static and dynamic first hyperpolarizabilities. International Journal of Quantum Chemistry, 2014, 114, 900-910.	2.0	51
141	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.	1.5	8
142	Linear and second-order nonlinear optical properties of ionic organic crystals. Journal of Chemical Physics, 2014, 141, 104109.	3.0	39
143	Resonant Raman spectra of molecules with diradical character: multiconfigurational wavefunction investigation of neutral viologens. Physical Chemistry Chemical Physics, 2014, 16, 21721-21731.	2.8	19
144	Analysis of the Resonant Raman Spectra of Viologens and of Their Radical Cations Using Range-Separated Hybrid Density Functionals. Journal of Physical Chemistry C, 2014, 118, 12469-12484.	3.1	15

#	Article	IF	Citations
145	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
146	All-Conjugated ABC-block-copolymer Formation with a Varying Sequence via an Unassociated Catalyst. Macromolecules, 2014, 47, 4668-4675.	4.8	39
147	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
148	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.	4.0	10
149	Origin of the Surface-Induced First Hyperpolarizability in the C₆₀/SiO₂ System: SCC-DFTB Insight. Journal of Physical Chemistry Letters, 2014, 5, 149-153.	4.6	10
150	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
151	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
152	A Multistate pHâ€Triggered Nonlinear Optical Switch. ChemPhysChem, 2014, 15, 2221-2224.	2.1	21
153	Effects of the basis set and of the exchangeâ€“correlation functional on the Inelastic Electron Tunneling signatures of 1,4-benzenedithiol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 34-41.	3.9	4
154	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.	2.6	7
155	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. Highlights in Theoretical Chemistry, 2014, , 225-239.	0.0	0
156	Diradicalology in thirdâ€order nonlinear optical systems: Second hyperpolarizabilities of acetyleneâ€linked phenalenylâ€based superpolyenes. International Journal of Quantum Chemistry, 2013, 113, 585-591.	2.0	4
157	SCC-DFTB calculation of the static first hyperpolarizability: From gas phase molecules to functionalized surfaces. Journal of Chemical Physics, 2013, 138, 204107.	3.0	16
158	Theoretical chemistry in Belgium. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	3
159	In situ nitroxideâ€mediated polymerization of styrene promoted by the Nâ€tertâ€butylâ€1â€isopropylnitrone/bpo pair: ESR investigations. Journal of Polymer Science Part A, 2013, 51, 1786-1795.	2.3	2
160	Design and Characterization of Molecular Nonlinear Optical Switches. Accounts of Chemical Research, 2013, 46, 2656-2665.	15.6	325
161	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
162	Theoretical study on the diradical characters and third-order nonlinear optical properties of transition-metal heterodinuclear systems. Chemical Physics Letters, 2013, 579, 73-77.	2.6	6

#	Article	IF	Citations
163	Vibrational Sumâ€Frequency Generation Activity of a 2,4â€Dinitrophenyl Phospholipid Hybrid Bilayer: Retrieving Orientational Parameters from a DFT Analysis of Experimental Data. ChemPhysChem, 2013, 14, 1227-1236.	2.1	6
164	Trivalent organophosphorus reagent induced pinacol rearrangement of 4H-cyclopenta[2,1-b:3,4-bâ€²]dithiophen-4-one. Tetrahedron Letters, 2013, 54, 526-529.	1.4	8
165	Theoretical study on the diradical characters and third-order nonlinear optical properties of cyclic thiazyl diradical compounds. Chemical Physics Letters, 2013, 585, 112-116.	2.6	14
166	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.	2.6	10
167	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
168	Understanding the Second-Order Nonlinear Optical Properties of One-Dimensional Ruthenium(II) Ammine Complexes. Journal of Physical Chemistry C, 2013, 117, 1833-1848.	3.1	25
169	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
170	Theoretical investigation of the first hyperpolarizability redox-switching in a ruthenium complex. Chemical Physics Letters, 2013, 574, 42-46.	2.6	15
171	Challenging Compounds for Calculating Hyperpolarizabilities: p-Quinodimethane Derivatives. Journal of Physical Chemistry A, 2013, 117, 4709-4715.	2.5	29
172	Reaction of 4H-cyclopenta[2,1-b:3,4-bâ€²]dithiophenes with NBSâ€”a route toward 2H-cyclopenta[2,1-b:3,4-bâ€²]dithiophene-2,6(4H)-diones. Tetrahedron, 2013, 69, 2260-2267.	1.9	5
173	Theoretical Insight into the Inelastic Electron Tunneling Spectra of an Anil Derivative. Journal of Physical Chemistry A, 2013, 117, 12783-12795.	2.5	4
174	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
175	Beta Sheets with a Twist: The Conformation of Helical Polyisocyanopeptides Determined by Using Vibrational Circular Dichroism. Chemistry - A European Journal, 2013, 19, 13168-13174.	3.3	15
176	Nanostructured Cocrystals of a Borazine with [60]Fullerene. Chemistry Letters, 2012, 41, 1210-1212.	1.3	10
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.	4.6	23
178	Theoretical Insight into the Second-Order NLO Response of the Bis{4-[2-(4-pyridyl)ethenyl]benzoato}-zinc(II) Metalâ€“Organic Framework. Journal of Physical Chemistry C, 2012, 116, 21973-21981.	3.1	25
179	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.	2.5	25
180	Theoretical Design of the Molecular Structure of Bent-Core Mesogens with Large Second-Order Nonlinear Optical Properties.. Journal of Physical Chemistry C, 2012, 116, 7552-7560.	3.1	18

