Anastasia V Bochenkova

List of Publications by Year
in descending order

59	1,111	394421 19	434195 31
papers	citations	h-index	g-index

64	64	64	992
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An Opsin Shift in Rhodopsin:â€‰ Retinal S0â^'S1 Excitation in Protein, in Solution, and in the Gas Phase. Journal of the American Chemical Society, 2007, 129, 13035-13042.	13.7	94
2	Origin of the Intrinsic Fluorescence of the Green Fluorescent Protein. Journal of the American Chemical Society, 2017, 139, 8766-8771.	13.7	75
3	Characterization of a complete cycle of acetylcholinesterase catalysis by ab initio QM/MM modeling. Journal of Molecular Modeling, 2008, 14, 409-416.	1.8	69
4	Ultrafast dual photoresponse of isolated biological chromophores: link to the photoinduced mode-specific non-adiabatic dynamics in proteins. Faraday Discussions, 2013, 163, 297.	3.2	59
5	Gas Phase Absorption Studies of Photoactive Yellow Protein Chromophore Derivatives. Journal of Physical Chemistry A, 2009, 113, 9442-9449.	2.5	56
6	Photoabsorption studies of neutral green fluorescent protein model chromophores in vacuo. Physical Chemistry Chemical Physics, 2009, 11, 9996.	2.8	41
7	Mode-Specific Vibrational Autodetachment Following Excitation of Electronic Resonances by Electrons and Photons. Physical Review Letters, 2020, 124, 203401.	7.8	41
8	Intrinsic photoisomerization dynamics of protonated Schiff-base retinal. Nature Communications, 2019, 10, 1210.	12.8	39
9	A QM/MM approach with effective fragment potentials applied to the dipeptideâ€“water structures. Computational and Theoretical Chemistry, 2002, 581, 167-175.	1.5	38
10	Mechanism of resonant electron emission from the deprotonated GFP chromophore and its biomimetics. Chemical Science, 2017, 8, 3154-3163.	7.4	38
11	Direct and Indirect Electron Emission from the Green Fluorescent Protein Chromophore. Physical Review Letters, 2012, 109, 128101.	7.8	37
12	UV Excitedâ€‰State Photoresponse of Biochromophore Negative Ions. Angewandte Chemie - International Edition, 2014, 53, 9797-9801.	13.8	36
13	Modeling Photoabsorption of the asFP595 Chromophore. Journal of Physical Chemistry A, 2008, 112, 8804-8810.	2.5	32
14	Hybrid diatomics-in-molecules-based quantum mechanical/molecular mechanical approach applied to the modeling of structures and spectra of mixed molecular clusters Arn(HCl)m and Arn(HF)m. Journal of Chemical Physics, 2004, 120, 3732-3743.	3.0	28
15	Hybrid DIM-based QM/MM approach applied to vibrational spectra and trapping site structures of HArF in solid argon. Chemical Physics Letters, 2005, 405, 165-171.	2.6	28
16	Modeling of the structure and electronic spectra of green fluorescent protein chromophore. Russian Journal of Physical Chemistry B, 2008, 2, 671-675.	1.3	25
17	HArF in Solid Argon Revisited: Transition from Unstable to Stable Configuration. Journal of Physical Chemistry A, 2009, 113, 7654-7659.	2.5	24
18	Decoupling Electronic versus Nuclear Photoresponse of Isolated Green Fluorescent Protein Chromophores Using Short Laser Pulses. Physical Review Letters, 2016, 117, 243004.	7.8	22

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19	The photophysics of isolated protein chromophores. European Physical Journal D, 2009, 51, 5-14.	1.3	20
20	Modeling reaction routes from rhodopsin to bathorhodopsin. Proteins: Structure, Function and Bioinformatics, 2010, 78, 614-622.	2.6	19
21	Direct Measurement of the Isomerization Barrier of the Isolated Retinal Chromophore. Angewandte Chemie - International Edition, 2015, 54, 4748-4752.	13.8	18
22	Photoresponse of the protonated Schiff-base retinal chromophore in the gas phase. Physical Chemistry Chemical Physics, 2013, 15, 19566.	2.8	17
23	The UV-visible action-absorption spectrum of all-trans and 11-cis protonated Schiff base retinal in the gas phase. Physical Chemistry Chemical Physics, 2018, 20, 7190-7194.	2.8	15
24	Electronic structure of the para-dinitrobenzene radical anion: a combined 2D photoelectron imaging and computational study. Physical Chemistry Chemical Physics, 2018, 20, 24019-24026.	2.8	15
25	Hindered rotation of HArF in solid argon: Infrared spectroscopy and a theoretical model. Physical Review B, 2008, 77, .	3.2	14
26	Hidden photoinduced reactivity of the blue fluorescent protein mKalama1. Physical Chemistry Chemical Physics, 2015, 17, 12472-12485.	2.8	14
27	Gas-Phase Spectroscopy of Protonated 3-OH Kynurenine and Argpyrimidine. Comparison of Experimental Results to Theoretical Modeling. Journal of Physical Chemistry A, 2007, 111, 10537-10543.	2.5	12
28	Light Driven Ultrafast Bioinspired Molecular Motors: Steering and Accelerating Photoisomerization Dynamics of Retinal. Journal of the American Chemical Society, 2022, 144, 69-73.	13.7	11
29	Structures of the Peptideâ€“Water Complexes Studied by the Hybrid Quantum Mechanicalâ€”Molecular Mechanical (QM/MM) Technique. Structural Chemistry, 2004, 15, 3-9.	2.0	10
30	Molecular Modeling the Reaction Mechanism of Serine-Carboxyl Peptidases. Journal of Chemical Theory and Computation, 2006, 2, 1168-1175.	5.3	10
31	Photodissociation pathways and lifetimes of protonated peptides and their dimers. Journal of Chemical Physics, 2012, 136, 014307.	3.0	10
32	How far can a single hydrogen bond tune the spectral properties of the GFP chromophore?. Physical Chemistry Chemical Physics, 2015, 17, 20056-20060.	2.8	10
33	A General Mechanism of Green-to-Red Photoconversions of GFP. Frontiers in Molecular Biosciences, 2020, 7, 176.	3.5	10
34	Insights into the Early-Time Excited-State Dynamics of Structurally Inhomogeneous Rhodopsin KR2. Journal of Physical Chemistry Letters, 2021, 12, 8664-8671.	4.6	10
35	Liquid-microjet photoelectron spectroscopy of the green fluorescent protein chromophore. Nature Communications, 2022, 13, 507.	12.8	10
36	Impact of Pyrophosphate andO-Ethyl-Substituted Pyrophosphate Groups on DNA Structure. Journal of Physical Chemistry B, 2007, 111, 432-438.	2.6	9

