Viktor N Staroverov

List of Publications by Year
in descending order

94	12,512	109137 35	38300 95
papers	citations	h-index	g-index

98	98	98	9578
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Climbing the Density Functional Ladder: Nonempirical Metaâ€“Generalized Gradient Approximation Designed for Molecules and Solids. Physical Review Letters, 2003, 91, 146401.	2.9	5,673
2	Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2003, 119, 12129-12137.	1.2	2,157
3	Prescription for the design and selection of density functional approximations: More constraint satisfaction with fewer fits. Journal of Chemical Physics, 2005, 123, 062201.	1.2	769
4	Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional. Journal of Chemical Physics, 2004, 120, 6898-6911.	1.2	431
5	Distribution of effectively unpaired electrons. Chemical Physics Letters, 2000, 330, 161-168.	1.2	197
6	Optimized effective potentials yielding Hartreeâ€“Fock energies and densities. Journal of Chemical Physics, 2006, 124, 141103.	1.2	175
7	Is the Hydrogen Bond in Water Dimer and Ice Covalent?. Journal of the American Chemical Society, 2000, 122, 1210-1214.	6.6	174
8	A Germanium(II)-Centered Dication. Journal of the American Chemical Society, 2007, 129, 15138-15139.	6.6	161
9	A Cryptand-Encapsulated Germanium(II) Dication. Science, 2008, 322, 1360-1363.	6.0	152
10	Diradical Character of the Cope Rearrangement Transition State. Journal of the American Chemical Society, 2000, 122, 186-187.	6.6	121
11	Exact-exchange energy density in the gauge of a semilocal density-functional approximation. Physical Review A, 2008, 77, .	1.0	104
12	Effect of Extended Ï€ Conjugation on the Spectroscopic and Electrochemical Properties of Boron Difluoride Formazanate Complexes. Journal of Organic Chemistry, 2015, 80, 5226-5235.	1.7	83
13	Effective local potentials for orbital-dependent density functionals. Journal of Chemical Physics, 2006, 125, 081104.	1.2	81
14	Transition Regions in the Cope Rearrangement of 1,5-Hexadiene and Its Cyano Derivatives. Journal of the American Chemical Society, 2000, 122, 7377-7385.	6.6	80
15	Band Gap Reduction in ZnO and ZnS by Creating Layered ZnO/ZnS Heterostructures. Journal of Physical Chemistry Letters, 2015, 6, 2075-2080.	2.1	75
16	Efficient electrochemiluminescence of a readily accessible boron difluoride formazanate dye. Chemical Communications, 2015, 51, 3766-3769.	2.2	75
17	How to tell when a model Kohnâ€“Sham potential is not a functional derivative. Journal of Chemical Physics, 2009, 131, 044107.	1.2	72
18	Assessment of simple exchange-correlation energy functionals of the one-particle density matrix. Journal of Chemical Physics, 2002, 117, 2489-2495.	1.2	62

