Tadeusz AndruniÃ³w

List of Publications by Year
in descending order

55 papers	2,021 citations	279798 23 h-index	243625 44 g-index
57 all docs	57 docs citations	57 times ranked	1520 citing authors

#	Article	IF	Citations
1	Tracking the excited-state time evolution of the visual pigment with multiconfigurational quantum chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7764-7769.	7.1	266
2	Structure, initial excited-state relaxation, and energy storage of rhodopsin resolved at the multiconfigurational perturbation theory level. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 17908-17913.	7.1	228
3	Properties of the Emitting State of the Green Fluorescent Protein Resolved at the CASPT2//CASSCF/CHARMM Level. Journal of the American Chemical Society, 2005, 127, 11534-11535.	13.7	142
4	Assessment of Approximate Coupled-Cluster and Algebraic-Diagrammatic-Construction Methods for Ground- and Excited-State Reaction Paths and the Conical-Intersection Seam of a Retinal-Chromophore Model. Journal of Chemical Theory and Computation, 2015, 11, 5758-5781.	5.3	123
5	Theoretical Determination of the Coâ^'C Bond Energy Dissociation in Cobalamins. Journal of the American Chemical Society, 2001, 123, 2679-2680.	13.7	98
6	Electronically Excited States of Vitamin B₁₂: Benchmark Calculations Including Time-Dependent Density Functional Theory and Correlated ab Initio Methods. Journal of Physical Chemistry A, 2011, 115, 1280-1292.	2.5	94
7	Density Functional Theory Analysis of Stereoelectronic Properties of Cobalaminsâ€. Journal of Physical Chemistry B, 2000, 104, 10921-10927.	2.6	67
8	Quantum Chemical Modeling and Preparation of a Biomimetic Photochemical Switch. Angewandte Chemie - International Edition, 2007, 46, 414-420.	13.8	60
9	Flavonesâ€™ and Flavonolsâ€™ Antiradical Structureâ€“Activity Relationshipâ€”A Quantum Chemical Study. Antioxidants, 2020, 9, 461.	5.1	60
10	Theoretical analysis of electronic absorption spectra of vitamin B12 models. Journal of Chemical Physics, 2001, 115, 7522-7533.	3.0	59
11	Vibrational Analysis of Methylcobalamin. Journal of Physical Chemistry A, 2002, 106, 1365-1373.	2.5	49
12	Photolysis of Methylcobalamin:Â Identification of the Relevant Excited States Involved in Coâ^'C Bond Scission. Journal of Physical Chemistry B, 2007, 111, 2419-2422.	2.6	48
13	Photodissociation of Coâ^'C Bond in Methyl- and Ethylcobalamin: An Insight from TD-DFT Calculations. Journal of Physical Chemistry B, 2009, 113, 6898-6909.	2.6	45
14	New light on the Coâ€“C bond activation in B12-dependent enzymes from density functional theory. Chemical Physics Letters, 2000, 331, 509-512.	2.6	43
15	Computational Photobiology and Beyond. Australian Journal of Chemistry, 2010, 63, 413.	0.9	36
16	Mechanism of Coâ€“C Bond Photolysis in the Base-On Form of Methylcobalamin. Journal of Physical Chemistry A, 2014, 118, 11718-11734.	2.5	36
17	Electronic and Structural Properties of Low-lying Excited States of Vitamin B₁₂. Journal of Physical Chemistry B, 2011, 115, 13304-13319.	2.6	35
18	Time-dependent density functional theory study of cobalt corrinoids: Electronically excited states of methylcobalamin. Journal of Chemical Physics, 2008, 129, 085101.	3.0	32

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19	DFTâ€“SQM force field for cobalt corrinoids. Chemical Physics Letters, 2000, 331, 502-508.	2.6	28
20	Density Functional Study of Absorption and Resonance Raman Spectra of Pyromellitic Diahydride (PMDA) Anion. Journal of Physical Chemistry A, 2000, 104, 845-851.	2.5	28
21	Assessment of Functionals for TDDFT Calculations of One- and Two-Photon Absorption Properties of Neutral and Anionic Fluorescent Proteins Chromophores. Journal of Chemical Theory and Computation, 2019, 15, 490-508.	5.3	27
22	Molecular orbital analysis of anomalous trans effect in cobalamins. Chemical Physics Letters, 2005, 410, 410-416.	2.6	26
23	Effects of the Protein Environment on the Spectral Properties of Tryptophan Radicals in Pseudomonas aeruginosa Azurin. Journal of the American Chemical Society, 2013, 135, 4822-4833.	13.7	26
24	Geometries and Vertical Excitation Energies in Retinal Analogues Resolved at the CASPT2 Level of Theory: Critical Assessment of the Performance of CASSCF, CC2, and DFT Methods. Journal of Chemical Theory and Computation, 2013, 9, 4915-4927.	5.3	26
25	Mechanism of the S1 excited state internal conversion in vitamin B12. Physical Chemistry Chemical Physics, 2014, 16, 18675-18679.	2.8	26
26	DFT Analysis of Coâ^'Alkyl and Coâ^'Adenosyl Vibrational Modes in B12-Cofactors. Inorganic Chemistry, 2006, 45, 5585-5590.	4.0	25
27	Time-dependent density functional theory study of cobalt corrinoids: Electronically excited states of coenzyme B[sub 12]. Journal of Chemical Physics, 2009, 131, 105105.	3.0	21
28	Recognition of the True and False Resonance Raman Optical Activity. Angewandte Chemie - International Edition, 2021, 60, 21205-21210.	13.8	21
29	Quantumâ€“classical simulations of rhodopsin reveal excited-state population splitting and its effects on quantum efficiency. Nature Chemistry, 2022, 14, 441-449.	13.6	20
30	On the Franck-Condon Effects in the Absorption Spectrum of C₁₀H₈Anion. the Analysis Based on the AB Initio MCSCF Method. Acta Physica Polonica A, 1998, 93, 707-715.	0.5	18
31	Resonance Raman study of Franck-Condon effects in the C10H8+ radical. Ab initio MCSCF calculations for the low-energy 2B2g and 2B3g symmetry states. Chemical Physics Letters, 1996, 259, 193-198.	2.6	17
32	The Franckâ€“Condon effect in the lowest energy state of tetracyanoquinodimethane anion. The resonance Raman studies in terms of density functional theory. Vibrational Spectroscopy, 1999, 21, 45-50.	2.2	17
33	Franckâ€“Condon effects in low-energy states of C10H8+ radical.. Chemical Physics, 1998, 236, 25-33.	1.9	16
34	Mechanism of the Initial Conformational Transition of a Photomodulable Peptide. Angewandte Chemie - International Edition, 2005, 44, 6077-6081.	13.8	13
35	How Does the Relocation of Internal Water Affect Resonance Raman Spectra of Rhodopsin? An Insight from CASSCF/Amber Calculations. Journal of Chemical Theory and Computation, 2009, 5, 3096-3104.	5.3	12
36	Initial Excited-State Dynamics of an N-Alkylated Indanylideneâ€“Pyrroline (NAIP) Rhodopsin Analog. Journal of Physical Chemistry B, 2014, 118, 12243-12250.	2.6	12

