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	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
2	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
3	Tuning Range-Separated Density Functional Theory for Photocatalytic Water Splitting Systems. Journal of Chemical Theory and Computation, 2015, 11, 1700-1709.	5.3	64
4	Chemical Bonding in Aqueous Ferrocyanide: Experimental and Theoretical X-ray Spectroscopic Study. Journal of Physical Chemistry B, 2014, 118, 1555-1563.	2.6	61
5	Direct Observation of Molecular Orbital Mixing in a Solvated Organometallic Complex. Angewandte Chemie - International Edition, 2013, 52, 9841-9844.	13.8	60
6	Multi-reference approach to the calculation of photoelectron spectra including spin-orbit coupling. Journal of Chemical Physics, 2015, 143, 074104.	3.0	48
7	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
8	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
9	Theoretical Xâ€ray spectroscopy of transition metal compounds. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1433.	14.6	44
10	2p x-ray absorption spectroscopy of 3d transition metal systems. Journal of Electron Spectroscopy and Related Phenomena, 2021, 249, 147061.	1.7	44
11	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
12	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
13	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
14	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
15	Electronic excitation spectrum of the photosensitizer [Ir(ppy)2(bpy)]+. Journal of Chemical Physics, 2012, 136, 214305.	3.0	37
16	Towards an ab initio theory for metal L-edge soft X-ray spectroscopy of molecular aggregates. Structural Dynamics, 2016, 3, 062601.	2.3	30
17	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
18	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

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19	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
20	Ground- and Excited-State Properties of Iron(II) Complexes Linked to Organic Chromophores. Inorganic Chemistry, 2020, 59, 14746-14761.	4.0	28
21	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
22	Intersystem Crossing and Triplet Dynamics in an Iron(II) N-Heterocyclic Carbene Photosensitizer. Inorganic Chemistry, 2020, 59, 14666-14678.	4.0	23
23	Distinct photodynamics of Î²-N and Î²-C pseudoisomeric iron(<scp>ii</scp>) complexes. Chemical Communications, 2021, 57, 6640-6643.	4.1	23
24	Mechanistic Study of Photocatalytic Hydrogen Generation with Simple Iron Carbonyls as Water Reduction Catalysts. ChemCatChem, 2016, 8, 404-411.	3.7	16
25	Multi-reference protocol for (auto)ionization spectra: Application to molecules. Journal of Chemical Physics, 2020, 152, 074108.	3.0	16
26	Quasi-classical approaches to vibronic spectra revisited. Journal of Chemical Physics, 2018, 148, 102337.	3.0	15
27	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
28	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
29	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
30	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
31	Ultrafast Spin-State Dynamics in Transition-Metal Complexes Triggered by Soft-X-Ray Light. Physical Review Letters, 2017, 118, 023001.	7.8	11
32	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
33	Chemical Tuning and Absorption Properties of Iridium Photosensitizers for Photocatalytic Applications. Inorganics, 2017, 5, 23.	2.7	10
34	Simulating vibronic spectra via Matsubara-like dynamics: Coping with the sign problem. Journal of Chemical Physics, 2018, 149, 194103.	3.0	10
35	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
36	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

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37	Ultrafast dissipative spin-state dynamics triggered by x-ray pulse trains. Physical Review A, 2018, 98, .	2.5	9
38	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
39	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
40	Density matrix-based time-dependent configuration interaction approach to ultrafast spin-flip dynamics. Molecular Physics, 2017, 115, 1898-1907.	1.7	8
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	BokarevetÂal.Reply. Physical Review Letters, 2014, 112, 129303.	7.8	5
49	Mapping Long-Lived Dark States in Copper Porphyrin Nanostructures. Journal of Physical Chemistry C, 2016, 120, 16977-16984.	3.1	5
50	A time-correlation function approach to nuclear dynamical effects in X-ray spectroscopy. Journal of Chemical Physics, 2017, 146, 224203.	3.0	5
51	Solvation and speciation of cobalt(II). A theoretical X-ray absorption and RIXS study. Chemical Physics, 2020, 532, 110681.	1.9	5
52	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
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 V: Oxalyl chloridefluoride (COClâ€“COF). Structural Chemistry, 2011, 22, 293-304.	2.0	4
54	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

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55	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
56	Effect of chemical structure on the ultrafast spin dynamics in core-excited states. Journal of Chemical Physics, 2020, 153, 044304.	3.0	3
57	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
58	Soft X-ray spectroscopy of transition metal compounds: a theoretical perspective. EPJ Web of Conferences, 2017, 132, 02004.	0.3	1