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19	Structurally Tunable 3â€Cyanoformazanate Boron Difluoride Dyes. Chemistry - A European Journal, 2014, 20, 11340-11344.	1.7	61
20	Reduction of Electronic Wave Functions to Kohn-Sham Effective Potentials. Physical Review Letters, 2015, 115, 083001.	2.9	61
21	The Cope rearrangement in theoretical retrospect. Computational and Theoretical Chemistry, 2001, 573, 81-89.	1.5	55
22	Accurate and Efficient Approximation to the Optimized Effective Potential for Exchange. Physical Review Letters, 2013, 111, 013001.	2.9	51
23	Optimization of density matrix functionals by the Hartreeâ€“Fockâ€“Bogoliubov method. Journal of Chemical Physics, 2002, 117, 11107-11112.	1.2	43
24	Exact expressions for the Kohnâ€“Sham exchange-correlation potential in terms of wave-function-based quantities. Molecular Physics, 2016, 114, 1050-1058.	0.8	41
25	Reconstruction of Density Functionals from Kohnâ^'Sham Potentials by Integration along Density Scaling Paths. Journal of Chemical Theory and Computation, 2009, 5, 699-707.	2.3	40
26	Reactivity Studies of N-Heterocyclic Carbene Complexes of Germanium(II). Organometallics, 2010, 29, 4871-4881.	1.1	40
27	Kohnâ€“Sham exchange-correlation potentials from second-order reduced density matrices. Journal of Chemical Physics, 2015, 143, 244116.	1.2	40
28	Improved method for generating exchange-correlation potentials from electronic wave functions. Journal of Chemical Physics, 2017, 146, 084103.	1.2	38
29	Hierarchy of model Kohnâ€“Sham potentials for orbital-dependent functionals: A practical alternative to the optimized effective potential method. Journal of Chemical Physics, 2014, 140, 18A535.	1.2	37
30	Assessment of the Tao-Mo nonempirical semilocal density functional in applications to solids and surfaces. Physical Review B, 2017, 95, .	1.1	37
31	Average local ionization energy generalized to correlated wavefunctions. Journal of Chemical Physics, 2014, 141, 084107.	1.2	36
32	Monitoring and Understanding the Paraelectricâ€“Ferroelectric Phase Transition in the Metalâ€“Organic Framework [NH₄][M(HCOO)₃] by Solidâ€State NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 14348-14361.	1.7	36
33	Structurally Diverse Boronâ€“Nitrogen Heterocycles from an N₂O₂^{3â^'} Formazanate Ligand. Angewandte Chemie - International Edition, 2017, 56, 8173-8177.	7.2	36
34	The effective local potential method: Implementation for molecules and relation to approximate optimized effective potential techniques. Journal of Chemical Physics, 2007, 126, 084107.	1.2	35
35	Improved Electronic Excitation Energies from Shape-Corrected Semilocal Kohn-Sham Potentials. Physical Review Letters, 2012, 108, 253005.	2.9	35
36	The reduced model space method in multireference second-order perturbation theory. Chemical Physics Letters, 1998, 296, 435-444.	1.2	34

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37	Virial exchange energies from model exact-exchange potentials. Journal of Chemical Physics, 2008, 128, 204101.	1.2	34
38	A family of model Kohnâ€“Sham potentials for exact exchange. Journal of Chemical Physics, 2008, 129, 134103.	1.2	34
39	Removal of Basis-Set Artifacts in Kohnâ€“Sham Potentials Recovered from Electron Densities. Journal of Chemical Theory and Computation, 2013, 9, 3959-3964.	2.3	33
40	Origin of the step structure of molecular exchangeâ€“correlation potentials. Physical Chemistry Chemical Physics, 2016, 18, 20938-20944.	1.3	32
41	Efficient construction of exchange and correlation potentials by inverting the Kohnâ€“Sham equations. Journal of Chemical Physics, 2013, 139, 074112.	1.2	29
42	A density functional method for degenerate spin-multiplet components. Chemical Physics Letters, 2001, 340, 142-150.	1.2	28
43	Optoelectronic, Aggregation, and Redox Properties of Doubleâ€Rotor Boron Difluoride Hydrazone Dyes. Chemistry - A European Journal, 2019, 25, 5994-6006.	1.7	28
44	Charge densities for singlet and triplet electron pairs. International Journal of Quantum Chemistry, 2000, 77, 651-660.	1.0	27
45	Pressure-Induced Polymorphic Transitions in Crystalline Diborane Deduced by Comparison of Simulated and Experimental Vibrational Spectra. Journal of Physical Chemistry C, 2013, 117, 2210-2215.	1.5	27
46	Structural Tuning of Boron Difluoride Formazanate Electrochemiluminescence Mediated by Tri-n-propylamine. Journal of Physical Chemistry C, 2018, 122, 1258-1266.	1.5	27
47	Visualizing atomic sizes and molecular shapes with the classical turning surface of the Kohnâ€“Sham potential. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E11578-E11585.	3.3	27
48	Formazanate Complexes of Hypervalent Group 14 Elements as Precursors to Electronically Stabilized Radicals. Angewandte Chemie - International Edition, 2018, 57, 9870-9874.	7.2	26
49	Determination of Kohnâ€“Sham effective potentials from electron densities using the differential virial theorem. Journal of Chemical Physics, 2012, 137, 164113.	1.2	25
50	Performance of a nonempirical density functional on molecules and hydrogen-bonded complexes. Journal of Chemical Physics, 2016, 145, 234306.	1.2	25
51	Aluminum Complexes of N₂O₂^{3â€“} Formazanate Ligands Supported by Phosphine Oxide Donors. Inorganic Chemistry, 2017, 56, 12436-12447.	1.9	25
52	Searching for stable fullerenes in space with computational chemistry. Monthly Notices of the Royal Astronomical Society, 2019, 485, 1137-1146.	1.6	23
53	Exact exchange-correlation potentials of singlet two-electron systems. Journal of Chemical Physics, 2017, 147, 164117.	1.2	22
54	Electron distributions in radicals. International Journal of Quantum Chemistry, 2000, 77, 316-323.	1.0	20

