Sergey I Bokarev

List of Publications by Year in descending order

58	1,851	304743	265206
papers	citations	22 h-index	42 g-index

68	68	68	2161
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	RhoDyn: A Ï•TD-RASCI Framework to Study Ultrafast Electron Dynamics in Molecules. Journal of Chemical Theory and Computation, 2022, 18, 46-58.	5.3	7
2	Probing the molecular structure of aqueous triiodide via X-ray photoelectron spectroscopy and correlated electron phenomena. Physical Chemistry Chemical Physics, 2022, 24, 15540-15555.	2.8	4
3	Multireference Approach to Normal and Resonant Auger Spectra Based on the One-Center Approximation. Journal of Chemical Theory and Computation, 2022, 18, 4387-4407.	5.3	9
4	Distinct photodynamics of Îº-N and Îº-C pseudoisomeric iron(<scp>ii</scp>) complexes. Chemical Communications, 2021, 57, 6640-6643.	4.1	23
5	Siteâ€Selective Realâ€Time Observation of Bimolecular Electron Transfer in a Photocatalytic System Using Lâ€Edge Xâ€Ray Absorption Spectroscopy**. ChemPhysChem, 2021, 22, 693-700.	2.1	5
6	2p x-ray absorption spectroscopy of 3d transition metal systems. Journal of Electron Spectroscopy and Related Phenomena, 2021, 249, 147061.	1.7	44
7	Theoretical Xâ€ray spectroscopy of transition metal compounds. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1433.	14.6	44
8	Effect of chemical structure on the ultrafast spin dynamics in core-excited states. Journal of Chemical Physics, 2020, 153, 044304.	3.0	3
9	The effect of N-heterocyclic carbene units on the absorption spectra of Fe(<scp>ii</scp>) complexes: a challenge for theory. Physical Chemistry Chemical Physics, 2020, 22, 27605-27616.	2.8	8
10	Intersystem Crossing and Triplet Dynamics in an Iron(II) N-Heterocyclic Carbene Photosensitizer. Inorganic Chemistry, 2020, 59, 14666-14678.	4.0	23
11	Ground- and Excited-State Properties of Iron(II) Complexes Linked to Organic Chromophores. Inorganic Chemistry, 2020, 59, 14746-14761.	4.0	28
12	Solvation and speciation of cobalt(II). A theoretical X-ray absorption and RIXS study. Chemical Physics, 2020, 532, 110681.	1.9	5
13	Multi-reference protocol for (auto)ionization spectra: Application to molecules. Journal of Chemical Physics, 2020, 152, 074108.	3.0	16
14	Multireference quantum chemistry protocol for simulating autoionization spectra: Test of ionization continuum models for the neon atom. Physical Review A, 2019, 100, .	2.5	14
15	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
16	Quasi-classical approaches to vibronic spectra revisited. Journal of Chemical Physics, 2018, 148, 102337.	3.0	15
17	Simulating vibronic spectra via Matsubara-like dynamics: Coping with the sign problem. Journal of Chemical Physics, 2018, 149, 194103.	3.0	10
18	Effective quenching and excited-state relaxation of a Cu(I) photosensitizer addressed by time-resolved spectroscopy and TDDFT calculations. Chemical Physics, 2018, 515, 557-563.	1.9	9

