Benoît Champagne

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

403 papers	12,256 citations	56 h-index	87 g-index
436 ext. papers	13,101 ext. citations	3.9 avg, IF	6.47 L-index

#	Paper	IF	Citations
403	Unraveling the Symmetry Effects on the Second-Order Nonlinear Optical Responses of Molecular Switches: The Case of Ruthenium Complexes.. *Inorganic Chemistry*, **2022**,	5.1	1
402	Unveiling the relationship between structural and polarization effects on the first hyperpolarizability of a merocyanine dye.. *Journal of Chemical Physics*, **2022**, 156, 014305	3.9	2
401	Lewis acid-catalyzed Diels–Alder cycloaddition of 2,5-dimethylfuran and ethylene: a density functional theory investigation. *Theoretical Chemistry Accounts*, **2022**, 141, 1	1.9	
400	A molecular loaded dice: When the π-conjugation breaks the statistical addressability of an octastate multimodal molecular switch. *Dyes and Pigments*, **2022**, 110270	4.6	0
399	Taming the Lewis Superacidity of Non-Planar Boranes: C-H Bond Activation and Non-Classical Binding Modes at Boron. *Angewandte Chemie - International Edition*, **2021**,	16.4	4
398	Simulation of absorption and scattering spectra of crystalline organic nanoparticles with the discrete dipole approximation: Effects of crystal shape, crystal size, and refractive index of the medium. *Journal of Chemical Physics*, **2021**, 155, 164703	3.9	
397	Self-aggregation of stilbazolium ion pairs in liquid chloroform. A molecular dynamics study. *Journal of Molecular Liquids*, **2021**, 344, 117735	6	
396	Second Harmonic Generation Responses of Ion Pairs Forming Dimeric Aggregates. *Journal of Physical Chemistry B*, **2021**, 125, 3386-3397	3.4	9
395	Combining Benzazolo-Oxazolidine Twins toward Multi-state Nonlinear Optical Switches. *Journal of Physical Chemistry B*, **2021**, 125, 3918-3931	3.4	4
394	Heavy-Atom-Free Bay-Substituted Perylene Diimide Donor-Acceptor Photosensitizers. *ChemPhysChem*, **2021**, 22, 1488-1496	3.2	1
393	Difluorodithieno[3,2-a:2?,3?-c]phenazine as a strong acceptor for materials displaying thermally activated delayed fluorescence or room temperature phosphorescence. *Dyes and Pigments*, **2021**, 190, 109301	4.6	2
392	Second-order nonlinear optical properties of Ξ-shaped pyrazine derivatives. *Dyes and Pigments*, **2021**, 184, 108850	4.6	3
391	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	4.6	7
390	Methylene Bridging Effect on the Structures, Lewis Acidities and Optical Properties of Semi-planar Triarylboranes. *Chemistry - A European Journal*, **2021**, 27, 1736-1743	4.8	
389	Self-assembling, structure and nonlinear optical properties of fluorescent organic nanoparticles in water. *Physical Chemistry Chemical Physics*, **2021**, 23, 23643-23654	3.6	3
388	Polar and Helical Isomorphous Crystals of Proline Derivatives: Influence of a Fluorine Atom on the Electric Susceptibility. *Chemistry Africa*, **2021**, 4, 553-562	2.2	0
387	Rational Development of a Metal-Free Bifunctional System for the C-H Activation of Methane: A Density Functional Theory Investigation. *ChemPhysChem*, **2021**, 22, 1958-1966	3.2	2