#	Article	IF	Citations
181	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
182	Towards modelling the vibrational signatures of functionalized surfaces: carboxylic acids on Hâ€“Si(111) surfaces. Journal of Physics Condensed Matter, 2012, 24, 124111.	1.8	5
183	Reference molecules for nonlinear optics: A joint experimental and theoretical investigation. Journal of Chemical Physics, 2012, 136, 024506.	3.0	144
184	Enhanced Intramolecular Charge Transfer in New Type Donorâ€“Acceptor Substituted Perylenes. Journal of Physical Chemistry C, 2012, 116, 22711-22719.	3.1	18
185	Nonlinear Optical Molecular Switches as Selective Cation Sensors. Journal of the American Chemical Society, 2012, 134, 8101-8103.	13.7	267
186	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	22
187	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
188	Full configuration interaction calculations of the second hyperpolarizabilities of the H4 model compound: Summation-over-states analysis and interplay with diradical characters. Journal of Chemical Physics, 2012, 136, 024315.	3.0	20
189	Functionalized Dithienylthiazolo[5,4â€d]thiazoles For Solutionâ€Processable Organic Fieldâ€Effect Transistors. ChemPlusChem, 2012, 77, 923-930.	2.8	12
190	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.	2.6	10
191	Enhancement of the second hyperpolarizability by dÏƒ electrons in one-dimensional tetrametallic transition-metal systems. Chemical Physics Letters, 2012, 527, 11-15.	2.6	8
192	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
193	Electron correlation effects on the first hyperpolarizability of pushâ€“pull Ï€-conjugated systems. Journal of Chemical Physics, 2011, 134, 074113.	3.0	174
194	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.	2.5	21
195	Theoretical Investigation of Raman Optical Activity Signatures of TrÃ¶gerâ€™s Base. Journal of Physical Chemistry A, 2011, 115, 13706-13713.	2.5	6
196	Amyloseâ€“Vanillin Complexation Assessed by a Joint Experimental and Theoretical Analysis. Journal of Physical Chemistry C, 2011, 115, 23315-23322.	3.1	19
197	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
198	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

#	Article	IF	Citations
199	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
200	(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
201	Theoretical assessment of new molecules for secondâ€order nonlinear optics. International Journal of Quantum Chemistry, 2011, 111, 1583-1595.	2.0	12
202	Calculating the secondâ€order nonlinear optical susceptibilities of 3â€methylâ€4â€nitropyridine Nâ€oxide, 2â€carboxylic acidâ€4â€nitropyridineâ€1â€oxide, 2â€methylâ€4â€nitroaniline, and mâ€nitroaniline crystals. International Journal of Quantum Chemistry, 2011, 111, 880-890.	2.0	13
203	Openâ€Shell Characters and Second Hyperpolarizabilities of Oneâ€Dimensional Graphene Nanoflakes Composed of Trigonal Graphene Units. ChemPhysChem, 2011, 12, 1697-1707.	2.1	46
204	Effects of the Nature and Length of the Ïâ€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
205	From Molecular to Macroscopic Engineering: Shaping Hydrogenâ€Bonded Organic Nanomaterials. Chemistry - A European Journal, 2011, 17, 3262-3273.	3.3	29
206	Extended Systems in Electrostatic Fields. Zeitschrift Fur Physikalische Chemie, 2010, 224, 617-630.	2.8	2
207	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
208	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
209	A joint theoretical and experimental investigation on the 13C and 1H NMR chemical shifts of coumarin derivatives. Theoretical Chemistry Accounts, 2010, 125, 461-470.	1.4	6
210	Electrostatic modeling of the linear optical susceptibilities of 2-methyl-4-nitroaniline, m-nitroaniline, 3-methyl-4-nitropyridine N-oxide and 2-carboxylic acid-4-nitropyridine-1-oxide crystals. Chemical Physics Letters, 2010, 487, 256-262.	2.6	23
211	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. Chemical Physics Letters, 2010, 489, 212-218.	2.6	90
212	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
213	Orientational Analysis of Dodecanethiol and pâ€Nitrothiophenol SAMs on Metals with Polarisationâ€Dependent SFG Spectroscopy. ChemPhysChem, 2010, 11, 607-615.	2.1	38
214	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
215	Selective detection of the antigenic polar heads of model lipid membranes supported on metals from their vibrational nonlinear optical response. Chemical Physics Letters, 2010, 489, 12-15.	2.6	9
216	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

