Benoît Champagne

List of Publications by Citations

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	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of Push-Pull π-Conjugated Systems. *Journal of Physical Chemistry A*, **2000**, 104, 4755-4763	2.8	473
402	Second hyperpolarizability (gamma) of singlet diradical system: dependence of gamma on the diradical character. *Journal of Physical Chemistry A*, **2005**, 109, 885-91	2.8	269
401	Design and characterization of molecular nonlinear optical switches. *Accounts of Chemical Research*, **2013**, 46, 2656-65	24.3	253
400	Synthesis and characterization of teranthene: a singlet biradical polycyclic aromatic hydrocarbon having Kekulé structures. *Journal of the American Chemical Society*, **2010**, 132, 11021-3	16.4	249
399	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	7.4	246
398	Nonlinear optical molecular switches as selective cation sensors. *Journal of the American Chemical Society*, **2012**, 134, 8101-3	16.4	213
397	Singlet Diradical Character from Experiment. *Journal of Physical Chemistry Letters*, **2010**, 1, 937-940	6.4	154
396	Electron correlation effects on the first hyperpolarizability of push-pull π-conjugated systems. *Journal of Chemical Physics*, **2011**, 134, 074113	3.9	152
395	Basis set and electron correlation effects on the polarizability and second hyperpolarizability of model open-shell pi-conjugated systems. *Journal of Chemical Physics*, **2005**, 122, 114315	3.9	129
394	Nonlinear optical properties of quasilinear conjugated oligomers, polymers and organic molecules. *International Reviews in Physical Chemistry*, **1997**, 16, 389-420	7	128
393	Two-way molecular switches with large nonlinear optical contrast. *Chemistry - A European Journal*, **2009**, 15, 2560-71	4.8	121
392	Reference molecules for nonlinear optics: a joint experimental and theoretical investigation. *Journal of Chemical Physics*, **2012**, 136, 024506	3.9	120
391	Electric Field Simulation of Substituents in Donor-Acceptor Polyenes:´ A Comparison with Ab Initio Predictions for Dipole Moments, Polarizabilities, and Hyperpolarizabilities. *Journal of the American Chemical Society*, **2000**, 122, 8007-8012	16.4	120
390	Theoretical Design of Open-Shell Singlet Molecular Systems for Nonlinear Optics. *Journal of Physical Chemistry Letters*, **2015**, 6, 3236-3256	6.4	116
389	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. *Theoretical Chemistry Accounts*, **2011**, 130, 711-724	1.9	114
388	Acido- and phototriggered NLO properties enhancement. *Journal of Physical Chemistry B*, **2005**, 109, 11139-50	3.4	114
387	In silico optimization of merocyanine-spiropyran compounds as second-order nonlinear optical molecular switches. *Physical Chemistry Chemical Physics*, **2008**, 10, 6223-32	3.6	113