386	Density Functional Theory Study of Substitution Effects on the Second-Order Nonlinear Optical Properties of Lindquist-Type Organo-Imido Polyoxometalates. *Symmetry*, **2021**, 13, 1636	2.7	0
385	All-Atom Quantum Mechanical Calculation of the Second-Harmonic Generation of Fluorescent Proteins. *Journal of Physical Chemistry Letters*, **2021**, 12, 9684-9690	6.4	2
384	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	3.4	2
383	Density functional theory investigation of the electronic and optical properties of metallo-phthalocyanine derivatives. *Optical Materials*, **2021**, 120, 111315	3.3	1
382	Concerted versus ionic mechanisms of the [illegible] and [illegible] extensions in uncatalyzed Mukaiyama reaction between [illegible] unsaturated bis silyl ketene acetal and benzaldehyde: A DFT study. *Computational and Theoretical Chemistry*, **2021**, 1204, 113395	2	
381	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	3.6	0
380	Topological investigation of the reaction mechanism of glycerol carbonate decomposition by bond evolution theory.. *RSC Advances*, **2021**, 11, 10083-10093	3.7	4
379	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	6.1	6
378	The effect of halogenation on PBDTT-TQxT based non-fullerene polymer solar cells [illegible] Chlorination vs fluorination. *Dyes and Pigments*, **2020**, 181, 108577	4.6	7
377	Dynamic Structural Effects on the Second-Harmonic Generation of Tryptophane-Rich Peptides and Gramicidin A. *Journal of Physical Chemistry B*, **2020**, 124, 2568-2578	3.4	8
376	Performance of DFT functionals for calculating the second-order nonlinear optical properties of dipolar merocyanines. *Physical Chemistry Chemical Physics*, **2020**, 22, 16579-16594	3.6	26
375	Near-Infrared BODIPY-Acridine Dyads Acting as Heavy-Atom-Free Dual-Functioning Photosensitizers. *Chemistry - A European Journal*, **2020**, 26, 15212-15225	4.8	4
374	Finding the optimal exchange-correlation functional to describe the excited state properties of push-pull organic dyes designed for thermally activated delayed fluorescence. *Physical Chemistry Chemical Physics*, **2020**, 22, 16387-16399	3.6	11
373	Second-Order Nonlinear Optical Properties of an Amphiphilic Dye Embedded in a Lipid Bilayer. A Combined Molecular Dynamics-Quantum Chemistry Study. *Journal of Physical Chemistry B*, **2020**, 124, 2101-2109	3.4	15
372	Controlled Generation of 9-Boratriptycene by Lewis Adduct Dissociation: Accessing a Non-Planar Triarylborane. *Angewandte Chemie*, **2020**, 132, 12502-12506	3.6	10
371	Controlled Generation of 9-Boratriptycene by Lewis Adduct Dissociation: Accessing a Non-Planar Triarylborane. *Angewandte Chemie - International Edition*, **2020**, 59, 12402-12406	16.4	16
370	Merocyanines in a Halogen-Bonded Network Involving Inorganic Building Blocks. *Crystal Growth and Design*, **2020**, 20, 608-616	3.5	6
369	Salicylideneaniline-Based Covalent Organic Frameworks: A New Family of Multistate Second-Order Nonlinear Optical Switches. *Journal of Physical Chemistry C*, **2020**, 124, 24451-24459	3.8	6

368	Innentitelbild: Controlled Generation of 9-Boratriptycene by Lewis Adduct Dissociation: Accessing a Non-Planar Triarylborane (Angew. Chem. 30/2020). *Angewandte Chemie*, **2020**, 132, 12322-12322	3.6	
367	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	2.8	6
366	New Insights into Photochromic Properties of N-Salicylideneaniline Derivatives Using a Cocrystal Engineering Approach. *Crystal Growth and Design*, **2019**, 19, 5544-5556	3.5	4
365	Magnetically-induced current density investigation in carbohelicenes and azahelicenes. *Physical Chemistry Chemical Physics*, **2019**, 21, 14678-14691	3.6	6
364	Nonlinear Optical Contrast in Azobenzene-Based Self-Assembled Monolayers. *Chemistry of Materials*, **2019**, 31, 6759-6769	9.6	17
363	First Principles Investigation of the Polarizability and First Hyperpolarizability of Anhydride Derivatives. *Chemistry Africa*, **2019**, 2, 443-453	2.2	11
362	All-polymer solar cells based on photostable bis(perylene diimide) acceptor polymers. *Solar Energy Materials and Solar Cells*, **2019**, 196, 178-184	6.4	7
361	Probing alkylsilane molecular structure on amorphous silica surfaces by sum frequency generation vibrational spectroscopy: First-principles calculations. *Journal of Chemical Physics*, **2019**, 150, 074703	3.9	2
360	Acido-triggered switching of the second-order nonlinear optical properties of a ferrocenyl-containing indolino-oxazolidine derivative. *Dyes and Pigments*, **2019**, 160, 641-646	4.6	8
359	Theoretical Assessment of the Second-Order Nonlinear Optical Responses of Lindqvist-Type Organoimido Polyoxometalates. *Inorganic Chemistry*, **2019**, 58, 11210-11219	5.1	10
358	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	3.9	4
357	Periodic DFT Study of the Effects of Co-Crystallization on a N-Salicylideneaniline Molecular Switch. *ChemPhysChem*, **2019**, 20, 2434-2442	3.2	1
356	A coloring tool for spiropyrans: solid state metal–organic complexation versus salification. *CrystEngComm*, **2019**, 21, 4925-4933	3.3	3
355	Synthesis and switching properties of new derivatives of azoresveratrol. *Dyes and Pigments*, **2019**, 171, 107666	4.6	1
354	Are Fully Conjugated Expanded Indenofluorenes Analogues and Diindeno[]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	2.8	5
353	Periodic DFT Study of the Effects of Co-Crystallization on a N-Salicylideneaniline Molecular Switch. *ChemPhysChem*, **2019**, 20, 2402-2402	3.2	
352	Pushing the Lewis Acidity Boundaries of Boron Compounds With Non-Planar Triarylboranes Derived from Triptycenes. *Angewandte Chemie*, **2019**, 131, 17045-17049	3.6	15
351	Pushing the Lewis Acidity Boundaries of Boron Compounds With Non-Planar Triarylboranes Derived from Triptycenes. *Angewandte Chemie - International Edition*, **2019**, 58, 16889-16893	16.4	33