#	Article	IF	Citations
217	NONLINEAR OPTICAL PROPERTIES OF mSTRAWBERRY AND mCHERRY FOR SECOND HARMONIC IMAGING. Journal of Nonlinear Optical Physics and Materials, 2010, 19, 1-13.	1.8	10
218	Raman Optical Activity Study of the Signatures Associated to (TG)[sub N] and (GG)[sub N] Conformations of Isotactic Polypropylene Chains using Mode Localization Method. , 2010, , .		1
219	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
220	A Three-Step Synthetic Approach to Asymmetrically Functionalized 4H-Cyclopenta[2,1-b:3,4-bâ€²]dithiophenes. Journal of Organic Chemistry, 2010, 75, 7202-7209.	3.2	24
221	Singlet Diradical Character from Experiment. Journal of Physical Chemistry Letters, 2010, 1, 937-940.	4.6	181
222	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
223	Investigation of the Resonance Raman Spectra and Excitation Profiles of a Monometallic Ruthenium(II) [Ru(bpy)₂(HAT)]²⁺ Complex by Time-Dependent Density Functional Theory. Journal of Physical Chemistry B, 2010, 114, 511-520.	2.6	28
224	Analysis of Vibrational Raman Optical Activity Signatures of the (TG)N and (GG)N Conformations of Isotactic Polypropylene Chains in Terms of Localized Modes. Journal of Physical Chemistry A, 2010, 114, 7198-7212.	2.5	21
225	Combined Experimental and Theoretical Study on the Raman and Raman Optical Activity Signatures of Pentamethylundecane Diastereoisomers. Journal of Physical Chemistry B, 2010, 114, 11753-11760.	2.6	12
226	Ring Current Model and Anisotropic Magnetic Response of Cyclopropane. Journal of Chemical Theory and Computation, 2010, 6, 2002-2018.	5.3	62
227	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
228	Nonlinear Optical Properties of Flavylium Salts: A Quantum Chemical Study. Journal of Physical Chemistry A, 2010, 114, 8474-8479.	2.5	19
229	Giant electric field effect on the second hyperpolarizability of symmetric singlet diradical molecules. Journal of Chemical Physics, 2010, 133, 154302.	3.0	38
230	Theoretical and experimental investigation of the structural and spectroscopic properties of coumarin 343 fluoroionophores. Physical Chemistry Chemical Physics, 2010, 12, 14172.	2.8	23
231	Nonlinear and Chiro-Optical Properties of Aromatic Foldamers. , 2009, , .		0
232	Third-Order Nonlinear Optical Properties of Open-Shell Systems: Diradical Character and Spin State Dependences. , 2009, , .		0
233	Study of Structural Effects in Poly(vinyl Chloride) by Theoretical Simulation and Interpretation of NMR Spectra. , 2009, , .		0
234	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

#	Article	IF	Citations
235	Electrostatic interaction schemes for evaluating the polarizability of silicon clusters. Journal of Chemical Physics, 2009, 130, 134715.	3.0	32
236	Twoâ€Way Molecular Switches with Large Nonlinear Optical Contrast. Chemistry - A European Journal, 2009, 15, 2560-2571.	3.3	132
237	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
238	Vibrational Raman optical activity of Ï€â€conjugated helical systems: Hexahelicene and heterohelicenes. Journal of Computational Chemistry, 2009, 30, 1261-1278.	3.3	34
239	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
240	Polarizabilities and second hyperpolarizabilities of hydrogen chains using the spinâ€componentâ€scaled MÃ¸llerâ€“Plesset secondâ€order method. International Journal of Quantum Chemistry, 2009, 109, 3103-3111.	2.0	22
241	Theoretical investigation on the polarizability and second hyperpolarizability of polysilole. Chemical Physics Letters, 2009, 471, 111-115.	2.6	33
242	Electron donor solvent effects on the (hyper)polarizabilities of a singlet diradical molecule involving a boron atom. Chemical Physics Letters, 2009, 477, 309-314.	2.6	9
243	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
244	Effect of the Dynamical Disorder on the Second-Order Nonlinear Optical Responses of Helicity-Encoded Polymer Strands. Journal of Physical Chemistry A, 2009, 113, 6552-6554.	2.5	25
245	Self-Assembled Film Organization in Fast Microcontact Printing Investigated by Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry C, 2009, 113, 9857-9864.	3.1	13
246	Conformation-controlled networking of H-bonded assemblies on surfaces. Chemical Communications, 2009, , 3525.	4.1	18
247	Theoretical investigation of the dynamic first hyperpolarizability of DHAâ€“VHF molecular switches. New Journal of Chemistry, 2009, 33, 1349.	2.8	61
248	Second-order nonlinear optical properties of fluorescent proteins for second-harmonic imaging. Journal of Materials Chemistry, 2009, 19, 7514.	6.7	42
249	Remarkable two-photon absorption in open-shell singlet systems. Journal of Chemical Physics, 2009, 131, 114316.	3.0	54
250	Nonlinear optical properties of photoswitchable fluorescent proteins. Proceedings of SPIE, 2009, , .	0.8	2
251	Methods for Simulating and Interpreting Vibrational Spectra of Molecules. , 2009, , .		0
252	Analytical Time-Dependent Hartree-Fock Scheme to Evaluate the Vibrational (Hyper)Polarizabilities. , 2009, , .		0

