Zilvinas Rinkevicius

List of Publications by Year
in descending order

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100 papers	3,391 citations	201674 27 h-index	149698 56 g-index
100 all docs	100 docs citations	100 times ranked	3617 citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	Two-photon absorption in solution by means of time-dependent density-functional theory and the polarizable continuum model. Journal of Chemical Physics, 2005, 122, 244104.	3.0	106
3	Restricted density functional theory of linear time-dependent properties in open-shell molecules. Journal of Chemical Physics, 2003, 119, 34-46.	3.0	91
4	Spin-flip time dependent density functional theory applied to excited states with single, double, or mixed electron excitation character. Journal of Chemical Physics, 2010, 133, 114104.	3.0	88
5	Breakdown of the first hyperpolarizability/bond-length alternation parameter relationship. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 16453-16458.	7.1	84
6	Density functional theory of nonlinear triplet response properties with applications to phosphorescence. Journal of Chemical Physics, 2003, 119, 11024-11034.	3.0	79
7	Calculations of nuclear magnetic shielding in paramagnetic molecules. Journal of Chemical Physics, 2003, 118, 2550.	3.0	71
8	Spatial Quantum Beats in Vibrational Resonant Inelastic Soft X-Ray Scattering at Dissociating States in Oxygen. Physical Review Letters, 2011, 106, 153004.	7.8	69
9	Hybrid density functional theory/molecular mechanics calculations of two-photon absorption of dimethylamino nitro stilbene in solution. Physical Chemistry Chemical Physics, 2011, 13, 12506.	2.8	64
10	Demystifying the solvatochromic reversal in Brookerâ€™s merocyanine dye. Physical Chemistry Chemical Physics, 2011, 13, 1290-1292.	2.8	55
11	Self-interaction-corrected time-dependent density-functional-theory calculations of x-ray-absorption spectra. Physical Review A, 2007, 76, .	2.5	52
12	Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. Journal of Physical Chemistry B, 2010, 114, 13349-13357.	2.6	52
13	Conformations, structural transitions and visible near-infrared absorption spectra of four-, five- and six-coordinated Cu(<scp>ii</scp>) aqua complexes. Physical Chemistry Chemical Physics, 2009, 11, 508-519.	2.8	51
14	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45
15	Modeling of EPR parameters of copper(II) aqua complexes. Chemical Physics, 2007, 332, 176-187.	1.9	41
16	Color modeling of protein optical probes. Physical Chemistry Chemical Physics, 2012, 14, 1107-1112.	2.8	40
17	The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. Journal of Physical Chemistry B, 2012, 116, 8169-8181.	2.6	40
18	Density functional theory for hyperfine coupling constants with the restricted-unrestricted approach. Journal of Chemical Physics, 2004, 121, 7614.	3.0	39

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19	A Hybrid Density Functional Theory/Molecular Mechanics Approach for Linear Response Properties in Heterogeneous Environments. Journal of Chemical Theory and Computation, 2014, 10, 989-1003.	5.3	39
20	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, 5145-5152.	2.5	39
21	Heisenberg Exchange in Dinuclear Manganese Complexes:â€‰ A Density Functional Theory Study. Journal of Chemical Theory and Computation, 2006, 2, 981-989.	5.3	37
22	Many-Photon Dynamics of Photobleaching. Journal of Physical Chemistry A, 2007, 111, 11961-11975.	2.5	37
23	Spin-flip time dependent density functional theory for singletâ€“triplet splittings in Ïƒ,Ïƒ-biradicals. Chemical Physics Letters, 2010, 491, 132-135.	2.6	35
24	Rearranging from 6- to 7-coordination initiates the catalytic activity: An EPR study on a Ru-bda water oxidation catalyst. Coordination Chemistry Reviews, 2017, 346, 206-215.	18.8	34
25	VeloxChem: A Pythonâ€driven densityâ€functional theory program for spectroscopy simulations in highâ€performance computing environments. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1457.	14.6	34
26	General excitations in time-dependent density functional theory. Journal of Chemical Physics, 2007, 126, 114101.	3.0	32
27	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. Journal of Physical Chemistry Letters, 2013, 4, 70-77.	4.6	29
28	Spin Multiplicity Dependence of Nonlinear Optical Properties. ChemPhysChem, 2009, 10, 817-823.	2.1	27
29	Association Dynamics and Linear and Nonlinear Optical Properties of an N-Acetylaladanamide Probe in a POPC Membrane. Journal of the American Chemical Society, 2013, 135, 13590-13597.	13.7	27
30	Restricted density-functional linear response theory calculations of electronic g-tensors. Journal of Chemical Physics, 2003, 119, 10489-10496.	3.0	26
31	Electronic g-tensors of solvated molecules using the polarizable continuum model. Journal of Chemical Physics, 2004, 121, 5051-5060.	3.0	26
32	Searching of potential energy curves for the benzene dimer using dispersion-corrected density functional theory. Physical Chemistry Chemical Physics, 2008, 10, 2715.	2.8	25
33	Solvatochromic shift of phenol blue in water from a combined Carâ€“Parrinello molecular dynamics hybrid quantum mechanics-molecular mechanics and <scp>ZINDO</scp> approach. Journal of Chemical Physics, 2010, 132, 234508.	3.0	25
34	Solvent Dependence on Bond Length Alternation and Charge Distribution in Phenol Blue: A Carâ€˜Parrinello Molecular Dynamics Investigation. Journal of Physical Chemistry A, 2009, 113, 4833-4839.	2.5	23
35	Theoretical Study of Specific Solvent Effects on the Optical and Magnetic Properties of Copper(II) Acetylacetonate. Journal of Physical Chemistry A, 2011, 115, 1331-1339.	2.5	22
36	Quantum Mechanical Studies of Intensity in Electronic Spectra of Fluorescein Dianion and Monoanion Forms. Structural Chemistry, 2003, 14, 643-648.	2.0	21

