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	Benchmarking ANO-R basis set for multiconfigurational calculations. Electronic Structure, 2022, 4, 014009.	2.8	2
2	A program system for self-consistent embedded potentials for ionic crystals. Chemical Physics, 2022, 562, 111549.	1.9	5
3	Is density functional theory accurate for lytic polysaccharide monooxygenase enzymes?. Dalton Transactions, 2020, 49, 1501-1512.	3.3	18
4	The ANO-R Basis Set. Journal of Chemical Theory and Computation, 2020, 16, 278-294.	5.3	31
5	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
6	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
7	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
8	Pyridine-cyanoanthracene bonded exciplex. AIP Conference Proceedings, 2019, , .	0.4	0
9	New compact density matrix averaged ANO basis sets for relativistic calculations. Journal of Chemical Physics, 2018, 149, 194102.	3.0	9
10	Multiscale study of crystal and electronic structure of Al defects in concrete. AIP Conference Proceedings, 2018, , .	0.4	0
11	Automatic procedure for generating symmetry adapted wavefunctions. Journal of Cheminformatics, 2017, 9, 8.	6.1	9
12	The electronic structure of negatively charged fullerenes: From monomers to dimers. AIP Conference Proceedings, 2017, , .	0.4	1
13	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
14	<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
15	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
16	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
17	The dipeptide conformations of all twenty amino acid types in the context of biosynthesis. SpringerPlus, 2015, 4, 668.	1.2	7
18	Luscus: molecular viewer and editor for MOLCAS. Journal of Cheminformatics, 2015, 7, 16.	6.1	25

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19	Atomistic modeling of crystal structure of Ca 1.67 SiH x. Cement and Concrete Research, 2015, 67, 197-203.	11.0	63
20	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
21	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
22	MOLCASâ€"a software for multiconfigurational quantum chemistry calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 143-149.	14.6	66
23	Parallelization of a multiconfigurational perturbation theory. Journal of Computational Chemistry, 2013, 34, 1937-1948.	3.3	35
24	The preferred conformation of dipeptides in the context of biosynthesis. Die Naturwissenschaften, 2013, 100, 853-859.	1.6	6
25	The binatural orbitals of electronic transitions. Molecular Physics, 2012, 110, 2455-2464.	1.7	17
26	How to select active space for multiconfigurational quantum chemistry?. International Journal of Quantum Chemistry, 2011, 111, 3329-3338.	2.0	178
27	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	3.3	1,485
28	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	2.8	84
29	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
30	Bond Length and Bond Order in One of the Shortest Crâ''Cr Bonds. Inorganic Chemistry, 2008, 47, 11455-11457.	4.0	64
31	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
32	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
33	Ab initio characterization of C5. Journal of Chemical Physics, 2007, 127, 154318.	3.0	23
34	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
35	How accurate is the CASPT2 method?. Physical Chemistry Chemical Physics, 2006, 8, 2727.	2.8	60
36	A theoretical study of singlet low-energy excited states of the benzene dimer. Chemical Physics Letters, 2006, 426, 268-272.	2.6	52

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37	New relativistic ANO basis sets for actinide atoms. Chemical Physics Letters, 2005, 409, 295-299.	2.6	253
38	New Relativistic ANO Basis Sets for Transition Metal Atoms. Journal of Physical Chemistry A, 2005, 109, 6575-6579.	2.5	938
39	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
40	2MOLCAS as a development platform for quantum chemistry software. International Journal of Quantum Chemistry, 2004, 100, 626-635.	2.0	310
41	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
42	MOLCAS: a program package for computational chemistry. Computational Materials Science, 2003, 28, 222-239.	3.0	1,689
43	Local characteristics of crystal electronic structure in the Hartree-Fock method. Physics of the Solid State, 1999, 41, 1286-1290.	0.6	33
44	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
45	Electronic Structure Investigation of Bulk ZnO and Its (1010) Surface. Physica Status Solidi (B): Basic Research, 1995, 189, K49.	1.5	4
46	Quantum chemical calculation of nickel and copper atomic valencies in crystalline oxides. International Journal of Quantum Chemistry, 1994, 52, 295-299.	2.0	4
47	Electronic structure and chemical bonding in Bi₂O₃. Physica Status Solidi (B): Basic Research, 1994, 183, K15.	1.5	12
48	The electronic structure of crystalline nickel oxides. Journal of Electron Spectroscopy and Related Phenomena, 1994, 68, 555-563.	1.7	10
49	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
50	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
51	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
52	Quantum-chemical definition of the atomic valence in molecules and crystals. Theoretica Chimica Acta, 1991, 81, 95-103.	0.8	47
53	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
54	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

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55	Simplifying the self-consistent procedure in crystal electronic-structure calculations. Journal of Structural Chemistry, 1988, 28, 810-810.	1.0	0