#	Article	IF	Citations
253	Resonance Raman Spectra and Raman Excitation Profiles of Rhodamine 6G from Timeâ€Đependent Density Functional Theory. ChemPhysChem, 2008, 9, 1667-1669.	2.1	33
254	Theoretical study on the second hyperpolarizability of open-shell singlet one-dimensional systems with a charged defect. Chemical Physics Letters, 2008, 451, 111-115.	2.6	13
255	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. Chemical Physics Letters, 2008, 454, 97-104.	2.6	36
256	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
257	Naphthidine di(radical cation)s-stabilized palladium nanoparticles for efficient catalytic Suzukiâ€“Miyaura cross-coupling reactions. Tetrahedron, 2008, 64, 372-381.	1.9	63
258	Investigation on the Second-Order Nonlinear Optical Responses in the Ketoâˆ’Enol Equilibrium of Anil Derivatives. Journal of Physical Chemistry C, 2008, 112, 5638-5645.	3.1	81
259	A Joined Theoreticalâˆ’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
260	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
261	In silico optimization of merocyanine-spiropyran compounds as second-order nonlinear optical molecular switches. Physical Chemistry Chemical Physics, 2008, 10, 6223.	2.8	153
262	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
263	Joint Theoretical Experimental Investigation of the Electron Spin Resonance Spectra of Nitroxyl Radicals: Application to Intermediates in in Situ Nitroxide Mediated Polymerization (in Situ NMP) of Vinyl Monomers. Journal of Physical Chemistry B, 2008, 112, 10432-10442.	2.6	9
264	Strong Two-Photon Circular Dichroism in Helicenes:â€‰ A Theoretical Investigation. Journal of Chemical Theory and Computation, 2008, 4, 457-467.	5.3	42
265	Theoretical investigation on the linear and nonlinear susceptibilities of urea crystal. Journal of Chemical Physics, 2008, 128, 244713.	3.0	26
266	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
267	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
268	Second-Harmonic Generation in GFP-like Proteins. Journal of the American Chemical Society, 2008, 130, 15713-15719.	13.7	66
269	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
270	Rototranslational sum rules for electromagnetic hypershielding at the nuclei and related atomic Cartesian derivatives of the optical rotatory power. Journal of Chemical Physics, 2008, 128, 244107.	3.0	2

#	Article	IF	Citations
271	Spin State Dependence of Second Hyperpolarizabilities of Zethrenes. AIP Conference Proceedings, 2008, , .	0.4	0
272	Multi-scale Approach to the Design of Ferroelectric Liquid Crystals for NLO Applications. AIP Conference Proceedings, 2008, , .	0.4	0
273	Ab initio investigation on the nonlinear optical properties of silicon clusters Sin (n=3â€“8). Journal of Computational Methods in Sciences and Engineering, 2008, 7, 297-304.	0.2	2
274	An analytical derivative procedure for the calculation of vibrational Raman optical activity spectra. Journal of Chemical Physics, 2007, 127, 204105.	3.0	79
275	Multi-scale simulations for materials and life sciences. AIP Conference Proceedings, 2007, , .	0.4	0
276	Theoretical Evaluation of the Faraday Effect in Organic Compounds. Computing Letters, 2007, 3, 193-200.	0.5	3
277	Second Hyperpolarizability of Zethrenes. Computing Letters, 2007, 3, 333-338.	0.5	60
278	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
279	Computing Oscillator Strengths and Related Properties. AIP Conference Proceedings, 2007, , .	0.4	0
280	Theoretical investigation of the EPR hyperfine coupling constants in amino derivatives. Physical Chemistry Chemical Physics, 2007, 9, 828.	2.8	17
281	Circular dichroism of helical structures using semiempirical methods. Journal of Chemical Physics, 2007, 127, 204101.	3.0	34
282	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
283	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
284	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
285	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
286	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.	2.5	25
287	Acido-Triggered Nonlinear Optical Switches:â€‰ Benzazolo-oxazolidines. Journal of Physical Chemistry B, 2007, 111, 9795-9802.	2.6	92
288	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

