

Sergey A Varganov

List of Publications by Citations

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49
papers

1,174
citations

19
h-index

33
g-index

55
ext. papers

1,317
ext. citations

4.4
avg, IF

4.51
L-index

#	Paper	IF	Citations
49	Where does the planar-to-nonplanar turnover occur in small gold clusters?. <i>Journal of the American Chemical Society</i> , 2005 , 127, 1049-52	16.4	198
48	The interaction of oxygen with small gold clusters. <i>Journal of Chemical Physics</i> , 2003 , 119, 2531-2537	3.9	113
47	A study of the reactions of molecular hydrogen with small gold clusters. <i>Journal of Chemical Physics</i> , 2004 , 120, 5169-75	3.9	90
46	Chiral Peropyrene: Synthesis, Structure, and Properties. <i>Journal of the American Chemical Society</i> , 2017 , 139, 13102-13109	16.4	75
45	Multireference second-order perturbation theory: how size consistent is "almost size consistent". <i>Journal of Chemical Physics</i> , 2005 , 122, 44105	3.9	68
44	Septulene: the heptagonal homologue of kekulene. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 12795-800	16.4	54
43	Nonadiabatic transition state theory: Application to intersystem crossings in the active sites of metal-sulfur proteins. <i>International Journal of Quantum Chemistry</i> , 2016 , 116, 750-761	2.1	51
42	Ab Initio Multiple Spawning Method for Intersystem Crossing Dynamics: Spin-Forbidden Transitions between (3)B1 and (1)A1 States of GeH2. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 2911-9	2.8	44
41	3D Printed Potential and Free Energy Surfaces for Teaching Fundamental Concepts in Physical Chemistry. <i>Journal of Chemical Education</i> , 2015 , 92, 2106-2112	2.4	33
40	Nonadiabatic transition state theory and trajectory surface hopping dynamics: intersystem crossing between (3)B1 and (1)A1 states of SiH2. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1332-8	2.8	33
39	Variational geminal-augmented multireference self-consistent field theory: two-electron systems. <i>Journal of Chemical Physics</i> , 2010 , 132, 054103	3.9	29
38	Interfacing the Ab initio multiple spawning method with electronic structure methods in GAMESS: Photodecay of trans-azomethane. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 10902-8	2.8	25
37	Resolutions of the Coulomb operator. <i>Journal of Chemical Physics</i> , 2008 , 128, 201104	3.9	25
36	Lactate Racemase Nickel-Pincer Cofactor Operates by a Proton-Coupled Hydride Transfer Mechanism. <i>Biochemistry</i> , 2018 , 57, 3244-3251	3.2	23
35	Protein induced singlet-triplet quasidegeneracy in the active site of [NiFe]-hydrogenase. <i>Chemical Physics Letters</i> , 2013 , 577, 138-141	2.5	22
34	Predicting Intersystem Crossing Rates with AIMS-DFT Molecular Dynamics. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 3480-3488	2.8	21
33	Accurate potential energy, dipole moment curves, and lifetimes of vibrational states of heteronuclear alkali dimers. <i>Journal of Chemical Physics</i> , 2014 , 140, 184315	3.9	21

