Bella L Grigorenko

List of Publications by Year in Descending Order

123 papers	2,552 citations	29 h-index	46 g-index
128 ext. papers	2,733 ext. citations	4.5 avg, IF	5.03 L-index

#	Paper	IF	Citations
123	QM/MM Approaches Shed Light on GFP Puzzles. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 271-292	0.7	2
122	Molecular Modeling Reveals the Mechanism of Ran-RanGAP-Catalyzed Guanosine Triphosphate Hydrolysis without an Arginine Finger. *ACS Catalysis*, **2021**, 11, 8985-8998	13.1	3
121	Stalling chromophore synthesis of the fluorescent protein Venus reveals the molecular basis of the final oxidation step. *Chemical Science*, **2021**, 12, 7735-7745	9.4	5
120	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	3.4	5
119	Modeling photophysical properties of the bacteriophytochrome-based fluorescent protein IFP1.4. *Journal of Chemical Physics*, **2021**, 154, 065101	3.9	1
118	Tuning Electrostatic Gating of Semiconducting Carbon Nanotubes by Controlling Protein Orientation in Biosensing Devices. *Angewandte Chemie - International Edition*, **2021**, 60, 20184-20189	16.4	3
117	Tuning Electrostatic Gating of Semiconducting Carbon Nanotubes by Controlling Protein Orientation in Biosensing Devices. *Angewandte Chemie*, **2021**, 133, 20346-20351	3.6	0
116	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	6.4	1
115	Theoretical characterization of the photochemical reaction CO2 + O(3P) -q CO + O2 related to experiments in solid krypton. *Chemical Physics Letters*, **2020**, 746, 137303	2.5	1
114	Structure of the Brain -Acetylaspartate Biosynthetic Enzyme NAT8L Revealed by Computer Modeling. *ACS Chemical Neuroscience*, **2020**, 11, 2296-2302	5.7	1
113	Study and modeling of mechanisms of cholinesterasis reactions in order to improve their catalytic properties in the neutralization reactions of organophosphorous compounds **2020**, 134-174		
112	Study and modeling of mechanisms of cholinesterasis reactions in order to improve their catalytic properties in the neutralization reactions of organophosphorus compounds **2020**, 140-180		
111	Human cholinesterases **2020**, 69-126		
110	ORGANOPHOSPHORUS NEUROTOXINS **2020**,		5
109	Human cholinesterases **2020**, 63-120		
108	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	3.4	7
107	Diversity of mechanisms in Ras-GAP catalysis of guanosine triphosphate hydrolysis revealed by molecular modeling. *Organic and Biomolecular Chemistry*, **2019**, 17, 4879-4891	3.9	10

106	Computer-designed active human butyrylcholinesterase double mutant with a new catalytic triad. *Chemico-Biological Interactions*, **2019**, 306, 138-146	5	30
105	Computational Challenges in Modeling of Representative Bioimaging Proteins: GFP-Like Proteins, Flavoproteins, and Phytochromes. *Journal of Physical Chemistry B*, **2019**, 123, 6133-6149	3.4	25
104	Modeling of the glycine tripeptide cyclization in the Ser65Gly/Tyr66Gly mutant of green fluorescent protein. *Mendeleev Communications*, **2019**, 29, 187-189	1.9	6
103	Computational Modeling Reveals the Mechanism of Fluorescent State Recovery in the Reversibly Photoswitchable Protein Dreiklang. *Journal of Physical Chemistry B*, **2019**, 123, 8901-8909	3.4	5
102	Effect of solvation water shells on enzyme active sites in zinc-dependent hydrolases. *Structural Chemistry*, **2019**, 30, 481-488	1.8	3
101	Optimization of Cholinesterase-Based Catalytic Bioscavengers Against Organophosphorus Agents. *Frontiers in Pharmacology*, **2018**, 9, 211	5.6	52
100	Mechanism of Metallo-β-Lactamase Inhibition by Oxacephalosporin Antibiotic. *Moscow University Chemistry Bulletin*, **2018**, 73, 155-157	0.5	0
99	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. *Chemical Physics Letters*, **2018**, 710, 59-63	2.5	12
98	Amide-imide tautomerization in the glutamine side chain in enzymatic and photochemical reactions in proteins. *Physical Chemistry Chemical Physics*, **2018**, 20, 23827-23836	3.6	17
97	Improving the Design of the Triple-Decker Motif in Red Fluorescent Proteins. *Journal of Physical Chemistry B*, **2017**, 121, 10602-10609	3.4	6
96	Molecular Modeling Clarifies the Mechanism of Chromophore Maturation in the Green Fluorescent Protein. *Journal of the American Chemical Society*, **2017**, 139, 10239-10249	16.4	31
95	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. *Chemical Reviews*, **2017**, 117, 758-795	55.1	154
94	Modeling hydrolysis of the cyclic dimeric guanosine monophosphate by phosphodiesterases. *Moscow University Chemistry Bulletin*, **2016**, 71, 12-15	0.5	1
93	Theoretical vibrational spectroscopy of intermediates and the reaction mechanism of the guanosine triphosphate hydrolysis by the protein complex Ras-GAP. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2016**, 166, 68-72	4.4	6
92	Computational characterization of the all-atom structure and the calcium binding sites of the LH1-RC core complex from Thermochromatium tepidum. *Journal of Theoretical and Computational Chemistry*, **2016**, 15, 1650020	1.8	2
91	Modeling the Complete Catalytic Cycle of Aspartoacylase. *Journal of Physical Chemistry B*, **2016**, 120, 4221-31	3.4	20
90	Analysis of proton wires in the enzyme active site suggests a mechanism of c-di-GMP hydrolysis by the EAL domain phosphodiesterases. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 1670-1680	4.2	4
89	A Light-Induced Reaction with Oxygen Leads to Chromophore Decomposition and Irreversible Photobleaching in GFP-Type Proteins. *Journal of Physical Chemistry B*, **2015**, 119, 5444-52	3.4	23