386	Density-functional theory (hyper)polarizabilities of push-pull pi-conjugated systems: treatment of exact exchange and role of correlation. *Journal of Chemical Physics*, **2005**, 123, 014319	3.9	113
385	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	3.9	107
384	Giant Enhancement of the Second Hyperpolarizabilities of Open-Shell Singlet Polyaromatic Diphenalenyl Diradicaloids by an External Electric Field and Donor–Acceptor Substitution. *Journal of Physical Chemistry Letters*, **2011**, 2, 1094-1098	6.4	104
383	Large Off-Diagonal Contribution to the Second-Order Optical Nonlinearities of -Shaped Molecules. *Journal of Physical Chemistry A*, **2003**, 107, 3942-3951	2.8	100
382	Theoretical and Experimental Investigation of Electric Field Induced Second Harmonic Generation in Tetrathia[7]helicenes. *Journal of Physical Chemistry C*, **2008**, 112, 7900-7907	3.8	96
381	Three-wave mixing in chiral liquids. *Physical Review Letters*, **2000**, 85, 4253-6	7.4	94
380	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. *Chemical Physics Letters*, **2008**, 467, 120-125	2.5	93
379	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. *Chemical Physics Letters*, **2010**, 489, 212-218	2.5	88
378	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	3.9	87
377	Second hyperpolarizabilities (gamma) of bisimidazole and bistriazole benzenes: diradical character, charged state, and spin state dependences. *Journal of Physical Chemistry A*, **2006**, 110, 4238-43	2.8	85
376	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. *Journal of Chemical Physics*, **2006**, 125, 074113	3.9	84
375	Acido-triggered nonlinear optical switches: benzazolo-oxazolidines. *Journal of Physical Chemistry B*, **2007**, 111, 9795-802	3.4	83
374	TDDFT investigation of the optical properties of cyanine dyes. *Chemical Physics Letters*, **2006**, 425, 105-109	2.5	83
373	Ab Initio Coupled Hartree–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	2.8	81
372	Theoretical study on the second hyperpolarizabilities of phenalenyl radical systems involving acetylene and vinylene linkers: diradical character and spin multiplicity dependences. *Journal of Physical Chemistry A*, **2007**, 111, 3633-41	2.8	80
371	Oxazines: A New Class of Second-Order Nonlinear Optical Switches. *Journal of the American Chemical Society*, **2016**, 138, 5052-62	16.4	76
370	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	3.9	76
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368	An analytical derivative procedure for the calculation of vibrational Raman optical activity spectra. *Journal of Chemical Physics*, **2007**, 127, 204105	3.9	75
367	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. *Journal of Chemical Physics*, **2010**, 132, 094107	3.9	74
366	Resonance Raman scattering of rhodamine 6G as calculated by time-dependent density functional theory: vibronic and solvent effects. *Journal of Physical Chemistry A*, **2008**, 112, 3215-23	2.8	74
365	Investigation on the Second-Order Nonlinear Optical Responses in the Keto–Enol Equilibrium of Anil Derivatives. *Journal of Physical Chemistry C*, **2008**, 112, 5638-5645	3.8	74
364	Theoretical study of the second-order nonlinear optical properties of [N]helicenes and [N]phenylenes. *Journal of Chemical Physics*, **2004**, 120, 2042-8	3.9	74
363	Vibrational polarizability and hyperpolarizability of p-nitroaniline. *Chemical Physics Letters*, **1996**, 261, 57-65	2.5	71
362	Evaluation of alternative sum-over-states expressions for the first hyperpolarizability of push-pull pi-conjugated systems. *Journal of Chemical Physics*, **2006**, 125, 24101	3.9	69
361	Multichromophoric Dendrimers as Single-Photon Sources: A Single-Molecule Study. *Journal of Physical Chemistry B*, **2004**, 108, 16686-16696	3.4	69
360	Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. *Chemical Physics Letters*, **2009**, 477, 355-359	2.5	68
359	Size dependences of the diradical character and the second hyperpolarizabilities in dicyclopenta-fused acenes: relationships with their aromaticity/antiaromaticity. *Physical Chemistry Chemical Physics*, **2011**, 13, 20575-83	3.6	64
358	Role of collective modes in vibrational polarizabilities and hyperpolarizabilities of polyacetylene and other quasilinear polymers. *Journal of Chemical Physics*, **1996**, 104, 4125-4136	3.9	63
357	Investigation of the UV/visible absorption spectra of merocyanine dyes using time-dependent density functional theory. *Journal of Physical Chemistry A*, **2006**, 110, 13007-13	2.8	62
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355	Ring Current Model and Anisotropic Magnetic Response of Cyclopropane. *Journal of Chemical Theory and Computation*, **2010**, 6, 2002-18	6.4	58
354	Second-harmonic generation in GFP-like proteins. *Journal of the American Chemical Society*, **2008**, 130, 15713-9	16.4	58
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352	Solvent Effects on the Second-Order Nonlinear Optical Responses in the Keto–Enol Equilibrium of a 2-Hydroxy-1-naphthaldehyde Derivative. *Journal of Physical Chemistry C*, **2010**, 114, 12760-12768	3.8	57
351	Naphthidine di(radical cation)s-stabilized palladium nanoparticles for efficient catalytic Suzuki–Miyaura cross-coupling reactions. *Tetrahedron*, **2008**, 64, 372-381	2.4	57

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319	Ab initio investigation on the second-order nonlinear optical responses in keto-enol equilibria of salicylideneanilines. *Journal of Physical Chemistry A*, **2007**, 111, 9914-23	2.8	44
318	Diradical character dependences of the first and second hyperpolarizabilities of asymmetric open-shell singlet systems. *Journal of Chemical Physics*, **2013**, 138, 244306	3.9	43
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