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37	Modeling solvatochromism of Nile red in water. International Journal of Quantum Chemistry, 2011, 111, 1521-1530.	2.0	21
38	Degenerate Perturbation Theory for Electronic g Tensors: Leading-Order Relativistic Effects. Journal of Chemical Theory and Computation, 2008, 4, 1810-1828.	5.3	20
39	Density Functional Theory/Molecular Mechanics Approach for Electronic g-Tensors of Solvated Molecules. Journal of Physical Chemistry B, 2011, 115, 4350-4358.	2.6	20
40	Extended Discrete Interaction Model: Plasmonic Excitations of Silver Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 28867-28880.	3.1	20
41	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. Journal of Chemical Theory and Computation, 2012, 8, 257-263.	5.3	19
42	Complex Polarization Propagator Approach in the Restricted Open-Shell, Self-Consistent Field Approximation: The Near K-Edge X-ray Absorption Fine Structure Spectra of Allyl and Copper Phthalocyanine. Journal of Physical Chemistry B, 2011, 115, 5096-5102.	2.6	18
43	Density Functional Restrictedâ€“Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. Journal of Chemical Theory and Computation, 2011, 7, 3261-3271.	5.3	18
44	Non-linear optical properties of molecules in heterogeneous environments: a quadratic density functional/molecular mechanics response theory. Physical Chemistry Chemical Physics, 2014, 16, 8981.	2.8	18
45	Hydrogen-bonding effects on electronicg-tensors of semiquinone anion radicals: Relativistic density functional investigation. International Journal of Quantum Chemistry, 2002, 90, 1404-1413.	2.0	17
46	Density functional restricted-unrestricted approach for nonlinear properties: Application to electron paramagnetic resonance parameters of square planar copper complexes. Journal of Chemical Physics, 2008, 129, 064109.	3.0	17
47	Novel Pathways for Enhancing Nonlinearity of Organics Utilizing Metal Clusters. Journal of Physical Chemistry A, 2010, 114, 7590-7594.	2.5	17
48	Electronic Circular Dichroism of Surface-Adsorbed Molecules by Means of Quantum Mechanics Capacitance Molecular Mechanics. Journal of Physical Chemistry C, 2014, 118, 5833-5840.	3.1	17
49	Density functional theory study of indirect nuclear spin-spin coupling constants with spin-orbit corrections. Journal of Chemical Physics, 2005, 123, 014101.	3.0	16
50	Optomagnetic Effect Induced by Magnetized Nanocavity Plasmon. Journal of the American Chemical Society, 2019, 141, 13795-13798.	13.7	16
51	Gator: A Pythonâ€driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528.	14.6	16
52	Time-dependent density functional theory with the generalized restricted-unrestricted approach. Journal of Chemical Physics, 2006, 124, 174103.	3.0	15
53	Hybrid density functionalâ€“molecular mechanics calculations for core-electron binding energies of glycine in water solution. Physical Chemistry Chemical Physics, 2013, 15, 244-254.	2.8	15
54	Zero-point vibrational corrections to isotropic hyperfine coupling constants in polyatomic molecules. Physical Chemistry Chemical Physics, 2011, 13, 696-707.	2.8	14