88	Modeling reactivation of the phosphorylated human butyrylcholinesterase by QM(DFTB)/MM calculations. *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550051	1.8	11
87	Why does mutation of Gln61 in Ras by the nitro analog NGln maintain activity of Ras-GAP in hydrolysis of guanosine triphosphate?. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 2091-9	4.2	9
86	Hydrolysis of Guanosine Triphosphate (GTP) by the Ras□GAP Protein Complex: Reaction Mechanism and Kinetic Scheme. *Journal of Physical Chemistry B*, **2015**, 119, 12838-45	3.4	37
85	Modeling the role of G12V and G13V Ras mutations in the Ras-GAP-catalyzed hydrolysis reaction of guanosine triphosphate. *Biochemistry*, **2014**, 53, 7093-9	3.2	31
84	All-atom structures and calcium binding sites of the bacterial photosynthetic LH1-RC core complex from Thermochromatium tepidum. *Journal of Molecular Modeling*, **2014**, 20, 2287	2	5
83	Catalytic Cycle of Penicillin Acylase from Escherichia coli: QM/MM Modeling of Chemical Transformations in the Enzyme Active Site upon Penicillin G Hydrolysis. *ACS Catalysis*, **2014**, 4, 2521-2529	13.1	19
82	The structure of the enzyme-substrate complex of the phosphodiesterase catalytic domain with cyclic diguanosine monophosphate. *Moscow University Chemistry Bulletin*, **2014**, 69, 1-4	0.5	1
81	Computer modeling of components of photoreceptor systems. *Russian Chemical Bulletin*, **2014**, 63, 1703-1709	1.7	1
80	Optical transitions in the light-harvesting complexes of bacterial photosynthetic centers. *Moscow University Chemistry Bulletin*, **2014**, 69, 152-154	0.5	2
79	First-principles characterization of the energy landscape and optical spectra of green fluorescent protein along the A-to-B proton transfer route. *Journal of the American Chemical Society*, **2013**, 135, 11541-9	10.4	55
78	Molecular model of LH1 light-harvesting complex of the photosynthetic center of Thermochromatium tepidum bacteria. *Moscow University Chemistry Bulletin*, **2013**, 68, 80-82	0.5	2
77	On quantum mechanical--molecular mechanical (QM/MM) approaches to model hydrolysis of acetylcholine by acetylcholinesterase. *Chemico-Biological Interactions*, **2013**, 203, 51-6	5	14
76	Thermal isomerization of the chromoprotein asFP595 and its kindling mutant A143G: QM/MM molecular dynamics simulations. *Journal of Physical Chemistry B*, **2013**, 117, 13507-14	3.4	7
75	Towards quantum-based modeling of enzymatic reaction pathways: Application to the acetylholinesterase catalysis. *Chemical Physics Letters*, **2013**, 556, 251-255	2.5	7
74	Unusual emitting states of the kindling fluorescent protein: appearance of the cationic chromophore in the GFP family. *Journal of Physical Chemistry B*, **2013**, 117, 7228-34	3.4	12
73	Triple-Decker Motif for Red-Shifted Fluorescent Protein Mutants. *Journal of Physical Chemistry Letters*, **2013**, 4, 1743-7	6.4	25
72	Minimum energy reaction profiles for the hydrolysis reaction of the cyclic guanosine monophosphate in water: Comparison of the results of two QM/MM approaches. *Computational and Theoretical Chemistry*, **2012**, 983, 88-94	2	7
71	Quantum chemistry behind bioimaging: insights from ab initio studies of fluorescent proteins and their chromophores. *Accounts of Chemical Research*, **2012**, 45, 265-75	24.3	114