#	Article	IF	Citations
19	Tuned Range-Separated Density Functional Theory and Dyson Orbital Formalism for Photoelectron Spectra. Journal of Chemical Theory and Computation, 2018, 14, 5870-5880.	5.3	13
20	Photoelectron shake-ups as a probe of molecular symmetry: 4d XPS analysis of I₃^{â”} in solution. Physical Chemistry Chemical Physics, 2018, 20, 19916-19921.	2.8	7
21	Ultrafast dissipative spin-state dynamics triggered by x-ray pulse trains. Physical Review A, 2018, 98, .	2.5	9
22	Ultrafast Spin-State Dynamics in Transition-Metal Complexes Triggered by Soft-X-Ray Light. Physical Review Letters, 2017, 118, 023001.	7.8	11
23	Nuclear Dynamical Correlation Effects in X-ray Spectroscopy from a Theoretical Time-Domain Perspective. Journal of Physical Chemistry Letters, 2017, 8, 992-996.	4.6	6
24	Density matrix-based time-dependent configuration interaction approach to ultrafast spin-flip dynamics. Molecular Physics, 2017, 115, 1898-1907.	1.7	8
25	Soft X-ray spectroscopy of transition metal compounds: a theoretical perspective. EPJ Web of Conferences, 2017, 132, 02004.	0.3	1
26	Light-induced relaxation dynamics of the ferricyanide ion revisited by ultrafast XUV photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 14248-14255.	2.8	28
27	Ultrafast Spin Crossover in [Fe^{II}(bpy)₃]²⁺: Revealing Two Competing Mechanisms by Extreme Ultraviolet Photoemission Spectroscopy. ChemPhysChem, 2017, 18, 465-469.	2.1	30
28	A time-correlation function approach to nuclear dynamical effects in X-ray spectroscopy. Journal of Chemical Physics, 2017, 146, 224203.	3.0	5
29	Ultrafast kinetics of linkage isomerism in Na2[Fe(CN)5NO] aqueous solution revealed by time-resolved photoelectron spectroscopy. Structural Dynamics, 2017, 4, 044031.	2.3	9
30	Chemical Tuning and Absorption Properties of Iridium Photosensitizers for Photocatalytic Applications. Inorganics, 2017, 5, 23.	2.7	10
31	Mapping Long-Lived Dark States in Copper Porphyrin Nanostructures. Journal of Physical Chemistry C, 2016, 120, 16977-16984.	3.1	5
32	Joint Analysis of Radiative and Non-Radiative Electronic Relaxation Upon X-ray Irradiation of Transition Metal Aqueous Solutions. Scientific Reports, 2016, 6, 24659.	3.3	38
33	Towards an ab initio theory for metal L-edge soft X-ray spectroscopy of molecular aggregates. Structural Dynamics, 2016, 3, 062601.	2.3	30
34	Mechanistic Study of Photocatalytic Hydrogen Generation with Simple Iron Carbonyls as Water Reduction Catalysts. ChemCatChem, 2016, 8, 404-411.	3.7	16
35	Multi-reference approach to the calculation of photoelectron spectra including spin-orbit coupling. Journal of Chemical Physics, 2015, 143, 074104.	3.0	48
36	Tuning Range-Separated Density Functional Theory for Photocatalytic Water Splitting Systems. Journal of Chemical Theory and Computation, 2015, 11, 1700-1709.	5.3	64

