Sergey A Varganov

List of Publications by Year in Descending Order

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	NAST: Nonadiabatic Statistical Theory Package for Predicting Kinetics of Spin-Dependent Processes.. *Topics in Current Chemistry*, **2022**, 380, 15	7.2	2
48	NAST: Nonadiabatic Statistical Theory Package for Predicting Kinetics of Spin-Dependent Processes. *Topics in Current Chemistry Collections*, **2022**, 79-103	1.8	
47	Intersystem crossing and internal conversion dynamics with GAIMS-TeraChem: Excited state relaxation in 2-cyclopentenone. *Journal of Chemical Physics*, **2021**, 155, 174107	3.9	3
46	Modeling Spin-Crossover Dynamics. *Annual Review of Physical Chemistry*, **2021**, 72, 515-540	15.7	7
45	Reaction Mechanisms of Anisole Pyrolysis at Different Temperatures: Experimental and Theoretical Studies. *Energy & Fuels*, **2021**, 35, 9994-10008	4.1	2
44	Intersystem crossing in tunneling regime: T -nS relaxation in thiophosgene. *Physical Chemistry Chemical Physics*, **2020**, 22, 5500-5508	3.6	15
43	Spin controlled surface chemistry: alkyl desorption from Si(100)-2□ by nonadiabatic hydrogen elimination. *Physical Chemistry Chemical Physics*, **2020**, 22, 16641-16647	3.6	2
42	Full Visible Spectrum and White Light Emission with a Single, Input-Tunable Organic Fluorophore. *Journal of the American Chemical Society*, **2020**,	16.4	9
41	Fluorescence and photoinduced proton transfer in the protolytic forms of fluorescein: Experimental and computational study. *Dyes and Pigments*, **2020**, 173, 107851	4.6	12
40	Locating Minimum Energy Crossings of Different Spin States Using the Fragment Molecular Orbital Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 6074-6084	6.4	8
39	Enhanced spin coherence of rubidium atoms in solid parahydrogen. *Physical Review B*, **2019**, 100,	3.3	5
38	In Silico Molecular Engineering of Dysprosocenium-Based Complexes to Decouple Spin Energy Levels from Molecular Vibrations. *Journal of Physical Chemistry Letters*, **2019**, 10, 7678-7683	6.4	20
37	Spin coherence and optical properties of alkali-metal atoms in solid parahydrogen. *Physical Review A*, **2019**, 100,	2.6	4
36	Electronic Transitions Responsible for C Diffuse Interstellar Bands. *Journal of Physical Chemistry Letters*, **2019**, 10, 115-120	6.4	14
35	Lactate Racemase Nickel-Pincer Cofactor Operates by a Proton-Coupled Hydride Transfer Mechanism. *Biochemistry*, **2018**, 57, 3244-3251	3.2	23
34	Predicting Intersystem Crossing Rates with AIMS-DFT Molecular Dynamics. *Journal of Physical Chemistry A*, **2018**, 122, 3480-3488	2.8	21
33	Ab initio calculations of spectroscopic constants and vibrational state lifetimes of diatomic alkali-alkaline-earth cations. *Journal of Chemical Physics*, **2017**, 147, 124304	3.9	8