70	Quantum chemical modelling in the research of molecular mechanisms of enzymatic catalysis. *Russian Chemical Reviews*, **2012**, 81, 1011-1025	6.8	26
69	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, 1912-20	6.4	22
68	Quantum mechanical/molecular mechanical analysis of mechanisms of enzyme action. Human acetylcholinesterase. *Russian Chemical Bulletin*, **2011**, 60, 2196-2204	1.7	1
67	Effect of protein environment on electronically excited and ionized states of the green fluorescent protein chromophore. *Journal of Physical Chemistry B*, **2011**, 115, 8296-303	3.4	82
66	Computational characterization of reaction intermediates in the photocycle of the sensory domain of the AppA blue light photoreceptor. *Photochemistry and Photobiology*, **2011**, 87, 564-73	3.6	23
65	Minimum energy reaction profiles for ATP hydrolysis in myosin. *Journal of Molecular Graphics and Modelling*, **2011**, 31, 1-4	2.8	24
64	Conformational partitioning in pH-induced fluorescence of the kindling fluorescent protein (KFP). *Journal of Physical Chemistry B*, **2011**, 115, 9195-201	3.4	11
63	Modeling of calcium binding in the light-harvesting complex of photosynthetic reaction center of the Thermochromatium tepidum bacterium. *Moscow University Chemistry Bulletin*, **2011**, 66, 80-82	0.5	4
62	Modeling the mechanism of hydrolysis of cyclic guanosine monophosphates in aqueous solution. *Moscow University Chemistry Bulletin*, **2011**, 66, 229-231	0.5	2
61	Coupling between the BLUF and EAL domains in the blue light-regulated phosphodiesterase BlrP1. *Journal of Molecular Modeling*, **2011**, 17, 1579-86	2	15
60	Modeling Structures and Spectra of Trapped Species in Low-Temperature Matrices **2011**, 447-468		
59	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, 2377-87	6.4	95
58	Algorithms of the flexible effective fragment method used for modeling of transformations in enzyme active sites. *Moscow University Chemistry Bulletin*, **2010**, 65, 355-357	0.5	1
57	Quantum Chemistry Calculations Provide Support to the Mechanism of the Light-Induced Structural Changes in the Flavin-Binding Photoreceptor Proteins. *Journal of Chemical Theory and Computation*, **2010**, 6, 2293-302	6.4	36
56	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	1.7	5
55	On photoabsorption of the neutral form of the green fluorescent protein chromophore. *Biophysical Chemistry*, **2009**, 145, 1-6	3.5	20
54	Biochemical evidence for the tyrosine involvement in cationic intermediate stabilization in mouse beta-carotene 15, 15-monooxygenase. *BMC Biochemistry*, **2009**, 10, 31	4.8	18
53	Simulated 18O kinetic isotope effects in enzymatic hydrolysis of guanosine triphosphate. *Biochemistry (Moscow)*, **2009**, 74, 1044-8	2.9	4