#	Article	IF	Citations
37	Quantum chemical study of the electronic properties of an Iridium-based photosensitizer bound to medium-sized silver clusters. Chemical Physics, 2015, 457, 1-6.	1.9	4
38	A theoretical perspective on charge transfer in photocatalysis. The example of Ir-based systems. Coordination Chemistry Reviews, 2015, 304-305, 133-145.	18.8	43
39	Unraveling the Electronic Structure of Photocatalytic Manganese Complexes by L-Edge X-ray Spectroscopy. Journal of Physical Chemistry C, 2015, 119, 19192-19200.	3.1	40
40	BokarevetÂal.Reply. Physical Review Letters, 2014, 112, 129303.	7.8	5
41	Chemical Bonding in Aqueous Ferrocyanide: Experimental and Theoretical X-ray Spectroscopic Study. Journal of Physical Chemistry B, 2014, 118, 1555-1563.	2.6	61
42	DFT-D investigation of the interaction between Ir (III) based photosensitizers and small silver clusters Agn (n=2â€“20,92). Chemical Physics, 2014, 435, 40-48.	1.9	10
43	Spin density distribution after electron transfer from triethylamine to an [Ir(ppy)2(bpy)]+ photosensitizer during photocatalytic water reduction. Physical Chemistry Chemical Physics, 2014, 16, 4789.	2.8	40
44	Electron- and Energy-Transfer Processes in a Photocatalytic System Based on an Ir(III)-Photosensitizer and an Iron Catalyst. Journal of Physical Chemistry Letters, 2014, 5, 1355-1360.	4.6	44
45	Direct Observation of Molecular Orbital Mixing in a Solvated Organometallic Complex. Angewandte Chemie - International Edition, 2013, 52, 9841-9844.	13.8	60
46	State-Dependent Electron Delocalization Dynamics at the Solute-Solvent Interface: Soft-X-Ray Absorption Spectroscopy andAbÂInitioCalculations. Physical Review Letters, 2013, 111, 083002.	7.8	74
47	Nature of the Chemical Bond of Aqueous Fe2+ Probed by Soft X-ray Spectroscopies and ab Initio Calculations. Journal of Physical Chemistry B, 2013, 117, 12613-12618.	2.6	44
48	Electronic excitation spectrum of the photosensitizer [Ir(ppy)2(bpy)]+. Journal of Chemical Physics, 2012, 136, 214305.	3.0	37
49	Electronic excitation spectra of the [Ir(ppy)2(bpy)]+ photosensitizer bound to small silver clusters Agn (n = 1â€“6). Physical Chemistry Chemical Physics, 2012, 14, 4977.	2.8	6
50	Vibronic spectra, ab initio calculations, and structures of conformationally non-rigid molecules of oxalyl halides in the ground and lowest excited electronic states â€“ Part VI: Oxalyl bromide (COBr)2 and summary. Journal of Molecular Spectroscopy, 2011, 269, 201-210.	1.2	2
51	Vibronic spectra, ab initio calculations, and structures of conformationally non-rigid molecules of oxalyl halides in the ground and lowest excited electronic states. Part V: Oxalyl chloridefluoride (COClâ€“COF). Structural Chemistry, 2011, 22, 293-304.	2.0	4
52	Vibronic spectra, ab initio calculations, and structures of conformationally non-rigid molecules of oxalyl halides in the ground and lowest excited electronic states. Part III: Theoretical investigation of oxalyl fluoride. Journal of Molecular Spectroscopy, 2010, 260, 50-56.	1.2	8
53	Vibronic spectra, ab initio calculations, and structures of conformationally non-rigid molecules of oxalyl halides in the ground and lowest excited electronic states. Part IV: Analysis of the absorption spectra of oxalyl fluoride in the gas phase. Journal of Molecular Spectroscopy, 2010, 260, 124-129.	1.2	6
54	Vibronic spectra, ab initio calculations, and structures of conformationally non-rigid molecules of oxalyl halides in the ground and lowest excited electronic states. Part II: Theoretical investigation of oxalyl chloride. Journal of Molecular Spectroscopy, 2009, 256, 247-255.	1.2	11

#	Article	IF	Citations
55	Molecular parameters of tetraatomic carbonyls X₂CO and XYCO (X, Y = H, F, Cl) in the ground and lowest excited electronic states, part 1: A test ofab initiomethods. International Journal of Quantum Chemistry, 2009, 109, 569-585.	2.0	25
56	Vibronic spectra, ab initio calculations, and structures of conformationally non-rigid molecules of oxalyl halides in the ground and lowest excited electronic states. Part I: Reanalysis of the 3680Ã... and 4100Ã... absorption systems of oxalyl chloride. Journal of Molecular Spectroscopy, 2009, 255, 39-44.	1.2	13
57	Structure and dynamics of acrolein in lowest excited ^{1,3}(n,Ï€*) electronic states: The quantumâ€chemical study. International Journal of Quantum Chemistry, 2008, 108, 2719-2731.	2.0	29
58	Theoretical study of structures of the X2CO and XYCO molecules (X and Y = H, F, or Cl) in the ground and lowest excited triplet electronic states. Russian Chemical Bulletin, 2005, 54, 2714-2725.	1.5	5