Vladimir A Mironov

List of Publications by Year
in descending order

37	1,070	840119	525886
papers	citations	11 h-index	27 g-index

38	38	38	1189
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structureâ€•and Interactionâ€Based Design of Antiâ€SARSâ€CoVâ€2 Aptamers. Chemistry - A European Journal, 2022, 28, .	1.7	9
2	The Photocycle of Bacteriophytochrome Is Initiated by Counterclockwise Chromophore Isomerization. Journal of Physical Chemistry Letters, 2022, 13, 4538-4542.	2.1	7
3	Computational approach to design of aptamers to the receptor binding domain of SARS-CoV-2. Siberian Medical Review, 2021, , 66-67.	0.1	1
4	Multi-Level Parallelization of the Fragment Molecular Orbital Method in GAMESS. , 2021, , 601-616.		1
5	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
6	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
7	Applying joint theoretical experimental research to aptamer modeling. Siberian Medical Review, 2021, , 105-106.	0.1	0
8	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
9	Computational Methods for Biochemical Simulations Implemented in GAMESS. Methods in Molecular Biology, 2020, 2114, 123-142.	0.4	7
10	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
11	The Parallel Hydrodynamic Code for Astrophysical Flow with Stellar Equations of State. Communications in Computer and Information Science, 2019, , 414-426.	0.4	2
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	Performance Evaluation of the Intel Optane DC Memory With Scientific Benchmarks. , 2019, , .		7
14	A systematic study of minima in alanine dipeptide. Journal of Computational Chemistry, 2019, 40, 297-309.	1.5	25
15	An efficient MPI/OpenMP parallelization of the Hartreeâ€“Fockâ€“Roothaan method for the first generation of IntelÂ® Xeon Phiâ„¢ processor architecture. International Journal of High Performance Computing Applications, 2019, 33, 212-224.	2.4	16
16	Evaluation of Intel Memory Drive Technology Performance for Computational Astrophysics. Communications in Computer and Information Science, 2019, , 563-572.	0.4	0
17	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
18	Evaluation of Intel Memory Drive Technology Performance for Scientific Applications. , 2018, , .		4

#	Article	IF	Citations
19	PaSTRI: Error-Bounded Lossy Compression for Two-Electron Integrals in Quantum Chemistry. , 2018, , .		19
20	Modeling structure and excitation of biliverdin-binding domains in infrared fluorescent proteins. Chemical Physics Letters, 2018, 710, 59-63.	1.2	14
21	Power Measurements of Hartree-Fock Algorithms Using Different Storage Devices. , 2017, , .		3
22	An efficient MPI/openMP parallelization of the Hartree-Fock method for the second generation of Intel ^{Â®} Xeon Phi ^{â„¢} processor. , 2017, , .		8
23	High temperature coolant demonstrated for a computational cluster. , 2016, , .		3
24	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
25	Server Level Liquid Cooling: Do Higher System Temperatures Improve Energy Efficiency?. Supercomputing Frontiers and Innovations, 2016, 3, .	0.5	4
26	Why does mutation of <scp>G</scp>ln61 in Ras by the nitro analog <scp>NG</scp>ln maintain activity of <scp>R</scp>asâ€<scp>GAP</scp> in hydrolysis of guanosine triphosphate?. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2091-2099.	1.5	9
27	On Quantum Chemistry Code Adaptation for RSC PetaStream Architecture. Lecture Notes in Computer Science, 2015, , 113-121.	1.0	4
28	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
29	Role of Zwitterions in Kindling Fluorescent Protein Photochemistry. Journal of Physical Chemistry B, 2015, 119, 2467-2474.	1.2	8
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 Performance Characterization of the RSC PetaStream Module. Lecture Notes in Computer Science, 2014, , 420-429.	1.0	7
32	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
33	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
34	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
35	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
36	Conformational Partitioning in pH-Induced Fluorescence of the Kindling Fluorescent Protein (KFP). Journal of Physical Chemistry B, 2011, 115, 9195-9201.	1.2	12

#	Article	IF	Citations
37	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