#	Article	IF	Citations
289	Second Hyperpolarizabilities (Î³) of 1,3-Dipole Systems: Diradical Character Dependence of Î³. AIP Conference Proceedings, 2007, , .	0.4	0
290	Multi-Scale Simulations For Materials and Life Sciences. AIP Conference Proceedings, 2007, , .	0.4	0
291	A joined theoreticalâ€“experimental investigation on the 1H and 13C NMR chemical shifts of chloro-alkenes. Chemical Physics Letters, 2007, 436, 388-393.	2.6	20
292	Theoretical investigation on bridged triarylamine helicenes: UV/visible and circular dichroism spectra. Chemical Physics Letters, 2007, 439, 213-218.	2.6	29
293	Theoretical design of sulfinate-based ferroelectric liquid crystals displaying second-order nonlinear optical properties. Chemical Physics Letters, 2007, 440, 116-120.	2.6	7
294	First and second hyperpolarizabilities of donorâ€“acceptor disubstituted diphenalenyl radical systems. Chemical Physics Letters, 2007, 443, 95-101.	2.6	43
295	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
296	Theoretical investigation on H1 and C13 NMR chemical shifts of small alkanes and chloroalkanes. Journal of Chemical Physics, 2006, 125, 144309.	3.0	37
297	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
298	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
299	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
300	Facile Synthesis and Characterization of Naphthidines as a New Class of Highly Nonplanar Electron Donors Giving Robust Radical Cations. Journal of Organic Chemistry, 2006, 71, 1351-1361.	3.2	25
301	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
302	Acidoswitchable NLO-phores:Â Benzimidazolo[2,3-b]oxazolidines. Journal of Physical Chemistry B, 2006, 110, 10672-10682.	2.6	54
303	Elongation method and supermolecule approach for the calculation of nonlinear susceptibilities. Application to the 3-Methyl-4-Nitropyridine 1-Oxide and 2-Methyl-4-Nitroaniline crystals. Journal of Computational Methods in Sciences and Engineering, 2006, 6, 171-188.	0.2	9
304	Density functional theory investigation of the alkylating strength of organoaluminum co-catalysts for Ziegler-Natta polymerization. International Journal of Quantum Chemistry, 2006, 106, 588-598.	2.0	9
305	Time-dependent density functional theory simulation of hyper-Raman spectra. International Journal of Quantum Chemistry, 2006, 106, 599-608.	2.0	18
306	Investigation of polyethylene helical conformations: Theoretical study by vibrational Raman optical activity. International Journal of Quantum Chemistry, 2006, 106, 3097-3107.	2.0	17

#	Article	IF	Citations
307	Theoretical investigation of the chain length effects on the NMR chemical shifts of oligomers. International Journal of Quantum Chemistry, 2006, 106, 3113-3121.	2.0	5
308	Second hyperpolarizability of phenalenyl radical system involving acetylene Ï€-conjugated bridge. Chemical Physics Letters, 2006, 420, 432-437.	2.6	33
309	TDDFT investigation of the optical properties of cyanine dyes. Chemical Physics Letters, 2006, 425, 105-109.	2.6	93
310	Theoretical design of molecular photo- and acido-triggered non-linear optical switches. Chemical Physics Letters, 2006, 427, 153-158.	2.6	13
311	Second hyperpolarizabilities of polycyclic diphenalenyl radicals: Effects of para/ortho-quinoid structures and central ring modification. Chemical Physics Letters, 2006, 429, 174-179.	2.6	20
312	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
313	Analysis of the VROA signals of helical heptasilanes using an atomistic approach. Vibrational Spectroscopy, 2006, 42, 309-316.	2.2	12
314	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
315	A Joint Theoreticalâ€“Experimental Investigation of the Faraday Effect in Benzene, Toluene, andp-Xylene. ChemPhysChem, 2006, 7, 1654-1656.	2.1	22
316	Theoretical Determination of the Vibrational Raman Optical Activity Signatures of Helical Polypropylene Chains. ChemPhysChem, 2006, 7, 2366-2376.	2.1	37
317	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
318	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
319	Nonlinear Optical Properties of Chiral Liquids. Challenges and Advances in Computational Chemistry and Physics, 2006, , 359-381.	0.6	1
320	Ab Initio Methods for Simulating and Interpreting hyper-Raman Spectra of Molecules. , 2006, , 317-323.		0
321	Theoretical Study on the Second Hyperpolarizabilities of Diphenalenyl Radical Systems. , 2006, , 231-240.		0
322	Rototranslational sum rules for static and dynamic polarisabilities. Computer Physics Communications, 2005, 173, 131-139.	7.5	1
323	Density functional theory investigation of the stereochemistry effects on 1H and 13C NMR chemical shifts of poly(vinyl chloride) oligomers. Chemical Physics Letters, 2005, 411, 207-213.	2.6	21
324	Large effect of dopant level on second hyperpolarizability of alkali-doped polyacetylene chains. Chemical Physics Letters, 2005, 412, 217-222.	2.6	33