350	Fingerprint of Aromaticity and Molecular Topology on the Photophysical Properties of Octaphyrins. *Journal of Physical Chemistry C*, **2019**, 123, 7318-7335	3.8	21
349	ONIOM Investigation of the Second-Order Nonlinear Optical Responses of Fluorescent Proteins. *Journal of Physical Chemistry B*, **2018**, 122, 4993-5005	3.4	12
348	The Impact of Acceptor-Acceptor Homocoupling on the Optoelectronic Properties and Photovoltaic Performance of PDTSQx Low Bandgap Polymers. *Macromolecular Rapid Communications*, **2018**, 39, e1800086	4.8	6
347	Acidochromic spiropyran–merocyanine stabilisation in the solid state. *CrystEngComm*, **2018**, 20, 3318-3327	3.3	11
346	DFT Investigation of the Diastereoselectivity of the MX and MX 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	2.8	3
345	Assessing the Structure of Octastate Molecular Switches Using 1H NMR Density Functional Theory Calculations. *Journal of Physical Chemistry C*, **2018**, 122, 1800-1808	3.8	2
344	Theoretical Study on Third-Order Nonlinear Optical Property of One-Dimensional Cyclic Thiazyl Radical Aggregates: Intermolecular Distance, Open-Shell Nature, and Spin State Dependences. *Journal of Physical Chemistry C*, **2018**, 122, 6779-6785	3.8	10
343	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	3.8	11
342	Coupled cluster evaluation of the second and third harmonic scattering responses of small molecules. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	6
341	Nonlinear optical responses of self-assembled monolayers functionalized with indolino-oxazolidine photoswitches. *Physical Chemistry Chemical Physics*, **2018**, 20, 21590-21597	3.6	10
340	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	2.3	4
339	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	2.8	12
338	Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on a Magnetically Induced Current. *Chemistry - A European Journal*, **2018**, 24, 13457-13466	4.8	10
337	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	2.8	12
336	Quantum Chemical Methods for Predicting and Interpreting Second-Order Nonlinear Optical Properties: From Small to Extended π-Conjugated Molecules **2018**, 117-138		13
335	Second-order nonlinear optical properties of Stenhouse photoswitches: insights from density functional theory. *Physical Chemistry Chemical Physics*, **2018**, 20, 27658-27667	3.6	24
334	Dynamical Behavior and Second Harmonic Generation Responses in Acido-Triggered Molecular Switches. *Journal of Physical Chemistry C*, **2018**, 122, 26160-26168	3.8	15
333	Aromaticity as a Guiding Concept for Spectroscopic Features and Nonlinear Optical Properties of Porphyrinoids. *Molecules*, **2018**, 23,	4.8	24

