Valera Veryazov

List of Publications by Year in descending order

55 papers	10,123 citations	218677 26 h-index	161849 54 g-index
64 all docs	64 docs citations	64 times ranked	6366 citing authors

#	Article	IF	Citations
1	MOLCAS: a program package for computational chemistry. Computational Materials Science, 2003, 28, 222-239.	3.0	1,689
2	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	3.3	1,485
3	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
4	Main Group Atoms and Dimers Studied with a New Relativistic ANO Basis Set. Journal of Physical Chemistry A, 2004, 108, 2851-2858.	2.5	1,200
5	New Relativistic ANO Basis Sets for Transition Metal Atoms. Journal of Physical Chemistry A, 2005, 109, 6575-6579.	2.5	938
6	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
7	New Relativistic Atomic Natural Orbital Basis Sets for Lanthanide Atoms with Applications to the Ce Diatom and LuF₃. Journal of Physical Chemistry A, 2008, 112, 11431-11435.	2.5	367
8	2MOLCAS as a development platform for quantum chemistry software. International Journal of Quantum Chemistry, 2004, 100, 626-635.	2.0	310
9	Relativistic atomic natural orbital type basis sets for the alkaline and alkaline-earth atoms applied to the ground-state potentials for the corresponding dimers. Theoretical Chemistry Accounts, 2004, 111, 345-351.	1.4	299
10	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
11	New relativistic ANO basis sets for actinide atoms. Chemical Physics Letters, 2005, 409, 295-299.	2.6	253
12	How to select active space for multiconfigurational quantum chemistry?. International Journal of Quantum Chemistry, 2011, 111, 3329-3338.	2.0	178
13	Not Innocent: Verdict from Ab Initio Multiconfigurational Second-Order Perturbation Theory on the Electronic Structure of Chloroiron Corrole. Journal of Physical Chemistry B, 2008, 112, 14099-14102.	2.6	87
14	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	2.8	84
15	MOLCASâ€"a software for multiconfigurational quantum chemistry calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 143-149.	14.6	66
16	Bond Length and Bond Order in One of the Shortest Crâ"Cr Bonds. Inorganic Chemistry, 2008, 47, 11455-11457.	4.0	64
17	Atomistic modeling of crystal structure of Ca 1.67 SiH x. Cement and Concrete Research, 2015, 67, 197-203.	11.0	63
18	How accurate is the CASPT2 method?. Physical Chemistry Chemical Physics, 2006, 8, 2727.	2.8	60

#	Article	IF	Citations
19	A theoretical study of singlet low-energy excited states of the benzene dimer. Chemical Physics Letters, 2006, 426, 268-272.	2.6	52
20	Potential Energy Surface of the Chromium Dimer Re-re-revisited with Multiconfigurational Perturbation Theory. Journal of Chemical Theory and Computation, 2016, 12, 1647-1655.	5.3	49
21	Quantum-chemical definition of the atomic valence in molecules and crystals. Theoretica Chimica Acta, 1991, 81, 95-103.	0.8	47
22	Hydration of trimethylamine-N-oxide and of dimethyldodecylamine-N-oxide: An ab initio study. Computational and Theoretical Chemistry, 2007, 808, 111-118.	1.5	35
23	Parallelization of a multiconfigurational perturbation theory. Journal of Computational Chemistry, 2013, 34, 1937-1948.	3.3	35
24	Local characteristics of crystal electronic structure in the Hartree-Fock method. Physics of the Solid State, 1999, 41, 1286-1290.	0.6	33
25	The ANO-R Basis Set. Journal of Chemical Theory and Computation, 2020, 16, 278-294.	5.3	31
26	A Combined Theoretical and Experimental Study of Simple Terminal Group 6 Nitride and Phosphide Nâ‰¡MX3 and Pâ‰¡MX3 Molecules. Journal of Physical Chemistry A, 2008, 112, 8030-8037.	2.5	27
27	Luscus: molecular viewer and editor for MOLCAS. Journal of Cheminformatics, 2015, 7, 16.	6.1	25
28	Investigation of the chemical bonding in nickel mixed oxides from electronic structure calculations. Journal of Physics and Chemistry of Solids, 1996, 57, 1839-1850.	4.0	23
29	Ab initio characterization of C5. Journal of Chemical Physics, 2007, 127, 154318.	3.0	23
30	Synthesis, spectroscopy and QM/MM simulations of a biomimetic ultrafast light-driven molecular motor. Photochemical and Photobiological Sciences, 2019, 18, 2259-2269.	2.9	23
31	Revised Atomistic Models of the Crystal Structure of Câ€“Sâ€“H with high C/S Ratio. Zeitschrift Fur Physikalische Chemie, 2016, 230, 1411-1424.	2.8	22
32	Analytical gradients of the second-order MÃ¸ller-Plesset energy using Cholesky decompositions. International Journal of Quantum Chemistry, 2014, 114, 321-327.	2.0	19
33	Is density functional theory accurate for lytic polysaccharide monooxygenase enzymes?. Dalton Transactions, 2020, 49, 1501-1512.	3.3	18
34	The Electronic Structure of Copper Oxide Crystalline Compounds. I. LUCâ€CNDO Approach to the Electronic Structure of Cu₂O and CuO Crystals. Physica Status Solidi (B): Basic Research, 1990, 157, 281-291.	1.5	17
35	The binatural orbitals of electronic transitions. Molecular Physics, 2012, 110, 2455-2464.	1.7	17
36	The Electronic Structure of Crystalline Lead Oxides. I. Crystal Structure and LUCâ€CNDO Calculations. Physica Status Solidi (B): Basic Research, 1991, 165, 401-410.	1.5	16