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55	Self-consistent effective local potentials. Journal of Chemical Physics, 2007, 127, 084113.	1.2	20
56	Contracted SchrÃ¶dinger equation and Kohnâ€“Sham effective potentials. Molecular Physics, 2019, 117, 1-5.	0.8	20
57	Generalized average local ionization energy and its representations in terms of Dyson and energy orbitals. Journal of Chemical Physics, 2016, 145, 074113.	1.2	19
58	Oxoborane Formation Turns on Formazanateâ€Based Photoluminescence. Chemistry - A European Journal, 2019, 25, 11015-11019.	1.7	19
59	Energy expressions for Kohnâ€“Sham potentials and their relation to the Slaterâ€“Janak theorem. Journal of Chemical Physics, 2012, 136, 124115.	1.2	18
60	Assessment of a density functional with full exact exchange and balanced non-locality of correlation. Molecular Physics, 2009, 107, 1077-1088.	0.8	17
61	Self-interaction correction scheme for approximate Kohn-Sham potentials. Physical Review A, 2012, 86, .	1.0	17
62	Effective local potentials for excited states. Journal of Chemical Physics, 2010, 133, 244104.	1.2	16
63	Two electrons in a cylindrical box: An exact configuration-interaction solution. Physical Review A, 2010, 81, .	1.0	15
64	Communication: Explicit construction of functional derivatives in potential-driven density-functional theory. Journal of Chemical Physics, 2010, 133, 101104.	1.2	15
65	Response to â€œComment on â€˜Kohnâ€“Sham exchange-correlation potentials from second-order reduced density matricesâ€™â€•[J. Chem. Phys. 145, 037101 (2016)]. Journal of Chemical Physics, 2016, 145, 037102.	1.2	15
66	Meta-Substituted Thienyl Benzenes: A Comparative Synthetic, Structural and Computational Study. Journal of Organic Chemistry, 2009, 74, 530-544.	1.7	14
67	Construction of integrable model Kohn-Sham potentials by analysis of the structure of functional derivatives. Physical Review A, 2011, 83, .	1.0	14
68	Cationic Boron Formazanate Dyes**. Angewandte Chemie - International Edition, 2021, 60, 5152-5156.	7.2	14
69	A generalized gradient approximation for exchange derived from the model potential of van Leeuwen and Baerends. Journal of Chemical Physics, 2012, 136, 064116.	1.2	13
70	Interelectron magnetic coupling in electrides with one-dimensional cavity-channel geometry. Physical Chemistry Chemical Physics, 2011, 13, 21615.	1.3	11
71	Structurally Diverse Boronâ€“Nitrogen Heterocycles from an N₂O₂^{3â^’} Formazanate Ligand. Angewandte Chemie, 2017, 129, 8285-8289.	1.6	11
72	Nearâ€Infrared Boron Difluoride Formazanate Dyes. Chemistry - A European Journal, 2021, 27, 2854-2860.	1.7	11

