Igor V Polyakov

List of Publications by Year
in descending order

35 papers	588 citations	758635 12 h-index	610482 24 g-index
40 all docs	40 docs citations	40 times ranked	624 citing authors

#	Article	IF	Citations
1	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore. 1. Electronically Excited and Ionized States of the Anionic Chromophore in the Gas Phase. Journal of Chemical Theory and Computation, 2009, 5, 1895-1906.	2.3	109
2	Potential Energy Landscape of the Electronic States of the GFP Chromophore in Different Protonation Forms: Electronic Transition Energies and Conical Intersections. Journal of Chemical Theory and Computation, 2010, 6, 2377-2387.	2.3	106
3	First-Principles Characterization of the Energy Landscape and Optical Spectra of Green Fluorescent Protein along the Aâ†’Iâ†’B Proton Transfer Route. Journal of the American Chemical Society, 2013, 135, 11541-11549.	6.6	64
4	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore: 2. <i>Cis</i>â^’<i>Trans</i> Isomerization in Water. Journal of Chemical Theory and Computation, 2009, 5, 1907-1914.	2.3	44
5	The effect of oxidation on the electronic structure of the green fluorescent protein chromophore. Journal of Chemical Physics, 2010, 132, 115104.	1.2	32
6	A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins. Journal of Physical Chemistry B, 2015, 119, 5444-5452.	1.2	28
7	Toward Molecular-Level Characterization of Photoinduced Decarboxylation of the Green Fluorescent Protein: Accessibility of the Charge-Transfer States. Journal of Chemical Theory and Computation, 2012, 8, 1912-1920.	2.3	25
8	Triple-Decker Motif for Red-Shifted Fluorescent Protein Mutants. Journal of Physical Chemistry Letters, 2013, 4, 1743-1747.	2.1	25
9	On photoabsorption of the neutral form of the green fluorescent protein chromophore. Biophysical Chemistry, 2009, 145, 1-6.	1.5	22
10	Unusual Emitting States of the Kindling Fluorescent Protein: Appearance of the Cationic Chromophore in the GFP Family. Journal of Physical Chemistry B, 2013, 117, 7228-7234.	1.2	14
11	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. Chemical Physics Letters, 2018, 710, 59-63.	1.2	14
12	Mechanisms of ATP to cAMP Conversion Catalyzed by the Mammalian Adenylyl Cyclase: A Role of Magnesium Coordination Shells and Proton Wires. Journal of Physical Chemistry B, 2020, 124, 451-460.	1.2	13
13	Interplay between Locally Excited and Charge Transfer States Governs the Photoswitching Mechanism in the Fluorescent Protein Dreiklang. Journal of Physical Chemistry B, 2021, 125, 757-770.	1.2	13
14	Computational Modeling Reveals the Mechanism of Fluorescent State Recovery in the Reversibly Photoswitchable Protein Dreiklang. Journal of Physical Chemistry B, 2019, 123, 8901-8909.	1.2	11
15	How Reproducible Are QM/MM Simulations? Lessons from Computational Studies of the Covalent Inhibition of the SARS-CoV-2 Main Protease by Carmofur. Journal of Chemical Theory and Computation, 2022, 18, 5056-5067.	2.3	9
16	Towards quantum-based modeling of enzymatic reaction pathways: Application to the acetylholinesterase catalysis. Chemical Physics Letters, 2013, 556, 251-255.	1.2	8
17	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. Journal of Physical Chemistry B, 2017, 121, 10602-10609.	1.2	8
18	Stalling chromophore synthesis of the fluorescent protein Venus reveals the molecular basis of the final oxidation step. Chemical Science, 2021, 12, 7735-7745.	3.7	8

#	Article	IF	Citations
19	Towards first-principles calculation of electronic excitations in the ring of the protein-bound bacteriochlorophylls. Chemical Physics, 2018, 505, 34-39.	0.9	6
20	Modeling of the mechanism of hydrolysis of succinylcholine in the active site of native and modified (Asp70Gly) human butyrylcholinesterase. Russian Chemical Bulletin, 2010, 59, 55-60.	0.4	5
21	Protonation States of Molecular Groups in the Chromophore-Binding Site Modulate Properties of the Reversibly Switchable Fluorescent Protein rsEGFP2. Journal of Physical Chemistry Letters, 2021, 12, 8263-8271.	2.1	5
22	Structure of the Brain <i>N</i>-Acetylaspartate Biosynthetic Enzyme NAT8L Revealed by Computer Modeling. ACS Chemical Neuroscience, 2020, 11, 2296-2302.	1.7	4
23	Model of the RNA Polymerase Complex of the SARS-CoV-2 Virus with Favipiravir. Russian Journal of Physical Chemistry B, 2021, 15, 103-107.	0.2	3
24	Algorithms of the flexible effective fragment method used for modeling of transformations in enzyme active sites. Moscow University Chemistry Bulletin, 2010, 65, 355-357.	0.2	2
25	Quantum chemical modeling of components of dye-sensitized solar cells. Moscow University Chemistry Bulletin, 2013, 68, 77-79.	0.2	2
26	Molecular model of LH1 light-harvesting complex of the photosynthetic center of Thermochromatium tepidum bacteria. Moscow University Chemistry Bulletin, 2013, 68, 80-82.	0.2	2
27	Structural forms of green fluorescent protein by quantum mechanics/molecular mechanics calculations. Russian Chemical Bulletin, 2010, 59, 61-65.	0.4	1
28	Computer modeling of components of photoreceptor systems. Russian Chemical Bulletin, 2014, 63, 1703-1709.	0.4	1
29	Modeling hydrolysis of the cyclic dimeric guanosine monophosphate by phosphodiesterases. Moscow University Chemistry Bulletin, 2016, 71, 12-15.	0.2	1
30	Theoretical characterization of the photochemical reaction CO2Â+ÂO(3P)Ââ†’ÂCOÂ+ÂO2 related to experiments in solid krypton. Chemical Physics Letters, 2020, 746, 137303.	1.2	1
31	Modeling photophysical properties of the bacteriophytochrome-based fluorescent protein IFP1.4. Journal of Chemical Physics, 2021, 154, 065101.	1.2	1
32	Computer Modeling of N-Acetylglutamate Synthase: From Primary Structure to Elemental Stages of Catalysis. Doklady Biochemistry and Biophysics, 2020, 495, 334-337.	0.3	1
33	Computer modeling of properties of complex molecular systems. AIP Conference Proceedings, 2015, , .	0.3	0
34	Modeling GTP hydrolysis in RasGAP protein complex. Moscow University Chemistry Bulletin, 2016, 71, 21-24.	0.2	0
35	Evaluation of the Q y absorption band maximum in a light-harvesting complex of the bacterial photosynthetic center Thermochromatium tepidum. Moscow University Chemistry Bulletin, 2017, 72, 111-114.	0.2	0