52	Conformation-dependent chemical reaction of formic acid with an oxygen atom. *Journal of Physical Chemistry A*, **2009**, 113, 8143-6	2.8	30
51	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore: 2. Cis-Trans Isomerization in Water. *Journal of Chemical Theory and Computation*, **2009**, 5, 1907-14	6.4	42
50	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, 1895-906	6.4	104
49	Opening the Arg-Glu salt bridge in myosin: computational study. *Physical Chemistry Chemical Physics*, **2009**, 11, 4804-7	3.6	6
48	Molecular models predict light-induced glutamine tautomerization in BLUF photoreceptors. *Biophysical Journal*, **2008**, 94, 3872-9	2.9	103
47	Conformation dependence of pKa of the chromophores from the purple asFP595 and yellow zFP538 fluorescent proteins. *Computational and Theoretical Chemistry*, **2008**, 863, 39-43		12
46	Theoretical characterization of the 1,3-diazaazulene molecule and its derivatives. *Computational and Theoretical Chemistry*, **2008**, 855, 40-44		4
45	Mechanisms of enzymatic hydrolysis of nucleoside triphosphates by quantum and molecular mechanics. *Russian Journal of General Chemistry*, **2008**, 78, 696-703	0.7	
44	Structure of the enzyme-substrate complex for guanosine triphosphate hydrolysis by elongation factor EF-Tu: Comparison of quantum mechanics/molecular mechanics and molecular dynamics results. *Moscow University Chemistry Bulletin*, **2008**, 63, 321-323	0.5	1
43	Photochemical synthesis of H2O2 from the H2O...O(3P) van der Waals complex: experimental observations in solid krypton and theoretical modeling. *Journal of Physical Chemistry A*, **2007**, 111, 11444-9	2.8	15
42	The role of magnesium in hydrolysis of triphosphates in water: Quantum mechanical/molecular mechanical modeling. *Moscow University Chemistry Bulletin*, **2007**, 62, 123-127	0.5	1
41	Implementation of a molecular dynamics approach with rigid fragments to simulation of chemical reactions in biomolecular systems. *Moscow University Chemistry Bulletin*, **2007**, 62, 177-179	0.5	2
40	Mechanism of the myosin catalyzed hydrolysis of ATP as rationalized by molecular modeling. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 7057-61	11.5	64
39	Investigation of matrix-isolated species: spectroscopy and molecular modelling. *Russian Chemical Reviews*, **2007**, 76, 1085-1092	6.8	4
38	Mechanisms of guanosine triphosphate hydrolysis by Ras and Ras-GAP proteins as rationalized by ab initio QM/MM simulations. *Proteins: Structure, Function and Bioinformatics*, **2007**, 66, 456-66	4.2	76
37	Mechanism of triphosphate hydrolysis in aqueous solution: QM/MM simulations in water clusters. *Journal of Physical Chemistry B*, **2006**, 110, 4407-12	3.4	56
36	Molecular Modeling the Reaction Mechanism of Serine-Carboxyl Peptidases. *Journal of Chemical Theory and Computation*, **2006**, 2, 1168-75	6.4	9
35	Ground-state structures and vertical excitations for the kindling fluorescent protein asFP595. *Journal of Physical Chemistry B*, **2006**, 110, 18635-40	3.4	29

34	Modeling dioxygen binding to the non-heme iron-containing enzymes. *International Journal of Quantum Chemistry*, **2006**, 106, 2184-2190	2.1	15
33	trans and cis Chromophore structures in the kindling fluorescent protein asFP595. *Chemical Physics Letters*, **2006**, 424, 184-188	2.5	21
32	Computational study of a transition state analog of phosphoryl transfer in the Ras-RasGAP complex: AlF(x) versus MgF3-. *Journal of Molecular Modeling*, **2005**, 11, 503-8	2	10
31	QM/MM modeling the Ras-GAP catalyzed hydrolysis of guanosine triphosphate. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 495-503	4.2	84
30	Structures of the Peptide–Water Complexes Studied by the Hybrid Quantum Mechanical–Molecular Mechanical (QM/MM) Technique. *Structural Chemistry*, **2004**, 15, 3-9	1.8	10
29	Modeling of serine protease prototype reactions with the flexible effective fragment potential quantum mechanical/molecular mechanical method. *Theoretical Chemistry Accounts*, **2004**, 111, 36-48	1.9	36
28	Quantum chemical modeling of the GTP hydrolysis by the RAS-GAP protein complex. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2004**, 1700, 125-36	4	40
27	QM/MM modeling of the glutathione–hydroxymethyl radical reaction in water. *Physical Chemistry Chemical Physics*, **2004**, 6, 1031-1038	3.6	9
26	Flexible effective fragment QM/MM method: validation through the challenging tests. *Journal of Computational Chemistry*, **2003**, 24, 1410-20	3.5	61
25	Quantum Chemical Simulations of the Proton Transfer in Water Wires Attached to Molecular Walls. *Journal of Physical Chemistry B*, **2003**, 107, 2958-2965	3.4	20
24	A QM/MM approach with effective fragment potentials applied to the dipeptide–water structures. *Computational and Theoretical Chemistry*, **2002**, 581, 167-175		37
23	On the Origin of Potential Barrier for the Reaction OH- + CO2 -→ HCO3- in Water: Studies by Using Continuum and Cluster Solvation Methods. *Journal of Physical Chemistry B*, **2002**, 106, 1734-1740	3.4	32
22	Modeling of Biomolecular Systems with the Quantum Mechanical and Molecular Mechanical Method Based on the Effective Fragment Potential Technique: Proposal of Flexible Fragments. *Journal of Physical Chemistry A*, **2002**, 106, 10663-10672	2.8	60
21	Intermolecular complexes of HXeOH with water: stabilization and destabilization effects. *Journal of the American Chemical Society*, **2002**, 124, 10706-11	16.4	86
20	Emission of SH radicals in solid krypton: mixed quantum-classical molecular dynamics simulations. *Chemical Physics Letters*, **2001**, 338, 317-322	2.5	4
19	An analysis of stationary points on the (HF)n potential surfaces (n≤3) predicted by the diatomics-in-ionic-systems model. *Computational and Theoretical Chemistry*, **2000**, 498, 47-60		5
18	Hydrogen bonding at the diatomics-in-molecules level: Water clusters. *Journal of Chemical Physics*, **2000**, 113, 2638-2647	3.9	16
17	A new hybrid approach for modeling reactions in molecular clusters: Application for the hydrogen bonded systems. *Journal of Chemical Physics*, **2000**, 112, 513-521	3.9	7