#	Article	IF	Citations
325	Hyper-Rayleigh scattering of neutral and charged helicenes. Chemical Physics Letters, 2005, 412, 274-279.	2.6	53
326	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
327	Simulation of UV/visible absorption spectra of (Î±-diimine)nickel(II) catalysts by time-dependent density functional theory. International Journal of Quantum Chemistry, 2005, 101, 840-848.	2.0	9
328	Hyperpolarizability density analysis of the enhancement of second hyperpolarizability of ?-conjugated oligomers by intermolecular interaction. International Journal of Quantum Chemistry, 2005, 102, 702-710.	2.0	20
329	Charge distributions in polyacetylene chains containing a positively charged defect. International Journal of Quantum Chemistry, 2005, 104, 354-366.	2.0	14
330	Introduction: Modeling vibrational spectroscopies. International Journal of Quantum Chemistry, 2005, 104, 587-588.	2.0	4
331	Mixed electric-magnetic second-order nonlinear optical response of helicenes. Journal of Chemical Physics, 2005, 122, 234713.	3.0	49
332	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
333	TDHF Evaluation of the Dipoleâ^'Quadrupole Polarizability and Its Geometrical Derivatives. Journal of Chemical Theory and Computation, 2005, 1, 444-452.	5.3	45
334	Acido- and Phototriggered NLO Properties Enhancement. Journal of Physical Chemistry B, 2005, 109, 11139-11150.	2.6	120
335	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
336	Comment on â€œPhysical Limits on Electronic Nonlinear Molecular Susceptibilitiesâ€• Physical Review Letters, 2005, 95, 109401; author reply 109402.	7.8	27
337	Vibrational Raman optical activity as a mean for revealing the helicity of oligosilanes: A quantum chemical investigation. Journal of Chemical Physics, 2005, 122, 214304.	3.0	23
338	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
339	Second-order nonlinear optical coefficient of polyphosphazene-based materials: A theoretical study. Journal of Chemical Physics, 2004, 120, 9401-9409.	3.0	34
340	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
341	Theoretical Study on Open-Shell Nonlinear Optical Systems. Materials Research Society Symposia Proceedings, 2004, 846, DD1.4.1.	0.1	2
342	Modelisation of the Electric Field Linear Response of an Infinite Aggregate of All-Trans Hexatriene Chains by Electrostatic Interaction Model. Structural Chemistry, 2004, 15, 385-390.	2.0	8

#	Article	IF	Citations
343	Ab initio investigation of the vibrational hyper-Raman spectra of ethylene, ethane, and dimethyl ether. Theoretical Chemistry Accounts, 2004, 111, 390-394.	1.4	9
344	Theoretical Design of Substituted Tetrathia-[7]-Helicenes with Large Second-Order Nonlinear Optical Responses. ChemPhysChem, 2004, 5, 1438-1442.	2.1	58
345	Structural properties of doped polyacetylene chains: a comparative theoretical investigation using Hartreeâ€“Fock, MÃllerâ€“Plesset second-order perturbation theory, and density functional theory approaches. Physical Chemistry Chemical Physics, 2004, 6, 3167-3174.	2.8	30
346	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
347	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
348	Multichromophoric Dendrimers as Single-Photon Sources:Â A Single-Molecule Study. Journal of Physical Chemistry B, 2004, 108, 16686-16696.	2.6	76
349	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
350	Identification of free radicals trapped in solid methacrylated resins. Journal of Polymer Science Part A, 2003, 41, 1691-1699.	2.3	42
351	Copolymerization Effects upon the Second-Order NLO Responses of Polyacetylene/Polymethineimine. Macromolecules, 2003, 36, 3980-3985.	4.8	16
352	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
353	Investigation of the configuration of alkyl phenyl ketone phenylhydrazones from ab initio 1H NMR chemical shiftsElectronic supplementary information (ESI) available: Full geometry optimization at the B3LYP/6-31G(d) level of approximation. See http://www.rsc.org/suppdata/ob/b3/b307528a/. Organic and Biomolecular Chemistry, 2003, 1, 3839.	2.8	16
354	Calculations of Nonlinear Optical Properties for the Solid State. Advances in Chemical Physics, 2003, , 41-92.	0.3	69
355	Electronic and Nonlinear Optical Properties of 2-Methyl-4-Nitroaniline Clusters. Computational Chemistry - Reviews of Current Trends, 2003, , 81-130.	0.4	1
356	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
357	Intramolecular charge transfer and first-order hyperpolarizability of planar and twisted sesquifulvalenes. Physical Chemistry Chemical Physics, 2002, 4, 5566-5571.	2.8	28
358	Integral algorithm and density matrix integration scheme forab initioband structure calculations on polymeric systems. Journal of Computational Chemistry, 2002, 23, 1430-1444.	3.3	10
359	Analytical TDHF second derivatives of dynamic electronic polarizability with respect to nuclear coordinates. Application to the dynamic ZPVA correction. Journal of Computational Chemistry, 2002, 23, 1495-1496.	3.3	5
360	Coupled-perturbed Hartree-Fock treatment of infinite periodic systems: Application to static polarizabilities and hyperpolarizabilities of polydiacetylene, polybutatriene, and interacting pairs of polyacetylene chains. International Journal of Quantum Chemistry, 2002, 90, 709-718.	2.0	25

