

# Edith Botek

## List of Publications by Year in descending order

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91  
papers

3,063  
citations

136950

32  
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161849

54  
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95  
all docs

95  
docs citations

95  
times ranked

2476  
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis and Characterization of Teranthrene: A Singlet Biradical Polycyclic Aromatic Hydrocarbon Having Kekulé Structures. <i>Journal of the American Chemical Society</i> , 2010, 132, 11021-11023.	13.7	285
2	Relationship between Third-Order Nonlinear Optical Properties and Magnetic Interactions in Open-Shell Systems: A New Paradigm for Nonlinear Optics. <i>Physical Review Letters</i> , 2007, 99, 033001.	7.8	258
3	Singlet Diradical Character from Experiment. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 937-940.	4.6	181
4	(Hyper)polarizability density analysis for open-shell molecular systems based on natural orbitals and occupation numbers. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 711-724.	1.4	125
5	Theoretical and Experimental Investigation of Electric Field Induced Second Harmonic Generation in Tetrathia[7]helicenes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 7900-7907.	3.1	104
6	Second Hyperpolarizabilities ( $\beta^3$ ) of Bisimidazole and Bistriazole Benzenes: A Diradical Character, Charged State, and Spin State Dependences. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4238-4243.	2.5	100
7	Theoretical study of third-order nonlinear optical properties in square nanographenes with open-shell singlet ground states. <i>Chemical Physics Letters</i> , 2008, 467, 120-125.	2.6	96
8	Signature of multiradical character in second hyperpolarizabilities of rectangular graphene nanoflakes. <i>Chemical Physics Letters</i> , 2010, 489, 212-218.	2.6	90
9	Origin of the enhancement of the second hyperpolarizability of singlet diradical systems with intermediate diradical character. <i>Journal of Chemical Physics</i> , 2006, 125, 074113.	3.0	88
10	Theoretical Study on the Second Hyperpolarizabilities of Phenalenyl Radical Systems Involving Acetylene and Vinylene Linkers: A Diradical Character and Spin Multiplicity Dependences. <i>Journal of Physical Chemistry A</i> , 2007, 111, 3633-3641.	2.5	84
11	Long-range corrected density functional theory study on static second hyperpolarizabilities of singlet diradical systems. <i>Journal of Chemical Physics</i> , 2010, 132, 094107.	3.0	82
12	Theoretical study on third-order nonlinear optical properties in hexagonal graphene nanoflakes: Edge shape effect. <i>Chemical Physics Letters</i> , 2009, 477, 355-359.	2.6	74
13	Second-Harmonic Generation in GFP-like Proteins. <i>Journal of the American Chemical Society</i> , 2008, 130, 15713-15719.	13.7	66
14	Second Hyperpolarizability of Zethrenes. <i>Computing Letters</i> , 2007, 3, 333-338.	0.5	60
15	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. <i>Chemical Physics Letters</i> , 2010, 493, 195-199.	2.6	59
16	Remarkable two-photon absorption in open-shell singlet systems. <i>Journal of Chemical Physics</i> , 2009, 131, 114316.	3.0	54
17	Theoretical consideration of singlet open-shell character of polyperiacenes using Clar's aromatic sextet valence bond model and quantum chemical calculations. <i>AIP Conference Proceedings</i> , 2012, , .	0.4	54
18	Theoretical Study on Second Hyperpolarizabilities of Singlet Diradical Square Planar Nickel Complexes Involving $\sigma$ -Semiquinonato Type Ligands. <i>Journal of Physical Chemistry A</i> , 2008, 112, 8423-8429.	2.5	49

