Rashid R Valiev

List of Publications by Year in descending order

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100 papers 2,470 citations

257450 24 h-index 223800 46 g-index

102 all docs

 $\begin{array}{c} 102 \\ \\ \text{docs citations} \end{array}$

102 times ranked

2617 citing authors

#	Article	IF	CITATIONS
1	Energy-Cascaded Upconversion in an Organic Dye-Sensitized Core/Shell Fluoride Nanocrystal. Nano Letters, 2015, 15, 7400-7407.	9.1	341
2	Dye-sensitized lanthanide-doped upconversion nanoparticles. Chemical Society Reviews, 2017, 46, 4150-4167.	38.1	281
3	Efficient Broadband Upconversion of Nearâ€Infrared Light in Dyeâ€Sensitized Core/Shell Nanocrystals. Advanced Optical Materials, 2016, 4, 1760-1766.	7.3	104
4	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. Journal of Physical Chemistry Letters, 2019, 10, 6701-6705.	4.6	103
5	First-principles method for calculating the rate constants of internal-conversion and intersystem-crossing transitions. Physical Chemistry Chemical Physics, 2018, 20, 6121-6133.	2.8	79
6	Aromaticity of the planar hetero[8] circulenes and their doubly charged ions: NICS and GIMIC characterization. Physical Chemistry Chemical Physics, 2014, 16, 15367-15374.	2.8	69
7	Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporphyrin. Physical Chemistry Chemical Physics, 2012, 14, 11508.	2.8	56
8	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	2.8	54
9	Molecular mechanism for rapid autoxidation in \hat{l}_{\pm} -pinene ozonolysis. Nature Communications, 2021, 12, 878.	12.8	47
10	Photon Upconversion Kinetic Nanosystems and Their Optical Response. Laser and Photonics Reviews, 2018, 12, 1700144.	8.7	42
11	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4756-4767.	2.5	41
12	Closed-shell paramagnetic porphyrinoids. Chemical Communications, 2017, 53, 9866-9869.	4.1	40
13	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. Journal of Physical Chemistry A, 2013, 117, 9062-9068.	2.5	38
14	Ab initio simulation of pyrene spectra in water matrices. RSC Advances, 2014, 4, 42054-42065.	3.6	38
15	Calculating rate constants for intersystem crossing and internal conversion in the Franck–Condon and Herzberg–Teller approximations. Physical Chemistry Chemical Physics, 2019, 21, 18495-18500.	2.8	38
16	Intersystem Crossings Drive Atmospheric Gas-Phase Dimer Formation. Journal of Physical Chemistry A, 2019, 123, 6596-6604.	2.5	35
17	Aromaticity of the completely annelated tetraphenylenes: NICS and GIMIC characterization. Journal of Molecular Modeling, 2015, 21, 136.	1.8	34
18	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	2.8	34

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19	The computational and experimental investigations of photophysical and spectroscopic properties of BF2 dipyrromethene complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 117, 323-329.	3.9	33
20	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. Physical Chemistry Chemical Physics, 2020, 22, 22314-22323.	2.8	32
21	Aromaticity of Even-Number Cyclo[$\langle i\rangle n\langle i\rangle$] carbons ($\langle i\rangle n\langle i\rangle$ = 6â \in "100). Journal of Physical Chemistry A, 2020, 124, 10849-10855.	2.5	30
22	New insights into aromatic pathways of carbachlorins and carbaporphyrins based on calculations of magnetically induced current densities. Physical Chemistry Chemical Physics, 2016, 18, 11932-11941.	2.8	28
23	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. Chemical Modelling, 0 , , 1 -42.	0.4	28
24	Predicting the degree of aromaticity of novel carbaporphyrinoids. Physical Chemistry Chemical Physics, 2015, 17, 14215-14222.	2.8	27
25	Can Plasmon Change Reaction Path? Decomposition of Unsymmetrical Iodonium Salts as an Organic Probe. Journal of Physical Chemistry Letters, 2020, 11, 5770-5776.	4.6	27
26	The aromatic character of thienopyrrole-modified 20Ï€-electron porphyrinoids. Physical Chemistry Chemical Physics, 2014, 16, 11010.	2.8	26
27	Application of a 2D Molybdenum Telluride in SERS Detection of Biorelevant Molecules. ACS Applied Materials & Samp; Interfaces, 2020, 12, 47774-47783.	8.0	25
28	Comparing Reaction Routes for ³ (RO···OR′) Intermediates Formed in Peroxy Radical Self- and Cross-Reactions. Journal of Physical Chemistry A, 2020, 124, 8305-8320.	2.5	24
29	Photolysis of diatomic molecules as a source of atoms in planetary exospheres. Astronomy and Astrophysics, 2020, 633, A39.	5.1	24
30	Aromatic Pathways in Carbathiaporphyrins. Journal of Physical Chemistry A, 2015, 119, 1201-1207.	2.5	23
31	Computational and Experimental Investigation of the Optical Properties of the Chromene Dyes. Journal of Physical Chemistry A, 2015, 119, 1948-1956.	2.5	23
32	Verdazyl Radical Building Blocks: Synthesis, Structure, and Sonogashira Crossâ€Coupling Reactions. European Journal of Organic Chemistry, 2018, 2018, 4802-4811.	2.4	23
33	2-lodoxybenzoic acid ditriflate: the most powerful hypervalent iodine(<scp>v</scp>) oxidant. Chemical Communications, 2019, 55, 7760-7763.	4.1	23
34	Non-intersecting ring currents in [12]infinitene. Physical Chemistry Chemical Physics, 2022, 24, 6404-6409.	2.8	23
35	DFT simulation of the heteroannelated octatetraenes vibronic spectra with the Franck–Condon and Herzberg–Teller approaches including Duschinsky effect. Chemical Physics, 2015, 459, 65-71.	1.9	22
36	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. Physical Chemistry Chemical Physics, 2018, 20, 17705-17713.	2.8	21