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37	Absorption and resonance Raman study of the pyromellitic diahydride anion via density functional theory. Chemical Physics Letters, 2000, 321, 485-490.	2.6	11
38	Toward a computational photobiology. Pure and Applied Chemistry, 2005, 77, 977-993.	1.9	10
39	The role of spin-orbit coupling in the photolysis of methylcobalamin. Journal of Chemical Physics, 2016, 144, 124305.	3.0	10
40	Assessing the Accuracy of Various Ab Initio Methods for Geometries and Excitation Energies of Retinal Chromophore Minimal Model by Comparison with CASPT3 Results. Journal of Chemical Theory and Computation, 2016, 12, 2346-2356.	5.3	10
41	Vibronic coupling effects in the low-energy and states of the C10H8+ radical. Chemical Physics, 1998, 236, 35-41.	1.9	8
42	Impacts of retinal polyene (de)methylation on the photoisomerization mechanism and photon energy storage of rhodopsin. Physical Chemistry Chemical Physics, 2015, 17, 17169-17181.	2.8	7
43	Illuminating the origins of twoâ€photon absorption properties in fluorescent protein chromophores. International Journal of Quantum Chemistry, 2020, 120, e26086.	2.0	7
44	QM/MM Studies of Light-responsive Biological Systems. Challenges and Advances in Computational Chemistry and Physics, 2021, , .	0.6	7
45	Vibrational analysis of a solvated green fluorescent protein chromophore. Journal of Molecular Modeling, 2007, 13, 775-783.	1.8	6
46	What is the Optimal Size of the Quantum Region in Embedding Calculations of Two-Photon Absorption Spectra of Fluorescent Proteins?. Journal of Chemical Theory and Computation, 2020, 16, 6439-6455.	5.3	6
47	Ab initio multireference study of Hetero-Diels-Alder reaction of buta-1,3-diene with alkyl glyoxylates. Journal of Molecular Modeling, 2008, 14, 727-733.	1.8	5
48	Removing artifacts in polarizable embedding calculations of one- and two-photon absorption spectra of fluorescent proteins. Journal of Chemical Physics, 2020, 153, 215102.	3.0	5
49	Excitedâ€state minima and emission energies of retinal chromophore analogues: Performance of CASSCF and CC2 methods as compared with CASPT2. Journal of Computational Chemistry, 2017, 38, 1799-1810.	3.3	4
50	The Role of Hydrogen Bonds and Electrostatic Interactions in Enhancing Twoâ€Photon Absorption in Green and Yellow Fluorescent Proteins. ChemPhysChem, 2022, 23, .	2.1	4
51	Is the choice of a standard zerothâ€order hamiltonian in CASPT2 ansatz optimal in calculations of excitation energies in protonated and unprotonated schiff bases of retinal?. Journal of Computational Chemistry, 2018, 39, 1470-1480.	3.3	3
52	Assessing Electronically Excited States of Cobalamins via Absorption Spectroscopy and Time-Dependent Density Functional Theory. Challenges and Advances in Computational Chemistry and Physics, 2019, , 219-258.	0.6	3
53	Initial excitedâ€state relaxation of locked retinal protonated schiff base chromophore. An insight from coupled cluster and multireference perturbation theory calculations. Journal of Computational Chemistry, 2018, 39, 1720-1727.	3.3	2
54	Erratum to â€œGeometries and Vertical Excitation Energies in Retinal Analogues Resolved at the CASPT2 Level of Theory: Critical Assessment of the Performance of CASSCF, CC2, and DFT Methodsâ€• Journal of Chemical Theory and Computation, 2014, 10, 5215-5215.	5.3	1

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55	Recognition of the True and False Resonance Raman Optical Activity. Angewandte Chemie, 2021, 133, 21375-21380.	2.0	0