32	Chiral Peropyrene: Synthesis, Structure, and Properties. *Journal of the American Chemical Society*, **2017**, 139, 13102-13109	16.4	75
31	Spin-Forbidden Transitions between Electronic States in the Active Site of Rubredoxin. *Journal of Physical Chemistry A*, **2016**, 120, 8691-8698	2.8	6
30	Nonadiabatic transition state theory: Application to intersystem crossings in the active sites of metal-sulfur proteins. *International Journal of Quantum Chemistry*, **2016**, 116, 750-761	2.1	51
29	Ab Initio Multiple Spawning Method for Intersystem Crossing Dynamics: Spin-Forbidden Transitions between (3)B1 and (1)A1 States of GeH2. *Journal of Physical Chemistry A*, **2016**, 120, 2911-9	2.8	44
28	Static polarization of the supramolecular dyads of fullerene C60 with porphyrin derivatives. *Journal of Porphyrins and Phthalocyanines*, **2015**, 19, 838-844	1.8	1
27	3D Printed Potential and Free Energy Surfaces for Teaching Fundamental Concepts in Physical Chemistry. *Journal of Chemical Education*, **2015**, 92, 2106-2112	2.4	33
26	Effect of H2 binding on the nonadiabatic transition probability between singlet and triplet states of the [NiFe]-hydrogenase active site. *Journal of Physical Chemistry A*, **2015**, 119, 1066-73	2.8	20
25	Nonadiabatic transition state theory and trajectory surface hopping dynamics: intersystem crossing between (3)B1 and (1)A1 states of SiH2. *Journal of Physical Chemistry A*, **2015**, 119, 1332-8	2.8	33
24	Accurate potential energy, dipole moment curves, and lifetimes of vibrational states of heteronuclear alkali dimers. *Journal of Chemical Physics*, **2014**, 140, 184315	3.9	21
23	A complex of ceftriaxone with Pb(II): synthesis, characterization, and antibacterial activity study. *Journal of Coordination Chemistry*, **2014**, 67, 2783-2794	1.6	9
22	SPIN-FORBIDDEN AND SPIN-ALLOWED CYCLOPROPENONE (c-H2C3O) FORMATION IN INTERSTELLAR MEDIUM. *Astrophysical Journal*, **2014**, 795, 173	4.7	10
21	Interfacing the Ab initio multiple spawning method with electronic structure methods in GAMESS: Photodecay of trans-azomethane. *Journal of Physical Chemistry A*, **2014**, 118, 10902-8	2.8	25
20	Protein induced singlet–triplet quasidegeneracy in the active site of [NiFe]-hydrogenase. *Chemical Physics Letters*, **2013**, 577, 138-141	2.5	22
19	Septulene: the heptagonal homologue of kekulene. *Angewandte Chemie - International Edition*, **2012**, 51, 12795-800	16.4	54
18	Septulene: The Heptagonal Homologue of Kekulene. *Angewandte Chemie*, **2012**, 124, 12967-12972	3.6	14
17	Innenrücktitelbild: Septulene: The Heptagonal Homologue of Kekulene (Angew. Chem. 51/2012). *Angewandte Chemie*, **2012**, 124, 13071-13071	3.6	
16	Variational geminal-augmented multireference self-consistent field theory: two-electron systems. *Journal of Chemical Physics*, **2010**, 132, 054103	3.9	29
15	Resolutions of the Coulomb operator. *Journal of Chemical Physics*, **2008**, 128, 201104	3.9	25

14	A generalized Poisson equation and short-range self-interaction energies. *Journal of Chemical Physics*, **2008**, 128, 241101	3.9	3
13	Scalable correlated electronic structure theory. *Journal of Physics: Conference Series*, **2006**, 46, 229-233	0.3	5
12	Effects of strong electron correlations in Ti8C12 Met-Car. *Chemical Physics*, **2006**, 326, 97-106	2.3	7
11	Predicted IR spectra of Ti8C12 and Ti8C12+. *Chemical Physics Letters*, **2006**, 429, 49-51	2.5	6
10	Where does the planar-to-nonplanar turnover occur in small gold clusters?. *Journal of the American Chemical Society*, **2005**, 127, 1049-52	16.4	198
9	The binding of the noble metal cations Au+ and Ag+ to propene. *Chemical Physics Letters*, **2005**, 412, 416-419	2.5	8
8	Multireference second-order perturbation theory: how size consistent is "almost size consistent". *Journal of Chemical Physics*, **2005**, 122, 44105	3.9	68
7	A study of the reactions of molecular hydrogen with small gold clusters. *Journal of Chemical Physics* , **2004**, 120, 5169-75	3.9	90
6	Reply to a comment: oxygen adsorption on Au clusters by W.T. Wallace, A.J. Leavitt, and R.J. Whetten. *Chemical Physics Letters*, **2003**, 368, 778-779	2.5	14
5	The interaction of oxygen with small gold clusters. *Journal of Chemical Physics*, **2003**, 119, 2531-2537	3.9	113
4	A study of the isomers of C36 fullerene using single and multireference MP2 perturbation theory. *Chemical Physics Letters*, **2002**, 362, 380-386	2.5	19
3	Possible scheme of synthesis-assembling of fullerenes. *Physics of the Solid State*, **2001**, 43, 973-981	0.8	9
2	Theoretical study of the toroidal forms of carbon and related endohedral complexes with lithium. *Physics of the Solid State*, **2001**, 43, 1982	0.8	4
1	Ab initio Calculations of the endo- and exohedral complexes of fullerene C60 with Zn atoms. *Journal of Structural Chemistry*, **2000**, 41, 687-691	0.9	3