#	Article	IF	Citations
361	Investigation of the frequency-dispersion effects on the Raman spectra of small polyenes. International Journal of Quantum Chemistry, 2002, 89, 341-348.	2.0	14
362	Convergence of exchange lattice summations in direct-space polymer calculations. International Journal of Quantum Chemistry, 2002, 89, 452-463.	2.0	9
363	Electronic excitations and first hyperpolarizability of 2-methyl-4-nitroaniline clusters. International Journal of Quantum Chemistry, 2002, 90, 1378-1387.	2.0	22
364	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
365	Theoretical approach to the design of organic molecular and polymeric nonlinear optical materials. , 2001, , 63-126.		64
366	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
367	MÃ¶bius strip versus linear and cyclic polyacenes: a HÃ¼ckel and semiempirical investigation. Theoretical Chemistry Accounts, 2001, 105, 431-436.	1.4	18
368	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
369	Long-range effects in optimizing the geometry of stereoregular polymers?IV: Explicit determination of the helical angle. International Journal of Quantum Chemistry, 2001, 85, 539-545.	2.0	6
370	Sum-frequency generation first hyperpolarizability from time-dependent Hartree-Fock method. International Journal of Quantum Chemistry, 2001, 85, 463-468.	2.0	11
371	Analytical TDHF second derivatives of dynamic electronic polarizability with respect to nuclear coordinates. Application to the dynamic ZPVA correction. Journal of Computational Chemistry, 2001, 22, 1920-1932.	3.3	29
372	Efficient treatment of the effect of vibrations on electrical, magnetic, and spectroscopic properties. Journal of Computational Chemistry, 2000, 21, 1572-1588.	3.3	48
373	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
374	Optimizing the geometry of stereoregular polymers. III. Polyyne and the basis set quasi-linear dependence. International Journal of Quantum Chemistry, 2000, 80, 863-870.	2.0	26
375	Hybridization effect upon the vibrational second hyperpolarizability: An ab initio study of acetylene, ethylene, and ethane. International Journal of Quantum Chemistry, 2000, 80, 871-881.	2.0	8
376	Vibrational second hyperpolarizability of symmetrically substituted `quadrupolar' Ï€-conjugated systems. Journal of Optics, 2000, 2, 247-254.	1.5	10
377	Large vibrational nonlinear optical properties ofC60:A combined Hartree-Fock/density-functional approach. Physical Review B, 2000, 61, 13137-13143.	3.2	17
378	Three-Wave Mixing in Chiral Liquids. Physical Review Letters, 2000, 85, 4253-4256.	7.8	115

#	Article	IF	Citations
379	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
380	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
381	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
382	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
383	Towards the Calculations of Polarizabilities of Stereoregular Polymers â™â™dedicated to Professor Yngve Ã–HRN at the occasion of his 65th birthday. Advances in Quantum Chemistry, 1999, , 95-110.	0.8	7
384	Static first hyperpolarizability of small all-trans polymethincimine oligomers. Basis set and electron correlation effects. Computational and Theoretical Chemistry, 1998, 425, 69-79.	1.5	20
385	Nonresonant frequency dispersion of the electronic second hyperpolarizability ofall-trans polysilane chains: An ab initio TDHF oligomeric approach. International Journal of Quantum Chemistry, 1998, 70, 751-761.	2.0	8
386	Ab initio determination of the vibrational and electronic first hyperpolarizabilities of reference compounds for non-linear optical (NLO) applications 3-Methyl 4-nitropyridine 1-oxide (POM) and N-(4-nitrophenyl)-(L)-prolinol (NPP). Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1547-1553.	1.7	27
387	Effect of solid-state interactions on the vibrational hyperpolarizability of all-trans polyacetylene chains from ab initio Hartreeâ€“Fock calculations. Journal of Chemical Physics, 1998, 109, 6450-6455.	3.0	14
388	Ab initio Hartree-Fock Investigation of Ï€-Conjugated Compounds Presenting Large Î²v/Î²e Ratio: Merocyanines. Collection of Czechoslovak Chemical Communications, 1998, 63, 1295-1308.	1.0	23
389	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
390	Nonlinear optical properties of quasilinear conjugated oligomers, polymers and organic molecules. International Reviews in Physical Chemistry, 1997, 16, 389-420.	2.3	133
391	Analysis of the vibrational static and dynamic second hyperpolarizabilities of polyacetylene chains. Synthetic Metals, 1997, 85, 1047-1050.	3.9	29
392	Static electronic and vibrational polarizabilities of poly(dimethylsilane) chains. Computational and Theoretical Chemistry, 1997, 391, 67-73.	1.5	6
393	Cluster size effects in models of the active site for stereospecific heterogeneous Ziegler-Natta polymerization. Journal of Molecular Catalysis A, 1997, 119, 235-244.	4.8	6
394	Electron correlation effects upon the static (hyper)polarizabilities of push-pull conjugated polyenes and polyynes. , 1997, 65, 679-688.		55
395	Vibrational versus electronic first hyperpolarizabilities of mono- and disubstituted benzenes: An ab initio coupled Hartree-Fock investigation. International Journal of Quantum Chemistry, 1997, 65, 689-696.	2.0	20
396	Electron correlation effects upon the static (hyper)polarizabilities of pushâ€pull conjugated polyenes and polyynes. International Journal of Quantum Chemistry, 1997, 65, 679-688.	2.0	2