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73	Optoelectronic Properties of Carbonâ€Bound Boron Difluoride Hydrazone Dimers. Chemistry - A European Journal, 2020, 26, 5522-5529.	1.7	10
74	X-ray Absorption Near-Edge Structure Spectroscopy of a Stable 6-Oxoverdazyl Radical and Its Diamagnetic Precursor. Journal of Physical Chemistry A, 2019, 123, 323-328.	1.1	9
75	Solution of the SchrÃ¶dinger equation for two electrons in axially symmetric cavities. Physical Review A, 2010, 82, .	1.0	7
76	Polymorphic transitions of diborane at sub- and near-megabar pressures. Scientific Reports, 2015, 5, 13929.	1.6	7
77	Construction of Fermi Potentials from Electronic Wave Functions. Journal of Chemical Theory and Computation, 2018, 14, 4246-4253.	2.3	7
78	What Is the Accuracy Limit of Adiabatic Linear-Response TDDFT Using Exact Exchangeâ€“Correlation Potentials and Approximate Kernels?. Journal of Chemical Theory and Computation, 2019, 15, 4956-4964.	2.3	7
79	Complete-active-space extended Koopmans theorem method. Journal of Chemical Physics, 2021, 155, 051102.	1.2	7
80	Elimination of Spurious Fractional Charges in Dissociating Molecules by Correcting the Shape of Approximate Kohnâ€“Sham Potentials. Journal of Chemical Theory and Computation, 2016, 12, 5361-5366.	2.3	6
81	Formazanate Complexes of Hypervalent Group 14 Elements as Precursors to Electronically Stabilized Radicals. Angewandte Chemie, 2018, 130, 10018-10022.	1.6	6
82	Unified construction of Fermi, Pauli and exchange-correlation potentials. Advances in Quantum Chemistry, 2019, , 201-219.	0.4	6
83	Asymptotic behavior of the average local ionization energy in finite basis sets. Journal of Chemical Physics, 2020, 153, 134109.	1.2	6
84	Pressure-Induced Polymorphic Transformations of Ethylenediamine Bisborane. Journal of Physical Chemistry C, 2021, 125, 18614-18622.	1.5	6
85	Exact relations between the electron density and external potential for systems of interacting and noninteracting electrons. International Journal of Quantum Chemistry, 2013, 113, 1626-1632.	1.0	5
86	Effects of Dispersion Corrections and Nonlocality on Density Functional Predictions of Pressure-Induced Polymorphic Transitions of Crystalline Diborane. Journal of Physical Chemistry C, 2018, 122, 14781-14787.	1.5	5
87	First Ionization Energy as the Asymptotic Limit of the Average Local Electron Energy. Journal of Chemical Theory and Computation, 2020, 16, 6886-6893.	2.3	5
88	A strongly Lewis-acidic and fluorescent borenium cation supported by a tridentate formazanate ligand. Chemical Communications, 2021, 57, 9530-9533.	2.2	5
89	Modified Slater exchange potential with correct uniform electron gas limit. Canadian Journal of Chemistry, 2015, 93, 91-97.	0.6	3
90	Cationic Boron Formazanate Dyes**. Angewandte Chemie, 2021, 133, 5212-5216.	1.6	2

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91	Accurate explicitly correlated wave functions for two electrons in a square. Journal of Chemical Physics, 2011, 135, 014106.	1.2	1
92	Do fractionally incremented nuclear charges improve time-dependent density functional theory excitation energies as reliably as fractional orbital populations?. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	1
93	Uniform electron gas limit of an exact expression for the Kohnâ€“Sham exchange-correlation potential. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	1
94	Frontispiece: Monitoring and Understanding the Paraelectric-Ferroelectric Phase Transition in the Metal-Organic Framework [NH4][M(HCOO)3] by Solid-State NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, n/a-n/a.	1.7	0