332	Predicting Keto-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	2.8	15
331	Theoretical investigation of curved π-conjugated fullerene flakes: open-shell character, aromaticity, and third-order nonlinear optical property. *Journal of Physical Organic Chemistry*, **2017**, 30, e3581	2.1	4
330	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	3.8	15
329	Simulation of the UV/Visible Absorption Spectra of Fluorescent Protein Chromophore Models. *ChemPhotoChem*, **2017**, 1, 281-296	3.3	13
328	A theoretical study on quasi-one-dimensional open-shell singlet ladder oligomers: multi-radical nature, aromaticity and second hyperpolarizability. *Organic Chemistry Frontiers*, **2017**, 4, 779-789	5.2	16
327	Assigning the stereochemistry of syn and anti 2-trimethylsiloxy-3-trimethylsilyl alkanoic acid silyl esters using GIAO 1 H NMR chemical shift calculations. *Journal of Molecular Structure*, **2017**, 1141, 436-440	2.4	2
326	Faraday Effect in Stacks of Aromatic Molecules. *Journal of Physical Chemistry C*, **2017**, 121, 15348-15352	3.8	13
325	Diradical and Ionic Characters of Open-Shell Singlet Molecular Systems. *Journal of Physical Chemistry A*, **2017**, 121, 861-873	2.8	14
324	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	3.8	39
323	How Dimerization Through a Spiro Junction Modifies the Nonlinear Optical Properties of a Push-Pull Organic Dye: Insights from Theory and Hyper-Rayleigh Scattering. *ChemPhotoChem*, **2017**, 1, 93-101	3.3	2
322	Electronic Band Structure of Helical Polyisocyanides. *Journal of Physical Chemistry A*, **2017**, 121, 7993-8002	2.8	1
321	Emergence of Nonlinear Optical Activity by Incorporation of a Linker Carrying the -Nitroaniline Motif in MIL-53 Frameworks. *Journal of Physical Chemistry C*, **2017**, 121, 25509-25519	3.8	12
320	Coupled-cluster sum-frequency generation nonlinear susceptibilities of methyl (CH) and methylene (CH) groups. *Physical Chemistry Chemical Physics*, **2017**, 19, 29822-29832	3.6	3
319	Tuning Nonlinear Optical Properties by Altering the Diradical and Charge-Transfer Characteristics of Chichibabin's Hydrocarbon Derivatives. *ChemPhysChem*, **2017**, 18, 142-148	3.2	10
318	A Structural Analysis of Spiropyran and Spirooxazine Compounds and Their Polymorphs. *Crystals*, **2017**, 7, 84	2.3	11
317	Nonlinear optical properties in open-shell molecular systems. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 198-210	7.9	47
316	Theoretical study on the spin state and open-shell character dependences of the second hyperpolarizability in hydrogen chain models. *Physical Review A*, **2016**, 94,	2.6	5
315	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, 5649-57	2.8	3