#	ARTICLE	IF	CITATIONS
19	Third-order nonlinear optical properties of trigonal, rhombic and bow-tie graphene nanoflakes with strong structural dependence of diradical character. <i>Chemical Physics Letters</i> , 2009, 480, 278-283.	2.6	49
20	Validation of reactive gases and aerosols in the MACC global analysis and forecast system. <i>Geoscientific Model Development</i> , 2015, 8, 3523-3543.	3.6	49
21	Open-shell Characters and Second Hyperpolarizabilities of One-dimensional Graphene Nanoflakes Composed of Trigonal Graphene Units. <i>ChemPhysChem</i> , 2011, 12, 1697-1707.	2.1	46
22	First and second hyperpolarizabilities of donor-acceptor disubstituted diphenalenyl radical systems. <i>Chemical Physics Letters</i> , 2007, 443, 95-101.	2.6	43
23	Second-order nonlinear optical properties of fluorescent proteins for second-harmonic imaging. <i>Journal of Materials Chemistry</i> , 2009, 19, 7514.	6.7	42
24	Finite-Field Spin-Flip Configuration Interaction Calculation of the Second Hyperpolarizabilities of Singlet Diradical Systems. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1699-1707.	5.3	41
25	Theoretical Investigation of the Second-Order Nonlinear Optical Properties of Helical Pyridine-Pyrimidine Oligomers. <i>Chemistry - A European Journal</i> , 2006, 12, 8687-8695.	3.3	38
26	Giant electric field effect on the second hyperpolarizability of symmetric singlet diradical molecules. <i>Journal of Chemical Physics</i> , 2010, 133, 154302.	3.0	38
27	Theoretical investigation on H1 and C13 NMR chemical shifts of small alkanes and chloroalkanes. <i>Journal of Chemical Physics</i> , 2006, 125, 144309.	3.0	37
28	Intermolecular interaction effects on the second hyperpolarizability of open-shell singlet diphenalenyl radical dimer. <i>Chemical Physics Letters</i> , 2008, 454, 97-104.	2.6	36
29	Second hyperpolarizabilities ( $\hat{\chi}^3$ ) of open-shell singlet one-dimensional systems: Intersite interaction effects on the average diradical character and size dependences of $\hat{\chi}^3$ . <i>Chemical Physics Letters</i> , 2006, 432, 473-479.	2.6	34
30	Circular dichroism of helical structures using semiempirical methods. <i>Journal of Chemical Physics</i> , 2007, 127, 204101.	3.0	34
31	Second hyperpolarizability of phenalenyl radical system involving acetylene $\pi$ -conjugated bridge. <i>Chemical Physics Letters</i> , 2006, 420, 432-437.	2.6	33
32	A Joined Theoretical-Experimental Investigation on the $^1\text{H}$ and $^{13}\text{C}$ NMR Signatures of Defects in Poly(vinyl chloride). <i>Journal of Physical Chemistry B</i> , 2008, 112, 14804-14818.	2.6	33
33	Approximate spin-projected spin-unrestricted density functional theory method: Application to the diradical character dependences of the (hyper)polarizabilities in p-quinodimethane models. <i>Chemical Physics Letters</i> , 2010, 501, 140-145.	2.6	32
34	Theoretical investigation on bridged triarylamine helicenes: UV/visible and circular dichroism spectra. <i>Chemical Physics Letters</i> , 2007, 439, 213-218.	2.6	29
35	From Molecular to Macroscopic Engineering: Shaping Hydrogen-Bonded Organic Nanomaterials. <i>Chemistry - A European Journal</i> , 2011, 17, 3262-3273.	3.3	29
36	Theoretical investigation on the linear and nonlinear susceptibilities of urea crystal. <i>Journal of Chemical Physics</i> , 2008, 128, 244713.	3.0	26

