Robert Zalesny

List of Publications by Year in Descending Order

77 papers	1,264 citations	22 h-index	29 g-index
84 ext. papers	1,482 ext. citations	4.1 avg, IF	4.45 L-index

#	Paper	IF	Citations
77	Infrared Spectra of Hydrogen-Bonded Molecular Complexes Under Spatial Confinement.. *Frontiers in Chemistry*, **2021**, 9, 801426	5	
76	Two-Photon Absorption Activity of BOPHY Derivatives: Insights from Theory. *Journal of Physical Chemistry A*, **2021**, 125, 2581-2587	2.8	2
75	Computational design of two-photon active organic molecules for infrared responsive materials. *Journal of Materials Chemistry C*, **2020**, 8, 9867-9873	7.1	1
74	Postsynthetic Framework Contraction Enhances the Two-Photon Absorption Properties of Pillar-Layered Metal□Organic Frameworks. *Chemistry of Materials*, **2020**, 32, 5682-5690	9.6	7
73	Predictions of High-Order Electric Properties of Molecules: Can We Benefit from Machine Learning?. *ACS Omega*, **2020**, 5, 5318-5325	3.9	6
72	Controlling Two-Photon Action Cross Section by Changing a Single Heteroatom Position in Fluorescent Dyes. *Journal of Physical Chemistry Letters*, **2020**, 11, 5920-5925	6.4	4
71	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. II. Halogen-bonded systems. *Physical Chemistry Chemical Physics*, **2020**, 22, 4225-4234	3.6	2
70	Interlayer-Sensitized Linear and Nonlinear Photoluminescence of Quasi-2D Hybrid Perovskites Using Aggregation-Induced Enhanced Emission Active Organic Cation Layers. *Advanced Functional Materials*, **2020**, 30, 1909375	15.6	8
69	A Computational Strategy for the Design of Photochromic Derivatives Based on Diarylethene and Nickel Dithiolene with Large Contrast in Nonlinear Optical Properties. *Journal of Physical Chemistry C*, **2020**, 124, 4221-4241	3.8	13
68	Multiscale Modeling of Two-Photon Probes for Parkinson□s Diagnostics Based on Monoamine Oxidase B Biomarker. *Journal of Chemical Information and Modeling*, **2020**, 60, 3854-3863	6.1	3
67	Accurate Nonlinear Optical Properties of Solvated -Nitroaniline Predicted by an Electrostatic Discrete Local Field Approach. *Journal of Physical Chemistry B*, **2020**, 124, 10195-10209	3.4	3
66	Second harmonic generation in nonlinear optical crystals formed from propellane-type molecules. *Journal of Materials Chemistry C*, **2019**, 7, 1255-1262	7.1	9
65	Can Density Functional Theory Be Trusted for High-Order Electric Properties? The Case of Hydrogen-Bonded Complexes. *Journal of Chemical Theory and Computation*, **2019**, 15, 3570-3579	6.4	11
64	Design of Two-Photon-Excited Fluorescent Dyes Containing Fluoroborylene Groups. *ChemPhotoChem*, **2019**, 3, 719-726	3.3	4
63	Electric properties of hydrated uracil: From micro- to macrohydration. *Journal of Molecular Liquids*, **2019**, 275, 338-346	6	2
62	Utilizing formation of dye aggregates with aggregation-induced emission characteristics for enhancement of two-photon absorption. *Journal of Materials Chemistry C*, **2018**, 6, 4384-4388	7.1	9
61	Partitioning of interaction-induced nonlinear optical properties of molecular complexes. I. Hydrogen-bonded systems. *Physical Chemistry Chemical Physics*, **2018**, 20, 19841-19849	3.6	9