16	Excited-state site effects in luminescence spectroscopy of SH radicals in krypton matrices: Experiment and simulations. *Journal of Chemical Physics*, **1999**, 110, 5836-5843	3.9	10
15	Diatomics-in-ionic-systems and ab initio predictions for the stationary points on potential energy surfaces of the (HF)n clusters (n=3). *Journal of Chemical Physics*, **1999**, 111, 4442-4452	3.9	13
14	ArHF vibrational predissociation dynamics using the diatomics-in-molecule potential energy surface. *Journal of Chemical Physics*, **1999**, 111, 2470-2477	3.9	22
13	Ab initio potential curves of the fragments and diatomics-in-molecules potential energy surfaces for the SH?Kr complex. *Chemical Physics Letters*, **1999**, 301, 287-296	2.5	13
12	MDDIM simulations of the 3(ion-pair)-a(valence) red-shifted transitions of Cl2 in neon matrices. *Chemical Physics Letters*, **1998**, 296, 84-92	2.5	9
11	Towards quantitative diatomics-in-molecules model for the water molecule. *Chemical Physics*, **1998**, 232, 321-328	2.3	6
10	Hydrogen bonding described through diatomics-in-ionic-systems: The HF dimer. *Journal of Chemical Physics*, **1998**, 108, 4413-4425	3.9	29
9	Modeling the spectra of matrix-isolated molecules. *Journal of Structural Chemistry*, **1997**, 38, 207-211	0.9	
8	Inclusion of ion-pair states in the diatomics-in-molecules description of potential energy surfaces: van der Waals complexes of He?Cl2 and Ar?Cl2. *Chemical Physics*, **1997**, 219, 161-172	2.3	30
7	Modeling properties of the HF dimer in argon clusters. *International Journal of Quantum Chemistry*, **1997**, 62, 55-65	2.1	6
6	Modelling trapping sites of (HF)2 in argon clusters. *Chemical Physics Letters*, **1997**, 270, 103-107	2.5	11
5	Ab initio potential functions for the ionic states of OH. *Chemical Physics Letters*, **1997**, 276, 171-176	2.5	16
4	Theoretical vibrational spectrum of (HF)2 in argon matrices. *Chemical Physics Letters*, **1996**, 250, 226-231	2.5	13
3	Many-body potentials and dynamics based on diatomics-in-molecules: Vibrational frequency shifts in ArnHF (n=1,62) clusters. *Journal of Chemical Physics*, **1996**, 104, 5510-5516	3.9	55
2	Properties of the NBr molecule in argon clusters. *Chemical Physics Letters*, **1995**, 233, 627-631	2.5	12
1	Effect of argon atoms on charge distributions in small lithium clusters. *Physical Review B*, **1994**, 50, 18666-18669	3.3	