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37	Second Hyperpolarizabilities of Singlet Polycyclic Diphenalenyl Radicals: Effects of the Nature of the Central Heterocyclic Ring and Substitution to Diphenalenyl Rings. <i>Journal of Physical Chemistry A</i> , 2007, 111, 9102-9110.	2.5	25
38	Effect of the Dynamical Disorder on the Second-Order Nonlinear Optical Responses of Helicity-Encoded Polymer Strands. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6552-6554.	2.5	25
39	A Three-Step Synthetic Approach to Asymmetrically Functionalized 4 <i>H</i> -Cyclopenta[2,1- <i>b</i> :3,4- <i>b'</i> ²]dithiophenes. <i>Journal of Organic Chemistry</i> , 2010, 75, 7202-7209.	3.2	24
40	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. <i>Chemical Physics Letters</i> , 2010, 487, 256-262.	2.6	23
41	Theoretical and experimental investigation of the structural and spectroscopic properties of coumarin 343 fluoroionophores. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14172.	2.8	23
42	A Joint Theoretical-Experimental Investigation of the Faraday Effect in Benzene, Toluene, and p-Xylene. <i>ChemPhysChem</i> , 2006, 7, 1654-1656.	2.1	22
43	Enhancement of Second Hyperpolarizabilities in Open-Shell Singlet Slipped-Stack Dimers Composed of Square Planar Nickel Complexes Involving <i>o</i> -Semiquinonato Type Ligands. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1117-1124.	2.5	21
44	Observations and Simulations of Dropout Events and Flux Decays in October 2013: Comparing MEO Equatorial With LEO Polar Orbit. <i>Journal of Geophysical Research: Space Physics</i> , 2021, 126, e2020JA028850.	2.4	21
45	Second hyperpolarizabilities of polycyclic diphenalenyl radicals: Effects of para/ortho-quinoid structures and central ring modification. <i>Chemical Physics Letters</i> , 2006, 429, 174-179.	2.6	20
46	A joined theoretical-experimental investigation on the <sup>1</sup> H and <sup>13</sup> C NMR chemical shifts of chloro-alkenes. <i>Chemical Physics Letters</i> , 2007, 436, 388-393.	2.6	20
47	Amylose-Vanillin Complexation Assessed by a Joint Experimental and Theoretical Analysis. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23315-23322.	3.1	19
48	ONIOM Investigation of the Second-Order Nonlinear Optical Responses of Fluorescent Proteins. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4993-5005.	2.6	18
49	Theoretical study on the second hyperpolarizability of open-shell singlet one-dimensional systems with a charged defect. <i>Chemical Physics Letters</i> , 2008, 451, 111-115.	2.6	13
50	One- and two-photon absorptions in open-shell singlet systems. <i>AIP Conference Proceedings</i> , 2012, , .	0.4	13
51	Electron Dropout Events and Flux Enhancements Associated With Geomagnetic Storms Observed by PROBA-V/Energetic Particle Telescope From 2013 to 2019. <i>Journal of Geophysical Research: Space Physics</i> , 2020, 125, e2020JA028487.	2.4	13
52	Functionalized Dithienylthiazolo[5,4- <i>d</i> ]thiazoles For Solution-Processable Organic Field-Effect Transistors. <i>ChemPlusChem</i> , 2012, 77, 923-930.	2.8	12
53	Observation of High-Energy Electrons Precipitated by NWC Transmitter From PROBA-V Low-Earth Orbit Satellite. <i>Geophysical Research Letters</i> , 2020, 47, e2020GL089077.	4.0	12
54	Evaluation of the Molecular Polarizability Using the IPPP-CLOPPA-INDO/S Method. Application to Molecules of Biological Interest. <i>Journal of Physical Chemistry A</i> , 2008, 112, 6992-6998.	2.5	11