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37	The Electronic Structure of Copper Oxide Crystalline Compounds. II. Chemical Bonding in Copperâ€“Oxygen Crystals. Physica Status Solidi (B): Basic Research, 1990, 158, 201-212.	1.5	15
38	Electronic structure and chemical bonding in Bi₂O₃. Physica Status Solidi (B): Basic Research, 1994, 183, K15.	1.5	12
39	The electronic structure of crystalline nickel oxides. Journal of Electron Spectroscopy and Related Phenomena, 1994, 68, 555-563.	1.7	10
40	In Search of the Reason for the Breathing Effect of MIL53 Metal-Organic Framework: An ab Initio Multiconfigurational Study. Frontiers in Chemistry, 2017, 5, 111.	3.6	10
41	The Electronic Structure and the Chemical Bonding in NiO and La₂NiO₄ Crystals. A Comparison with CuO and La₂CuO₄. Physica Status Solidi (B): Basic Research, 1993, 179, 441-451.	1.5	9
42	Automatic procedure for generating symmetry adapted wavefunctions. Journal of Cheminformatics, 2017, 9, 8.	6.1	9
43	New compact density matrix averaged ANO basis sets for relativistic calculations. Journal of Chemical Physics, 2018, 149, 194102.	3.0	9
44	The dipeptide conformations of all twenty amino acid types in the context of biosynthesis. SpringerPlus, 2015, 4, 668.	1.2	7
45	The Electronic Structure of Crystalline Lead Oxides. II. Chemical Bonding in the Crystalline Lead Oxides. Physica Status Solidi (B): Basic Research, 1991, 165, 411-418.	1.5	6
46	The preferred conformation of dipeptides in the context of biosynthesis. Die Naturwissenschaften, 2013, 100, 853-859.	1.6	6
47	A program system for self-consistent embedded potentials for ionic crystals. Chemical Physics, 2022, 562, 111549.	1.9	5
48	Quantum chemical calculation of nickel and copper atomic valencies in crystalline oxides. International Journal of Quantum Chemistry, 1994, 52, 295-299.	2.0	4
49	Electronic Structure Investigation of Bulk ZnO and Its (1010) Surface. Physica Status Solidi (B): Basic Research, 1995, 189, K49.	1.5	4
50	A new module for constrained multiâ€fragment geometry optimization in internal coordinates implemented in the MOLCAS package. Journal of Computational Chemistry, 2013, 34, 2657-2665.	3.3	4
51	Benchmarking ANO-R basis set for multiconfigurational calculations. Electronic Structure, 2022, 4, 014009.	2.8	2
52	The electronic structure of negatively charged fullerenes: From monomers to dimers. AIP Conference Proceedings, 2017, , .	0.4	1
53	Simplifying the self-consistent procedure in crystal electronic-structure calculations. Journal of Structural Chemistry, 1988, 28, 810-810.	1.0	0
54	Multiscale study of crystal and electronic structure of Al defects in concrete. AIP Conference Proceedings, 2018, , .	0.4	0

#	Article	IF	Citations
55	Pyridine-cyanoanthracene bonded exciplex. AIP Conference Proceedings, 2019, , .	0.4	0