32	Effect of H ₂ binding on the nonadiabatic transition probability between singlet and triplet states of the [NiFe]-hydrogenase active site. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1066-73	2.8	20
31	In Silico Molecular Engineering of Dysprosocenium-Based Complexes to Decouple Spin Energy Levels from Molecular Vibrations. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 7678-7683	6.4	20
30	A study of the isomers of C ₃₆ fullerene using single and multireference MP2 perturbation theory. <i>Chemical Physics Letters</i> , 2002 , 362, 380-386	2.5	19
29	Intersystem crossing in tunneling regime: T- τ s relaxation in thiophosgene. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 5500-5508	3.6	15
28	Septulene: The Heptagonal Homologue of Kekulene. <i>Angewandte Chemie</i> , 2012 , 124, 12967-12972	3.6	14
27	Reply to a comment: oxygen adsorption on Au clusters by W.T. Wallace, A.J. Leavitt, and R.J. Whetten. <i>Chemical Physics Letters</i> , 2003 , 368, 778-779	2.5	14
26	Electronic Transitions Responsible for C Diffuse Interstellar Bands. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 115-120	6.4	14
25	Fluorescence and photoinduced proton transfer in the protolytic forms of fluorescein: Experimental and computational study. <i>Dyes and Pigments</i> , 2020 , 173, 107851	4.6	12
24	SPIN-FORBIDDEN AND SPIN-ALLOWED CYCLOPROPENONE (c-H ₂ C ₃ O) FORMATION IN INTERSTELLAR MEDIUM. <i>Astrophysical Journal</i> , 2014 , 795, 173	4.7	10
23	A complex of ceftriaxone with Pb(II): synthesis, characterization, and antibacterial activity study. <i>Journal of Coordination Chemistry</i> , 2014 , 67, 2783-2794	1.6	9
22	Possible scheme of synthesis-assembling of fullerenes. <i>Physics of the Solid State</i> , 2001 , 43, 973-981	0.8	9
21	Full Visible Spectrum and White Light Emission with a Single, Input-Tunable Organic Fluorophore. <i>Journal of the American Chemical Society</i> , 2020 ,	16.4	9
20	Ab initio calculations of spectroscopic constants and vibrational state lifetimes of diatomic alkali-alkaline-earth cations. <i>Journal of Chemical Physics</i> , 2017 , 147, 124304	3.9	8
19	Locating Minimum Energy Crossings of Different Spin States Using the Fragment Molecular Orbital Method. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6074-6084	6.4	8
18	The binding of the noble metal cations Au ⁺ and Ag ⁺ to propene. <i>Chemical Physics Letters</i> , 2005 , 412, 416-419	2.5	8
17	Effects of strong electron correlations in Ti ₈ C ₁₂ Met-Car. <i>Chemical Physics</i> , 2006 , 326, 97-106	2.3	7
16	Modeling Spin-Crossover Dynamics. <i>Annual Review of Physical Chemistry</i> , 2021 , 72, 515-540	15.7	7
15	Spin-Forbidden Transitions between Electronic States in the Active Site of Rubredoxin. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 8691-8698	2.8	6

14	Predicted IR spectra of Ti ₈ C ₁₂ and Ti ₈ C ₁₂ +. <i>Chemical Physics Letters</i> , 2006 , 429, 49-51	2.5	6
13	Scalable correlated electronic structure theory. <i>Journal of Physics: Conference Series</i> , 2006 , 46, 229-233	0.3	5
12	Enhanced spin coherence of rubidium atoms in solid parahydrogen. <i>Physical Review B</i> , 2019 , 100,	3.3	5
11	Theoretical study of the toroidal forms of carbon and related endohedral complexes with lithium. <i>Physics of the Solid State</i> , 2001 , 43, 1982	0.8	4
10	Spin coherence and optical properties of alkali-metal atoms in solid parahydrogen. <i>Physical Review A</i> , 2019 , 100,	2.6	4
9	A generalized Poisson equation and short-range self-interaction energies. <i>Journal of Chemical Physics</i> , 2008 , 128, 241101	3.9	3
8	Ab initio Calculations of the endo- and exohedral complexes of fullerene C ₆₀ with Zn atoms. <i>Journal of Structural Chemistry</i> , 2000 , 41, 687-691	0.9	3
7	Intersystem crossing and internal conversion dynamics with GAUSS-TeraChem: Excited state relaxation in 2-cyclopentenone. <i>Journal of Chemical Physics</i> , 2021 , 155, 174107	3.9	3
6	Spin controlled surface chemistry: alkyl desorption from Si(100)-2x1 by nonadiabatic hydrogen elimination. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 16641-16647	3.6	2
5	Reaction Mechanisms of Anisole Pyrolysis at Different Temperatures: Experimental and Theoretical Studies. <i>Energy & Fuels</i> , 2021 , 35, 9994-10008	4.1	2
4	NAST: Nonadiabatic Statistical Theory Package for Predicting Kinetics of Spin-Dependent Processes.. <i>Topics in Current Chemistry</i> , 2022 , 380, 15	7.2	2
3	Static polarization of the supramolecular dyads of fullerene C ₆₀ with porphyrin derivatives. <i>Journal of Porphyrins and Phthalocyanines</i> , 2015 , 19, 838-844	1.8	1
2	Innenstruktur: Septulene: The Heptagonal Homologue of Kekulene (Angew. Chem. 51/2012). <i>Angewandte Chemie</i> , 2012 , 124, 13071-13071	3.6	
1	NAST: Nonadiabatic Statistical Theory Package for Predicting Kinetics of Spin-Dependent Processes. <i>Topics in Current Chemistry Collections</i> , 2022 , 79-103	1.8	