# Valera Veryazov

List of Publications by Year
in descending order



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|---|---|---|---|
| 55 papers | 10,123 citations | 218381 26 h-index | 161609 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. | 1.4 | 1,689 |
| 2 | MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247. | 1.5 | 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. | 1.5 | 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. | 1.1 | 1,200 |
| 5 | New Relativistic ANO Basis Sets for Transition Metal Atoms. Journal of Physical Chemistry A, 2005, 109, 6575-6579. | 1.1 | 938 |
| 6 | OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964. | 2.3 | 661 |
| 7 | New Relativistic Atomic Natural Orbital Basis Sets for Lanthanide Atoms with Applications to the Ce Diatom and LuF<sub>3</sub>. Journal of Physical Chemistry A, 2008, 112, 11431-11435. | 1.1 | 367 |
| 8 | 2MOLCAS as a development platform for quantum chemistry software. International Journal of Quantum Chemistry, 2004, 100, 626-635. | 1.0 | 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. | 0.5 | 299 |
| 10 | Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117. | 1.2 | 281 |
| 11 | New relativistic ANO basis sets for actinide atoms. Chemical Physics Letters, 2005, 409, 295-299. | 1.2 | 253 |
| 12 | How to select active space for multiconfigurational quantum chemistry?. International Journal of Quantum Chemistry, 2011, 111, 3329-3338. | 1.0 | 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. | 1.2 | 87 |
| 14 | Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896. | 1.3 | 84 |
| 15 | MOLCASâ€"a software for multiconfigurational quantum chemistry calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 143-149. | 6.2 | 66 |
| 16 | Bond Length and Bond Order in One of the Shortest Crâ‚‚Cr Bonds. Inorganic Chemistry, 2008, 47, 11455-11457. | 1.9 | 64 |
| 17 | Atomistic modeling of crystal structure of Ca 1.67 SiH x. Cement and Concrete Research, 2015, 67, 197-203. | 4.6 | 63 |
| 18 | How accurate is the CASPT2 method?. Physical Chemistry Chemical Physics, 2006, 8, 2727. | 1.3 | 60 |

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|---|---|---|---|
| 19 | A theoretical study of singlet low-energy excited states of the benzene dimer. Chemical Physics Letters, 2006, 426, 268-272. | 1.2 | 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. | 2.3 | 49 |
| 21 | Quantum-chemical definition of the atomic valence in molecules and crystals. Theoretica Chimica Acta, 1991, 81, 95-103. | 0.9 | 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. | 1.5 | 35 |
| 24 | Local characteristics of crystal electronic structure in the Hartree-Fock method. Physics of the Solid State, 1999, 41, 1286-1290. | 0.2 | 33 |
| 25 | The ANO-R Basis Set. Journal of Chemical Theory and Computation, 2020, 16, 278-294. | 2.3 | 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. | 1.1 | 27 |
| 27 | Luscus: molecular viewer and editor for MOLCAS. Journal of Cheminformatics, 2015, 7, 16. | 2.8 | 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. | 1.9 | 23 |
| 29 | Ab initio characterization of C5. Journal of Chemical Physics, 2007, 127, 154318. | 1.2 | 23 |
| 30 | Synthesis, spectroscopy and QM/MM simulations of a biomimetic ultrafast light-driven molecular motor. Photochemical and Photobiological Sciences, 2019, 18, 2259-2269. | 1.6 | 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. | 1.4 | 22 |
| 32 | Analytical gradients of the second-order MÃ¸ller-Plesset energy using Cholesky decompositions. International Journal of Quantum Chemistry, 2014, 114, 321-327. | 1.0 | 19 |
| 33 | Is density functional theory accurate for lytic polysaccharide monooxygenase enzymes?. Dalton Transactions, 2020, 49, 1501-1512. | 1.6 | 18 |
| 34 | The Electronic Structure of Copper Oxide Crystalline Compounds. I. LUCâ€€NDO Approach to the Electronic Structure of Cu<sub>2</sub>O and CuO Crystals. Physica Status Solidi (B): Basic Research, 1990, 157, 281-291. | 0.7 | 17 |
| 35 | The binatural orbitals of electronic transitions. Molecular Physics, 2012, 110, 2455-2464. | 0.8 | 17 |
| 36 | The Electronic Structure of Crystalline Lead Oxides. I. Crystal Structure and LUCâ€€NDO Calculations. Physica Status Solidi (B): Basic Research, 1991, 165, 401-410. | 0.7 | 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. | 0.7 | 15 |
| 38 | Electronic structure and chemical bonding in Bi<sub>2</sub>O<sub>3</sub>. Physica Status Solidi (B): Basic Research, 1994, 183, K15. | 0.7 | 12 |
| 39 | The electronic structure of crystalline nickel oxides. Journal of Electron Spectroscopy and Related Phenomena, 1994, 68, 555-563. | 0.8 | 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. | 1.8 | 10 |
| 41 | The Electronic Structure and the Chemical Bonding in NiO and La<sub>2</sub>NiO<sub>4</sub> Crystals. A Comparison with CuO and La<sub>2</sub>CuO<sub>4</sub>. Physica Status Solidi (B): Basic Research, 1993, 179, 441-451. | 0.7 | 9 |
| 42 | Automatic procedure for generating symmetry adapted wavefunctions. Journal of Cheminformatics, 2017, 9, 8. | 2.8 | 9 |
| 43 | New compact density matrix averaged ANO basis sets for relativistic calculations. Journal of Chemical Physics, 2018, 149, 194102. | 1.2 | 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. | 0.7 | 6 |
| 46 | The preferred conformation of dipeptides in the context of biosynthesis. Die Naturwissenschaften, 2013, 100, 853-859. | 0.6 | 6 |
| 47 | A program system for self-consistent embedded potentials for ionic crystals. Chemical Physics, 2022, 562, 111549. | 0.9 | 5 |
| 48 | Quantum chemical calculation of nickel and copper atomic valencies in crystalline oxides. International Journal of Quantum Chemistry, 1994, 52, 295-299. | 1.0 | 4 |
| 49 | Electronic Structure Investigation of Bulk ZnO and Its (1010) Surface. Physica Status Solidi (B): Basic Research, 1995, 189, K49. | 0.7 | 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. | 1.5 | 4 |
| 51 | Benchmarking ANO-R basis set for multiconfigurational calculations. Electronic Structure, 2022, 4, 014009. | 1.0 | 2 |
| 52 | The electronic structure of negatively charged fullerenes: From monomers to dimers. AIP Conference Proceedings, 2017, , . | 0.3 | 1 |
| 53 | Simplifying the self-consistent procedure in crystal electronic-structure calculations. Journal of Structural Chemistry, 1988, 28, 810-810. | 0.3 | 0 |
| 54 | Multiscale study of crystal and electronic structure of Al defects in concrete. AIP Conference Proceedings, 2018, , . | 0.3 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Pyridine-cyanoanthracene bonded exciplex. AIP Conference Proceedings, 2019, , . | 0.3 | 0 |