314	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	3.8	42
313	Second-order nonlinear optical responses of heptahelicene and heptathiahelicene derivatives. *Chemical Physics Letters*, **2016**, 644, 195-200	2.5	9
312	Oxazines: A New Class of Second-Order Nonlinear Optical Switches. *Journal of the American Chemical Society*, **2016**, 138, 5052-62	16.4	76
311	Second-Order Nonlinear Optical Susceptibilities of Metal□Organic Frameworks Using a Combined Local Field Theory/Charge Embedding Electrostatic Scheme. *Journal of Physical Chemistry C*, **2016**, 120, 6741-6749	3.8	15
310	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	3.8	25
309	Fourier Space Uncoupled Hartree□Fock Polarizabilities of One-Dimensionally Periodic Systems. Polyethylene and Polysilane Revisited. *Zeitschrift Fur Physikalische Chemie*, **2016**, 230, 589-632	3.1	1
308	Challenging compounds for calculating molecular second hyperpolarizabilities: the triplet state of the trimethylenemethane diradical and two derivatives. *Physical Chemistry Chemical Physics*, **2016**, 18, 6420-9	3.6	5
307	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	3.9	7
306	Elucidating Batch-to-Batch Variation Caused by Homocoupled Side Products in Solution-Processable Organic Solar Cells. *Chemistry of Materials*, **2016**, 28, 9088-9098	9.6	17
305	Third-Order Nonlinear Optical Properties of Asymmetric Non-Alternant Open-Shell Condensed-Ring Hydrocarbons: Effects of Diradical Character, Asymmetricity, and Exchange Interaction. *Journal of Physical Chemistry C*, **2016**, 120, 1193-1207	3.8	31
304	ZIF-8 as Nonlinear Optical Material: Influence of Structure and Synthesis. *Chemistry of Materials*, **2016**, 28, 3203-3209	9.6	46
303	Synthetic, Optical and Theoretical Study of Alternating Ethylenedioxythiophene-Pyridine Oligomers: Evolution from Planar Conjugated to Helicoidal Structure towards a Chiral Configuration. *ChemPhysChem*, **2016**, 17, 4090-4101	3.2	5
302	Investigating the first hyperpolarizability of liquid carbon tetrachloride. *RSC Advances*, **2016**, 6, 99558-99563	3.7	3
301	Origin of the Enhancement of the Second Hyperpolarizabilities of Metal-Carbon Bonds. *Journal of Physical Chemistry A*, **2016**, 120, 6838-45	2.8	
300	Switching of the Nonlinear Optical Responses of Anil Derivatives: From Dilute Solutions to the Solid State **2016**, 175-202		7
299	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. *Journal of Physical Chemistry Letters*, **2015**, 6, 3236-3256	6.4	116
298	Spectroscopic and second-order nonlinear optical properties of Ruthenium(ii) complexes: a DFT/MRCI and ADC(2) study. *Physical Chemistry Chemical Physics*, **2015**, 17, 18908-12	3.6	11
297	Which charge definition for describing the crystal polarizing field and the □(1)) and □(2)) of organic crystals?. *Physical Chemistry Chemical Physics*, **2015**, 17, 19546-56	3.6	19

296	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, 23634-42	3.6	28
295	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-b?]dithiophene-alt-quinoxaline) copolymers. *Journal of Materials Chemistry A*, **2015**, 3, 2960-2970	13	30
294	Inelastic Electron Tunneling of C60 on Gold Surfaces from First-Principles Calculations. *Journal of Physical Chemistry C*, **2015**, 119, 803-818	3.8	3
293	Pigment violet 19 - 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, 444-56	4.2	10
292	Modeling of structural, energetic, and dynamic properties of few-atom silver clusters embedded in polynucleotide strands by using molecular dynamics. *ChemPhysChem*, **2015**, 16, 360-9	3.2	2
291	Second-Order Nonlinear Optical Properties of a Dithienylethene-Indolinooxazolidine Hybrid: A Joint Experimental and Theoretical Investigation. *Chemistry - A European Journal*, **2015**, 21, 18749-57	4.8	25
290	PPV Polymerization through the Gilch Route: Diradical Character of Monomers. *Chemistry - A European Journal*, **2015**, 21, 19176-85	4.8	8
289	The Fourier Space Restricted Hartree□ock Method for the Electronic Structure Calculation of One-Dimensionally Periodic Systems. *Advances in Quantum Chemistry*, **2015**, 71, 153-194	1.4	
288	Explicit versus implicit solvation effects on the first hyperpolarizability of an organic biphotochrome. *Journal of Physical Chemistry A*, **2015**, 119, 5496-503	2.8	25
287	Frequency dispersion of the first hyperpolarizabilities of reference molecules for nonlinear optics. *Journal of Chemical Physics*, **2015**, 142, 194102	3.9	19
286	Numerical differentiation method to calculate molecular properties at ground and excited states □ Application to Julolidinemalononitrile. *Chemical Physics Letters*, **2015**, 634, 249-254	2.5	2
285	Diradical character dependence of third-harmonic generation spectra in open-shell singlet systems. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	9
284	Theoretical Investigation of Vibrational Sum-Frequency Generation Signatures of Functionalized H□i(111). *Journal of Physical Chemistry C*, **2015**, 119, 3180-3191	3.8	9
283	N-acyl-dithieno[3,2-b:2□3□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	6.4	12
282	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, 7083-8	3.6	57
281	Enhanced open-circuit voltage in polymer solar cells by dithieno[3,2-b:2?,3?-d]pyrrole N-acylation. *Journal of Materials Chemistry A*, **2014**, 2, 7535-7545	13	30
280	Evaluation of the molecular static and dynamic first hyperpolarizabilities. *International Journal of Quantum Chemistry*, **2014**, 114, 900-910	2.1	42
279	Natural orbital functional calculations of molecular polarizabilities and second hyperpolarizabilities. The hydrogen molecule as a test case. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2014**, 47, 015101	1.3	8

