

Vladimir A Mironov

List of Publications by Year in descending order

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37
papers

1,070
citations

840119

11
h-index

525886

27
g-index

38
all docs

38
docs citations

38
times ranked

1189
citing authors

#	ARTICLE	IF	CITATIONS
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
2	Modeling the Role of G12V and G13V Ras Mutations in the Ras-GAP-Catalyzed Hydrolysis Reaction of Guanosine Triphosphate. Biochemistry, 2014, 53, 7093-7099.	1.2	40
3	Exploring Structural and Optical Properties of Fluorescent Proteins by Squeezing: Modeling High-Pressure Effects on the mStrawberry and mCherry Red Fluorescent Proteins. Journal of Physical Chemistry B, 2012, 116, 12426-12440.	1.2	32
4	A systematic study of minima in alanine dipeptide. Journal of Computational Chemistry, 2019, 40, 297-309.	1.5	25
5	Computational characterization of the chemical step in the GTP hydrolysis by Ras-GAP for the wild-type and G13V mutated Ras. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1046-1053.	1.5	19
6	PaSTRI: Error-Bounded Lossy Compression for Two-Electron Integrals in Quantum Chemistry. , 2018, , .		19
7	Molecular Electrostatic Potential and Electron Density of Large Systems in Solution Computed with the Fragment Molecular Orbital Method. Journal of Physical Chemistry A, 2019, 123, 6281-6290.	1.1	18
8	An efficient MPI/OpenMP parallelization of the Hartree-Fock-Roothaan method for the first generation of Intel® Xeon Phi, processor architecture. International Journal of High Performance Computing Applications, 2019, 33, 212-224.	2.4	16
9	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. Chemical Physics Letters, 2018, 710, 59-63.	1.2	14
10	The role of SAXS and molecular simulations in 3D structure elucidation of a DNA aptamer against lung cancer. Molecular Therapy - Nucleic Acids, 2021, 25, 316-327.	2.3	14
11	Conformational Partitioning in pH-Induced Fluorescence of the Kindling Fluorescent Protein (KFP). Journal of Physical Chemistry B, 2011, 115, 9195-9201.	1.2	12
12	Multithreaded parallelization of the energy and analytic gradient in the fragment molecular orbital method. International Journal of Quantum Chemistry, 2019, 119, e25937.	1.0	11
13	Thermal Isomerization of the Chromoprotein asFP595 and Its Kindling Mutant A143G: QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 13507-13514.	1.2	10
14	Why does mutation of Gln61 in Ras by the nitro analog NGln maintain activity of Ras in hydrolysis of guanosine triphosphate?. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2091-2099.	1.5	9
15	Structure- and Interaction-Based Design of Anti-SARS-CoV-2 Aptamers. Chemistry - A European Journal, 2022, 28, .	1.7	9
16	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.	0.6	8
17	Modeling absorption of the kindling fluorescent protein with the neutral form of the chromophore. International Journal of Quantum Chemistry, 2012, 112, 2947-2951.	1.0	8
18	Role of Zwitterions in Kindling Fluorescent Protein Photochemistry. Journal of Physical Chemistry B, 2015, 119, 2467-2474.	1.2	8

#	ARTICLE	IF	CITATIONS
19	An efficient MPI/openMP parallelization of the Hartree-Fock method for the second generation of Intel [®] Xeon Phi [™] processor. , 2017, , .		8
20	The Performance Characterization of the RSC PetaStream Module. Lecture Notes in Computer Science, 2014, , 420-429.	1.0	7
21	Performance Evaluation of the Intel Optane DC Memory With Scientific Benchmarks. , 2019, , .		7
22	Computational Methods for Biochemical Simulations Implemented in GAMESS. Methods in Molecular Biology, 2020, 2114, 123-142.	0.4	7
23	The Photocycle of Bacteriophytochrome Is Initiated by Counterclockwise Chromophore Isomerization. Journal of Physical Chemistry Letters, 2022, 13, 4538-4542.	2.1	7
24	On Quantum Chemistry Code Adaptation for RSC PetaStream Architecture. Lecture Notes in Computer Science, 2015, , 113-121.	1.0	4
25	Evaluation of Intel Memory Drive Technology Performance for Scientific Applications. , 2018, , .		4
26	Server Level Liquid Cooling: Do Higher System Temperatures Improve Energy Efficiency?. Supercomputing Frontiers and Innovations, 2016, 3, .	0.5	4
27	High temperature coolant demonstrated for a computational cluster. , 2016, , .		3
28	Power Measurements of Hartree-Fock Algorithms Using Different Storage Devices. , 2017, , .		3
29	Luminescent Zero-Dimensional Hybrid Lead Thiohalide Nanostructures for High Quantum Yield and Broadband Excitation. ACS Applied Nano Materials, 2021, 4, 3654-3663.	2.4	3
30	The photoreaction mechanism in the bacterial blue light receptor BLUF according to metadynamics modeling. Moscow University Chemistry Bulletin, 2014, 69, 149-151.	0.2	2
31	The Parallel Hydrodynamic Code for Astrophysical Flow with Stellar Equations of State. Communications in Computer and Information Science, 2019, , 414-426.	0.4	2
32	Computational approach to design of aptamers to the receptor binding domain of SARS-CoV-2. Siberian Medical Review, 2021, , 66-67.	0.1	1
33	Multi-Level Parallelization of the Fragment Molecular Orbital Method in GAMESS. , 2021, , 601-616.		1
34	3-D electronic density maps for enzyme reaction intermediates: big data and high performance computing services in a virtualized environment. Journal of Physics: Conference Series, 2019, 1392, 012049.	0.3	1
35	Methodological aspects of the calculation of the free energy profile of guanosine triphosphate hydrolysis by Ras-GAP protein complex. Moscow University Chemistry Bulletin, 2016, 71, 283-286.	0.2	0
36	Applying joint theoretical experimental research to aptamer modeling. Siberian Medical Review, 2021, , 105-106.	0.1	0

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37	Evaluation of Intel Memory Drive Technology Performance for Computational Astrophysics. Communications in Computer and Information Science, 2019, , 563-572.	0.4	0