60	Unusual binding-site-specific photophysical properties of a benzothiazole-based optical probe in amyloid beta fibrils. *Physical Chemistry Chemical Physics*, **2018**, 20, 20334-20339	3.6	7
59	Benchmarking the Performance of Exchange-Correlation Functionals for Predicting Two-Photon Absorption Strengths. *Journal of Chemical Theory and Computation*, **2018**, 14, 3677-3685	6.4	30
58	Photophysical Properties of Phenacylphenantridine Difluoroboranyls: Effect of Substituent and Double Benzannulation. *Journal of Organic Chemistry*, **2017**, 82, 1529-1537	4.2	28
57	Two-photon absorption of BF-carrying compounds: insights from theory and experiment. *Physical Chemistry Chemical Physics*, **2017**, 19, 5705-5708	3.6	12
56	Two-photon absorption of the spatially confined LiH molecule. *Physical Chemistry Chemical Physics*, **2017**, 19, 7568-7575	3.6	8
55	Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples. *Journal of Chemical Theory and Computation*, **2017**, 13, 4347-4356	6.4	14
54	Vibrational nonlinear optical properties of spatially confined weakly bound complexes. *Physical Chemistry Chemical Physics*, **2017**, 19, 24276-24283	3.6	7
53	Nonempirical Simulations of Inhomogeneous Broadening of Electronic Transitions in Solution: Predicting Band Shapes in One- and Two-Photon Absorption Spectra of Chalcones. *Molecules*, **2017**, 22,	4.8	8
52	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. *Physical Chemistry Chemical Physics*, **2016**, 18, 22467-77	3.6	10
51	First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF2) Core Complex. *Journal of Physical Chemistry B*, **2016**, 120, 2323-32	3.4	21
50	Elucidating the Mechanism of Zn(2+) Sensing by a Bipyridine Probe Based on Two-Photon Absorption. *Journal of Physical Chemistry B*, **2016**, 120, 9067-75	3.4	12
49	Comparison of Property-Oriented Basis Sets for the Computation of Electronic and Nuclear Relaxation Hyperpolarizabilities. *Journal of Chemical Theory and Computation*, **2015**, 11, 4119-28	6.4	13
48	On the particular importance of vibrational contributions to the static electrical properties of model linear molecules under spatial confinement. *Physical Chemistry Chemical Physics*, **2015**, 17, 21782-6	3.6	16
47	Relation between Nonlinear Optical Properties of Push-Pull Molecules and Metric of Charge Transfer Excitations. *Journal of Chemical Theory and Computation*, **2015**, 11, 4182-8	6.4	32
46	Toward fully nonempirical simulations of optical band shapes of molecules in solution: a case study of heterocyclic ketoimine difluoroborates. *Journal of Physical Chemistry A*, **2015**, 119, 5145-52	2.8	35
45	Toward assessment of density functionals for vibronic coupling in two-photon absorption: A case study of 4-nitroaniline. *Journal of Computational Chemistry*, **2015**, 36, 1124-31	3.5	12
44	Influence of substituent and benzoannulation on photophysical properties of 1-benzoylmethyleneisoquinoline difluoroborates. *Journal of Organic Chemistry*, **2015**, 80, 2072-80	4.2	36
43	One- and two-photon absorption of a spiropyran-merocyanine system: experimental and theoretical studies. *Journal of Physical Chemistry B*, **2015**, 119, 1515-22	3.4	16

42	On the nonlinear electrical properties of molecules in confined spaces From cylindrical harmonic potential to carbon nanotube cages. *Chemical Physics*, **2014**, 428, 19-28	2.3	24
41	Promising two-photon probes for in vivo detection of amyloid deposits. *Chemical Communications*, **2014**, 50, 11694-7	5.8	21
40	Chelation-Induced Quenching of Two-Photon Absorption of Azacrown Ether Substituted Distyryl Benzene for Metal Ion Sensing. *Journal of Chemical Theory and Computation*, **2014**, 10, 778-88	6.4	9
39	Molecular structure-optical property relationships for a series of non-centrosymmetric two-photon absorbing push-pull triarylamine molecules. *Scientific Reports*, **2014**, 4, 4447	4.9	40
38	Anharmonicity contributions to the vibrational first and second hyperpolarizability of para-disubstituted benzenes. *Chemical Physics Letters*, **2014**, 595-596, 109-112	2.5	7
37	Comparative assessment of density functionals for excited-state dipole moments. *Chemical Physics Letters*, **2013**, 584, 58-62	2.5	8
36	The BHB bridging interaction in B-substituted oxazaborolidine borane complexes: a theoretical study. *Structural Chemistry*, **2013**, 24, 1485-1492	1.8	7
35	Revealing the Electronic and Molecular Structure of Randomly Oriented Molecules by Polarized Two-Photon Spectroscopy. *Journal of Physical Chemistry Letters*, **2013**, 4, 1753-9	6.4	16
34	Substituent effects on the photophysical properties of fluorescent 2-benzoylmethylenequinoline difluoroboranes: A combined experimental and quantum chemical study. *Dyes and Pigments*, **2013**, 99, 957-965	4.6	37
33	On the nature of unusual intensity changes in the infrared spectra of the enflurane acetone complexes. *Physical Chemistry Chemical Physics*, **2013**, 15, 6001-7	3.6	13
32	Two-photon solvatochromism II: experimental and theoretical study of solvent effects on the two-photon absorption spectrum of Reichardt's dye. *ChemPhysChem*, **2013**, 14, 3731-9	3.2	23
31	Towards first-principles based modeling of poly-3-alkylthiophenes: The nature of interactions in 2,2?-bithiophene dimer. *Chemical Physics Letters*, **2013**, 566, 67-70	2.5	1
30	The effect of intermolecular interactions on the electric dipole polarizabilities of nucleic acid base complexes. *Chemical Physics Letters*, **2013**, 555, 230-234	2.5	14
29	On the performance of long-range-corrected density functional theory and reduced-size polarized LPol-n basis sets in computations of electric dipole (hyper)polarizabilities of conjugated molecules. *Journal of Computational Chemistry*, **2013**, 34, 819-26	3.5	24
28	Performance of density functional theory in computing nonresonant vibrational (hyper)polarizabilities. *Journal of Computational Chemistry*, **2013**, 34, 1775-84	3.5	39
27	Revealing spectral features in two-photon absorption spectrum of Hoechst 33342: a combined experimental and quantum-chemical study. *Journal of Physical Chemistry B*, **2013**, 117, 12013-9	3.4	18
26	Resonant and Nonresonant Hyperpolarizabilities of Spatially Confined Molecules: A Case Study of Cyanoacetylene. *Journal of Chemical Theory and Computation*, **2013**, 9, 3463-72	6.4	25
25	New basis sets for the evaluation of interaction-induced electric properties in hydrogen-bonded complexes. *Journal of Computational Chemistry*, **2013**, 34, 275-83	3.5	12