278	Linear and second-order nonlinear optical properties of ionic organic crystals. *Journal of Chemical Physics*, **2014**, 141, 104109	3.9	31
277	Resonant Raman spectra of molecules with diradical character: multiconfigurational wavefunction investigation of neutral viologens. *Physical Chemistry Chemical Physics*, **2014**, 16, 21721-31	3.6	15
276	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	3.8	11
275	Second-order Nonlinear Optical Susceptibilities and Refractive Indices of Organic Crystals from a Multiscale Numerical Simulation Approach. *Advanced Optical Materials*, **2014**, 2, 1000-1006	8.1	31
274	All-Conjugated ABC-block-copolymer Formation with a Varying Sequence via an Unassociated Catalyst. *Macromolecules*, **2014**, 47, 4668-4675	5.5	33
273	Third-order nonlinear optical properties of one-dimensional open-shell molecular aggregates composed of phenalenyl radicals. *Chemistry - A European Journal*, **2014**, 20, 11129-36	4.8	42
272	Open-shell character and second hyperpolarizabilities of one-dimensional chromium(II) chains: size dependence and bond-length alternation effect. *Inorganic Chemistry*, **2014**, 53, 8700-7	5.1	9
271	Origin of the Surface-Induced First Hyperpolarizability in the C60/SiO2 System: SCC-DFTB Insight. *Journal of Physical Chemistry Letters*, **2014**, 5, 149-53	6.4	9
270	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	3.8	25
269	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, 2114-24	6.4	46
268	A multistate pH-triggered nonlinear optical switch. *ChemPhysChem*, **2014**, 15, 2221-4	3.2	19
267	Effects of the basis set and of the exchange-correlation functional on the Inelastic Electron Tunneling signatures of 1,4-benzenedithiol. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 119, 34-41	4.4	3
266	Axial ligand effects on the diradical characters and second hyperpolarizabilities of open-shell singlet transition-metal dinuclear complexes. *Chemical Physics Letters*, **2014**, 608, 68-73	2.5	7
265	Nonlinear optical molecular switches for alkali ion identification. *Molecules*, **2014**, 19, 10574-86	4.8	12
264	Ab initio simulation of the sum-frequency generation response of optically active liquids in the presence of a dc electric field□determination of the absolute molecular configuration. *Science China Chemistry*, **2014**, 57, 1405-1408	7.9	
263	Feature issue introduction: chirality in optics. *Optical Materials Express*, **2014**, 4, 2663	2.6	6
262	QM/MM investigation of the concentration effects on the second-order nonlinear optical responses of solutions. *Journal of Chemical Physics*, **2014**, 141, 234104	3.9	18
261	Linear and nonlinear optical properties of arylvinyldiazine dyes: A theoretical investigation. *Dyes and Pigments*, **2014**, 110, 256-260	4.6	34

260	Implementation in the Pyvib2 program of the localized mode method and application to a helicene. *Highlights in Theoretical Chemistry*, **2014**, 225-239		
259	Diradicalology in third-order nonlinear optical systems: Second hyperpolarizabilities of acetylene-linked phenalenyl-based superpolyenes. *International Journal of Quantum Chemistry*, **2013**, 113, 585-591	2.1	3
258	SCC-DFTB calculation of the static first hyperpolarizability: from gas phase molecules to functionalized surfaces. *Journal of Chemical Physics*, **2013**, 138, 204107	3.9	13
257	In situ nitroxide-mediated polymerization of styrene promoted by the N-tert-butyl-□sopropylnitrone/bpo pair: ESR investigations. *Journal of Polymer Science Part A*, **2013**, 51, 1786-1795	2.5	2
256	Design and characterization of molecular nonlinear optical switches. *Accounts of Chemical Research*, **2013**, 46, 2656-65	24.3	253
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