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55	NMR Spinâ€“Spin Coupling Constants in Polymethine Dyes as Polarity Indicators. Chemistry - A European Journal, 2012, 18, 11677-11684.	3.3	14
56	Quantum Mechanics/Molecular Mechanics Modeling of Photoelectron Spectra: The Carbon 1s Coreâ€“Electron Binding Energies of Ethanolâ€“Water Solutions. Journal of Physical Chemistry B, 2014, 118, 13217-13225.	2.6	14
57	Two-Photon Absorption of Metal-Assisted Chromophores. Journal of Chemical Theory and Computation, 2014, 10, 5630-5639.	5.3	14
58	Plasmonic nano-shells: atomistic discrete interaction versus classic electrodynamics models. Physical Chemistry Chemical Physics, 2020, 22, 13467-13473.	2.8	14
59	Symmetry-forbidden x-ray Raman scattering induced by a strong infrared-laser field. Physical Review A, 2008, 77, .	2.5	13
60	Internal symmetry and selection rules in resonant inelastic soft x-ray scattering. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 161002.	1.5	13
61	Time-dependent density-functional theory calculations of triplet-triplet absorption. Journal of Chemical Physics, 2005, 122, 224104.	3.0	12
62	Modelling the visible absorption spectra of copper(II) acetylacetonate by Density Functional Theory. Chemical Physics Letters, 2010, 492, 14-18.	2.6	12
63	Time-dependent density functional theory for nonlinear properties of open-shell systems. Journal of Chemical Physics, 2007, 127, 114101.	3.0	11
64	Hybrid Complex Polarization Propagator/Molecular Mechanics Method for Heterogeneous Environments. Journal of Chemical Theory and Computation, 2016, 12, 2661-2667.	5.3	10
65	An algorithm for the efficient evaluation of two-electron repulsion integrals over contracted Gaussian-type basis functions. Journal of Chemical Physics, 2012, 137, 234105.	3.0	9
66	Optical Properties of Gold Nanoclusters Functionalized with a Small Organic Compound: Modeling by an Integrated Quantum-Classical Approach. Journal of Chemical Theory and Computation, 2016, 12, 3325-3339.	5.3	9
67	Antibacterial Activity of Silver and Gold Particles Formed on Titania Thin Films. Nanomaterials, 2022, 12, 1190.	4.1	9
68	Influence of Hydrogen Bonding in the Paramagnetic NMR Shieldings of Nitronylnitroxide Derivative Molecules. Journal of Physical Chemistry B, 2004, 108, 1197-1206.	2.6	8
69	Modeling two photon absorption cross sections of open-shell systems. Journal of Chemical Physics, 2009, 130, 014103.	3.0	8
70	Binding Mechanism and Magnetic Properties of a Multifunctional Spin Label for Targeted EPR Imaging of Amyloid Proteins: Insight from Atomistic Simulations and First-Principles Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4766-4774.	5.3	8
71	Spectral character of intermediate state in solid-state photoarrangement of Î±-santonin. Chemical Physics, 2012, 405, 40-45.	1.9	8
72	Formation of N-oxide in the third oxidation of [Ru^{II}(tpy)(L)(OH₂)]²⁺. Chemical Communications, 2017, 53, 5622-5624.	4.1	8