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37	A PYP chromophore acts as a â€˜photoacidâ€™ in an isolated hydrogen bonded complex. Physical Chemistry Chemical Physics, 2016, 18, 9909-9913.	2.8	9
38	The origin of radiationless conversion of the excited state in the kindling fluorescent protein (KFP): femtosecond studies and quantum modeling. Laser Physics Letters, 2011, 8, 469-474.	1.4	8
39	Probing the Barrier for Internal Rotation of the Retinal Chromophore. Angewandte Chemie - International Edition, 2012, 51, 8757-8761.	13.8	8
40	Excited-state locked amino analogues of the green fluorescent protein chromophore with a giant Stokes shift. RSC Advances, 2019, 9, 38730-38734.	3.6	8
41	Photo-initiated Dynamics and Spectroscopy of the Deprotonated Green Fluorescent Protein Chromophore. Physical Chemistry in Action, 2013, , 67-103.	0.6	7
42	Potential functions of internal rotation of the methacryloyl fluoride molecule in the ground (S0) and excited (S1) electronic states. Journal of Molecular Structure, 2019, 1181, 228-234.	3.6	7
43	Investigation of matrix-isolated species: spectroscopy and molecular modelling. Russian Chemical Reviews, 2007, 76, 1085-1092.	6.5	6
44	Accurate modeling of the S 0 -S 1 photo-absorption in biological chromophores. , 2007, , .		6
45	On the temperature of large biomolecules in ion-storage rings. European Physical Journal D, 2022, 76, 1.	1.3	5
46	QM/MM modeling of the structures and properties of the Î²-diketonate-based lanthanide complexes. International Journal of Quantum Chemistry, 2005, 104, 203-213.	2.0	4
47	Controlling Lightâ€Induced Proton Transfer from the GFP Chromophore. ChemPhysChem, 2021, 22, 833-841.	2.1	4
48	A photoelectron imaging study of the deprotonated GFP chromophore anion and RNA fluorescent tags. Physical Chemistry Chemical Physics, 2021, 23, 19911-19922.	2.8	3
49	Action-Absorption Spectroscopy at the Band Origin of the Deprotonated Green Fluorescent Protein Chromophore In Vacuo. Journal of Physical Chemistry Letters, 0, , 6683-6685.	4.6	3
50	Role of the Protein Environment in Photoisomerization of Type I and Type II Rhodopsins: a Theoretical Perspective. Moscow University Chemistry Bulletin, 2021, 76, 407-416.	0.6	2
51	Designing Red-Shifted Molecular Emitters Based on the Annulated Locked GFP Chromophore Derivatives. International Journal of Molecular Sciences, 2021, 22, 13645.	4.1	2
52	The role of magnesium in hydrolysis of triphosphates in water: Quantum mechanical/molecular mechanical modeling. Moscow University Chemistry Bulletin, 2007, 62, 123-127.	0.6	1
53	Plasmon-Enhanced Fluorescence of EGFP on Short-Range Ordered Ag Nanohole Arrays. Nanomaterials, 2020, 10, 2563.	4.1	1
54	Controlling Lightâ€Induced Proton Transfer from the GFP Chromophore. ChemPhysChem, 2021, 22, 807-807.	2.1	1

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55	Remarkably efficient acid generation in chemically amplified resist from quantum chemistry modeling. Journal of Vacuum Science & Technology B, 2007, 25, 58.	1.3	0
56	Computational approaches in modeling spectra of biological chromophores. Proceedings of SPIE, 2008, , .	0.8	0
57	Frontispiece: Direct Measurement of the Isomerization Barrier of the Isolated Retinal Chromophore. Angewandte Chemie - International Edition, 2015, 54, .	13.8	0
58	Direct Measurement of the Isomerization Barrier of the Isolated Retinal Chromophore. Journal of Physics: Conference Series, 2015, 635, 032034.	0.4	0
59	Protein Mobility Measurements through Oxidative Green-to-Red Photoconversion of EGFP. Journal of Physical Chemistry B, 0, , .	2.6	0