#	Article	IF	Citations
397	Electronic first hyperpolarizability of polymethineimine chains with donor and acceptor groups. Synthetic Metals, 1996, 80, 205-210.	3.9	21
398	Ab initio dynamic polarizabilities of polymers. I. Hydrogen chain models. International Journal of Quantum Chemistry, 1996, 57, 811-821.	2.0	24
399	Curvature versus nuclear relaxation contributions to the static vibrational polarizability of polyacetylene chains. Chemical Physics Letters, 1996, 248, 301-308.	2.6	20
400	Vibrational polarizability and hyperpolarizability of p-nitroaniline. Chemical Physics Letters, 1996, 261, 57-65.	2.6	79
401	Exploratory Pariser-Parr-Pople investigation of the static first hyperpolarizability of polymethineimine chains. Chemical Physics, 1996, 213, 217-228.	1.9	13
402	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
403	Abinitioinvestigation of the electronic properties of planar and twisted polyparaphenylenes. Physical Review B, 1996, 54, 2381-2389.	3.2	29
404	<title>Model calculations of the first hyperpolarisability per unit cell of finite and infinite polymethineimine chains</title>. , 1995, , .		19
405	Density functional study of the static longitudinal polarizability of model polymeric chains. International Journal of Quantum Chemistry, 1995, 56, 117-130.	2.0	12
406	On the convergence of the exchange-like sums in the random phase approximation applied to stereoregular polymers. International Journal of Quantum Chemistry, 1995, 56, 429-435.	2.0	5
407	Molecular orbital expressions for approximate uncoupled Hartree-Fock second hyperpolarizabilities. A Pariser-Parr-Pople assessment for model polyacetylene chains. Chemical Physics, 1995, 197, 107-127.	1.9	11
408	About the relations between polarizability and Hartreeâ€"Fock instabilities. Part 1. The hydrogen molecule. Computational and Theoretical Chemistry, 1995, 332, 93-104.	1.5	5
409	Electron-correlation effects on the static longitudinal polarizability of polymeric chains. II. Bond-length-alternation effects. Physical Review A, 1995, 52, 1039-1053.	2.5	26
410	Electron-correlation effects on the static longitudinal polarizability of polymeric chains. Physical Review A, 1995, 52, 178-188.	2.5	46
411	Electron propagator theory and application. Theoretica Chimica Acta, 1995, 90, 397-419.	0.8	14
412	Static vibrational polarizability of all-trans polyethylene and polysilane. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 1641-1646.	1.7	20
413	Study of excited states of polyethylene in the Hartreeâ€"Fock, Tammâ€"Dancoff, and randomâ€phase approximations. Journal of Chemical Physics, 1995, 102, 6831-6836.	3.0	15
414	Ab initio investigation of the static polarizability of planar and twisted infinite polythiophene chains. International Journal of Quantum Chemistry, 1994, 52, 451-467.	2.0	18

#	Article	IF	Citations
415	Ab initio longitudinal polarizabilities of conjugated stereoregular polymers with a carbon backbone. Chemical Physics Letters, 1994, 217, 551-558.	2.6	24
416	Vibrational polarizability of polyacetylene chains. Journal of Chemical Physics, 1994, 101, 10796-10807.	3.0	55
417	ELECTRONIC AND VIBRATIONAL POLARIZABILITIES OF BUCKMINSTERFULLERENE. Bulletin Des SociÃ©tÃ©s Chimiques Belges, 1994, 103, 135-141.	0.0	1
418	The convergence of the direct lattice sums in the random phase approximation method applied to periodic infinite systems. Chemical Physics Letters, 1993, 210, 232-242.	2.6	9
419	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
420	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
421	Efficient computation of electron-repulsion integrals inab initio studies of polymeric systems. International Journal of Quantum Chemistry, 1993, 48, 793-806.	2.0	9
422	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
423	Determination of ab initio polarizabilities of polymers: Application to polyethylene and polysilane. International Journal of Quantum Chemistry, 1992, 42, 1009-1024.	2.0	48
424	Model calculations of polarizabilities of polyene chains: Oligomers and infinite polymers. International Journal of Quantum Chemistry, 1990, 38, 859-871.	2.0	15