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73	Mechanistic Studies on NaHCO₃ Hydrogenation and HCOOH Dehydrogenation Reactions Catalysed by a Fe^{II} Linear Tetraphosphine Complex. Chemistry - A European Journal, 2018, 24, 5366-5372.	3.3	8
74	Nuclear Magnetic Shielding of the 113Cd(II) Ion in Aqua Solution: A Combined Molecular Dynamics/Density Functional Theory Study. Journal of Physical Chemistry B, 2008, 112, 11347-11352.	2.6	7
75	Theoretical Studies on the Photoinduced Rearrangement Mechanism of Î±â€Šantonin. ChemPhysChem, 2012, 13, 353-362.	2.1	7
76	Quantum mechanics capacitance molecular mechanics modeling of core-electron binding energies of methanol and methyl nitrite on Ag(111) surface. Journal of Chemical Physics, 2016, 145, 024703.	3.0	7
77	Fine and hyperfine structure in three low-lying3Î£+states of molecular hydrogen. Molecular Physics, 2003, 101, 2335-2346.	1.7	6
78	Two-photon-induced x-ray emission in neon atoms. Physical Review A, 2010, 82, .	2.5	6
79	Role of zero-point vibrational corrections to carbon hyperfine coupling constants in organic Ï€ radicals. Journal of Chemical Physics, 2013, 138, 054310.	3.0	6
80	Formation of Au nanostructures on the surfaces of annealed <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow><mml:mi mathvariant="normal">TiO</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> thin films. Surfaces and Interfaces, 2021, 25, 101239.	3.0	6
81	A time-dependent density-functional theory and complete active space self-consistent field method study of vibronic absorption and emission spectra of coumarin. Journal of Chemical Physics, 2014, 141, 014306.	3.0	5
82	Origin of the Absorption Band of Bromophenol Blue in Acidic and Basic pH: Insight from a Combined Molecular Dynamics and TD-DFT/MM Study. Journal of Physical Chemistry A, 2016, 120, 7175-7182.	2.5	5
83	Theoretical study of para-nitro-aniline adsorption on the Au(111) surface. Surface Science, 2016, 649, 124-132.	1.9	5
84	Size-dependent polarizabilities and van der Waals dispersion coefficients of fullerenes from large-scale complex polarization propagator calculations. Journal of Chemical Physics, 2021, 154, 074304.	3.0	5
85	Single-spin measurements for quantum computation using magnetic resonance force microscopy. Superlattices and Microstructures, 2003, 34, 509-511.	3.1	4
86	Paramagnetic Perturbation of the 19F NMR Chemical Shift in Fluorinated Cysteine by O2: A Theoretical Study. Journal of Physical Chemistry B, 2009, 113, 10916-10922.	2.6	4
87	EPR spin Hamiltonian parameters of encapsulated spin-labels: impact of the hydrogen bonding topology. Physical Chemistry Chemical Physics, 2013, 15, 2427.	2.8	4
88	On the magnetic properties of nanodiamonds: Electronic g-tensor calculations. Journal of Chemical Physics, 2019, 151, 044305.	3.0	4
89	Electronic g-tensors of nanodiamonds: Dependence on the size, shape, and surface functionalization. Journal of Chemical Physics, 2019, 151, 144305.	3.0	3
90	Efficient implementation of isotropic cubic response functions for two-photon absorption cross sections within the self-consistent field approximation. Journal of Chemical Physics, 2021, 154, 024111.	3.0	3

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91	Quantum Chemical Design of Light Driven Molecular Logical Machines. , 2002, , 209-219.		2
92	Kohnâ€“Sham Time-Dependent Density Functional Theory with Applications to Linear and Nonlinear Properties. Challenges and Advances in Computational Chemistry and Physics, 2006, , 151-209.	0.6	2
93	Resonant inelastic X-ray Raman scattering induced by Rabi flopping of core holes. Chemical Physics Letters, 2008, 453, 117-121.	2.6	2
94	Role of the³(Ï€Ï€*) State in Photolysis of Lumisantonin: Insight from ab Initio Studies. Journal of Physical Chemistry A, 2011, 115, 7815-7822.	2.5	2
95	Ï€-Stacking effects on the EPR parameters of a prototypical DNA spin label. Physical Chemistry Chemical Physics, 2013, 15, 10466.	2.8	2
96	Computational study on the electronic g-tensors of hydrophilic and hydrophobic nanodiamonds interacting with water. Journal of Chemical Physics, 2020, 152, 144302.	3.0	2
97	Electronic g-Tensor Calculations for Dangling Bonds in Nanodiamonds. Journal of Physical Chemistry A, 2021, 125, 8249-8260.	2.5	2
98	Restricted Density Functional Response Theory for Open-Shell Systems. Advances in Quantum Chemistry, 2005, 50, 271-288.	0.8	1
99	Time-dependent closed and open-shell density functional theory from the perspective of partitioning techniques and projections. Computational and Theoretical Chemistry, 2009, 914, 50-59.	1.5	1
100	Finite-Time Stabilization of the Fractional Model of the Driven Dissipative Nonlinear Pendulum. International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 2022, 32, .	1.7	1