24	Quantum chemical study of hole transfer coupling in nucleic acid base complexes containing 7-deazaadenine. *Chemical Physics Letters*, **2012**, 537, 94-100	2.5	3
23	Experimental and theoretical study on the one- and two-photon absorption properties of novel organic molecules based on phenylacetylene and azoaromatic moieties. *Journal of Physical Chemistry B*, **2012**, 116, 14677-88	3.4	22
22	Electric dipole (hyper)polarizabilities of spatially confined LiH molecule. *Journal of Chemical Physics*, **2012**, 137, 094307	3.9	25
21	Electronic structure, bonding, spectra, and linear and nonlinear electric properties of Ti@C28. *Journal of Physical Chemistry A*, **2011**, 115, 10370-81	2.8	33
20	Long-range corrected DFT calculations of charge-transfer integrals in model metal-free phthalocyanine complexes. *Journal of Molecular Modeling*, **2011**, 17, 2143-9	2	21
19	Large changes of static electric properties induced by hydrogen bonding: an ab initio study of linear HCN oligomers. *Journal of Physical Chemistry A*, **2011**, 115, 4691-700	2.8	23
18	Two-photon absorption spectra of carotenoids compounds. *Journal of Applied Physics*, **2011**, 109, 103529	2.5	20
17	Linear and nonlinear optical properties of triphenylamine-functionalized C60: insights from theory and experiment. *Physical Chemistry Chemical Physics*, **2010**, 12, 373-81	3.6	39
16	Electronic and vibrational contributions to first hyperpolarizability of donor-acceptor-substituted azobenzene. *Journal of Chemical Physics*, **2010**, 133, 244308	3.9	47
15	Theoretical insights into the nature of intermolecular interactions in cytosine dimer. *Biophysical Chemistry*, **2009**, 139, 137-43	3.5	14
14	Nucleic Acid Base Complexes: Elucidation of the Physical Origins of Their Stability **2009**, 387-397		
13	The post-SCF quantum chemistry characteristics of the guanine-guanine stacking B-DNA. *Physical Chemistry Chemical Physics*, **2008**, 10, 2665-72	3.6	24
12	On the electron correlation effects on electronic and vibrational hyperpolarizability of merocyanine dyes. *Journal of Chemical Physics*, **2008**, 129, 134310	3.9	15
11	On the influence of confinement effects on electric properties: An ab initio study. *Chemical Physics Letters*, **2007**, 449, 314-318	2.5	28
10	The nature of interactions in uracil dimer: An ab initio study. *Chemical Physics Letters*, **2007**, 450, 132-137	2.5	25
9	Experimental and theoretical investigations of spectroscopic properties of azobenzene derivatives in solution. *Journal of Molecular Modeling*, **2007**, 13, 785-91	2	14
8	Computational insight into relations between electronic and vibrational polarizabilities within the two-state valence-bond charge-transfer model. *Chemical Physics*, **2007**, 337, 77-80	2.3	14
7	SOS Methods in Calculations of Electronic NLO Properties. *Challenges and Advances in Computational Chemistry and Physics*, **2006**, 129-150	0.7	5

6	Quantum-chemical insight into the design of molecular optoelectrical switch. *Chemical Physics*, **2005**, 316, 267-278	2.3	31
5	First-order hyperpolarizability of pyridinium N-phenolate betaine dye: Ab initio study. *Chemical Physics Letters*, **2005**, 411, 8-13	2.5	11
4	Performance of the reduced-size polarized Z3PolX basis set in calculations of vibrational polarizabilities, infrared, and Raman intensities: Application to formaldehyde molecule. *International Journal of Quantum Chemistry*, **2005**, 104, 660-666	2.1	5
3	Size-Nonextensive Contributions in Singles-Only CI. *Structural Chemistry*, **2004**, 15, 379-384	1.8	2
2	Ab initio calculations of doubly resonant sum-frequency generation second-order polarizabilities of LiH. *Chemical Physics Letters*, **2003**, 380, 549-555	2.5	10
1	Less is more: on the effect of benzannulation on the solid-state emission of difluoroborates. *Journal of Materials Chemistry C*,	7.1	1