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55	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
56	Dynamics of Megaelectron Volt Electrons Observed in the Inner Belt by PROBA-2/EPT. Journal of Geophysical Research: Space Physics, 2019, 124, 1651-1659.	2.4	10
57	Improving Predictions of the 3D Dynamic Model of the Plasmasphere. Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	10
58	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
59	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
60	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
61	Fingerprints for Structural Defects in Poly(thienylene vinylene) (PTV): A Joint Theoretical-Experimental NMR Study on Model Molecules. Journal of Physical Chemistry B, 2011, 115, 12040-12050.	2.6	8
62	Links of the Plasmopause With Other Boundary Layers of the Magnetosphere: Ionospheric Convection, Radiation Belt Boundaries, Auroral Oval. Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	7
63	A joint theoretical and experimental investigation on the <sup>13</sup> C and <sup>1</sup> H NMR chemical shifts of coumarin derivatives. Theoretical Chemistry Accounts, 2010, 125, 461-470.	1.4	6
64	Combined experimental-theoretical NMR study on 2,5-bis(5-aryl-2-hexylthiophen-2-yl)thiazolo[5,4-d]thiazole derivatives for printable electronics. Magnetic Resonance in Chemistry, 2012, 50, 379-387.	1.9	6
65	Assessment of the Earth's Cold Plasmatrough Modeling by Using Van Allen Probes/EMFISIS and Arase/PWE Electron Density Data. Journal of Geophysical Research: Space Physics, 2021, 126, e2021JA029737.	2.4	6
66	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
67	Theoretical Evaluation of the Faraday Effect in Organic Compounds. Computing Letters, 2007, 3, 193-200.	0.5	3
68	Prediction of first hyperpolarizability of fluorescent proteins. AIP Conference Proceedings, 2015, , .	0.4	3
69	Electron donor solvent effects on the (Hyper) polarizabilities of a solute presenting singlet diradical character. AIP Conference Proceedings, 2012, , .	0.4	2
70	In situ nitroxide-mediated polymerization of styrene promoted by the N-tert-butyl- $\alpha$ -isopropylnitron/bpo pair: ESR investigations. Journal of Polymer Science Part A, 2013, 51, 1786-1795.	2.3	2
71	Approximate spin projected spin-unrestricted density functional theory method: Application to diradical character dependences of second hyperpolarizabilities. , 2015, , .		1
72	Modeling the space environment and its effects on spacecraft and astronauts using SPENVIS. , 2018, , .		1

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73	Second Hyperpolarizabilities ( $\hat{\chi}^3$ ) of 1,3-Dipole Systems: Diradical Character Dependence of $\hat{\chi}^3$ . AIP Conference Proceedings, 2007, , .	0.4	0
74	Spin State Dependence of Second Hyperpolarizabilities of Zethrenes. AIP Conference Proceedings, 2008, , .	0.4	0
75	Nonlinear and Chiro-Optical Properties of Aromatic Foldamers. , 2009, , .		0
76	Third-Order Nonlinear Optical Properties of Open-Shell Systems: Diradical Character and Spin State Dependences. , 2009, , .		0
77	Study of Structural Effects in Poly(vinyl Chloride) by Theoretical Simulation and Interpretation of NMR Spectra. , 2009, , .		0
78	A Singlet Biradical Polycyclic Aromatic Hydrocarbon. Synfacts, 2010, 2010, 1238-1238.	0.0	0
79	Spin polarization and third-order nonlinear optical properties of open-shell singlet graphene nanoflakes. , 2012, , .		0
80	Electron spin resonance spectra of nitroxyl radicals. , 2012, , .		0
81	Second hyperpolarizabilities of singlet diradical compounds and their radical ions. , 2012, , .		0
82	Long-range-corrected UDFT study on second hyperpolarizabilities of open-shell singlet systems. , 2012, , .		0
83	Theoretical aspects on the evaluation and interpretation of the third-order nonlinear optical properties of diradical compounds. , 2012, , .		0
84	Linear and nonlinear second order susceptibilities of molecular crystals. , 2012, , .		0
85	Second-order nonlinear optical responses of flexible pyridine-pyrimidine foldamers. , 2012, , .		0
86	Relationship between second hyperpolarizability and diradical character in open-shell singlet metal-metal multiply bonded systems. , 2015, , .		0
87	Theoretical Study on the Second Hyperpolarizabilities of Diphenalenyl Radical Systems. , 2006, , 231-240.		0
88	Static electric field effect on third-order nonlinear optical (NLO) properties of singlet diradical molecules: Toward the realization of an electric field induced open-shell NLO switch. , 2015, , .		0
89	Mixed Electric-Magnetic Second Order Response of Helicenes. , 2019, , 769-770.		0
90	Evaluation of Second-Order Susceptibilities of 2-methyl-4-nitroaniline (MNA) and 3-methyl-4-nitropyridine-l-oxyde (POM) Crystals. , 2019, , 783-786.		0

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91	Observations of Electron Fluxes in the Radiation Belts with PROBA-V/EPT at Polar Low Earth Orbit and Van Allen Probes/MagEIS at Near Equatorial Elliptical Orbit. , 2022, , .		0