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37	Interlayerâ€Sensitized Linear and Nonlinear Photoluminescence of Quasiâ€2D Hybrid Perovskites Using Aggregationâ€Induced Enhanced Emission Active Organic Cation Layers. Advanced Functional Materials, 2020, 30, 1909375.	14.9	21
38	The influence of benzene rings on aromatic pathways in the porphyrins. International Journal of Quantum Chemistry, 2013, 113, 2563-2567.	2.0	19
39	Lasing of pyrromethene 567 in solid matrices. Chemical Physics Letters, 2013, 588, 184-187.	2.6	19
40	Optical and magnetic properties of antiaromatic porphyrinoids. Physical Chemistry Chemical Physics, 2017, 19, 25979-25988.	2.8	19
41	Aromaticity and photophysics of tetrasila- and tetragerma-annelated tetrathienylenes as new representatives of the hetero[8]circulene family. Physical Chemistry Chemical Physics, 2019, 21, 9246-9254.	2.8	19
42	Plasmon-assisted MXene grafting: tuning of surface termination and stability enhancement. 2D Materials, 2021, 8, 045037.	4.4	19
43	When are Antiaromatic Molecules Paramagnetic?. Journal of Physical Chemistry C, 2020, 124, 21027-21035.	3.1	18
44	Theoretical and experimental investigation of photophysical properties of Zn(DFP SAMQ)2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 137-140.	3.9	17
45	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. New Journal of Chemistry, 2017, 41, 2717-2723.	2.8	16
46	Relations between the aromaticity and magnetic dipole transitions in the electronic spectra of hetero[8]circulenes. Physical Chemistry Chemical Physics, 2018, 20, 30239-30246.	2.8	16
47	Fast estimation of the internal conversion rate constant in photophysical applications. Physical Chemistry Chemical Physics, 2021, 23, 6344-6348.	2.8	16
48	Perhalophenyl Three-Coordinate Gold(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints. Inorganic Chemistry, 2020, 59, 14236-14244.	4.0	15
49	Integration of global ring currents using the Ampère–Maxwell law. Physical Chemistry Chemical Physics, 2022, 24, 624-628.	2.8	15
50	Electroluminescence of Halogen Complexes with Monovalent Copper: OLED Devices and DFT Modeling. Russian Physics Journal, 2016, 58, 1205-1211.	0.4	14
51	Computational Investigation of the Formation of Peroxide (ROOR) Accretion Products in the OH- and NO ₃ -Initiated Oxidation of α-Pinene. Journal of Physical Chemistry A, 2021, 125, 10632-10639.	2.5	13
52	Electronic absorption spectrum of monoamine tetraphenylporphyrin with the complexon of ethylenediaminetetraacetic acid as substitute. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 87, 40-45.	3.9	12
53	Photolysis of metal oxides as a source of atoms in planetary exospheres. Planetary and Space Science, 2017, 145, 38-48.	1.7	12
54	Thermally activated delayed fluorescence in dibenzothiophene sulfone derivatives: Theory and experiment. Chemical Physics Letters, 2019, 717, 53-58.	2.6	11

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55	The blue vibronically resolved electroluminescence of azatrioxa[8]circulene. Chemical Physics Letters, 2019, 732, 136667.	2.6	10
56	Impact of heteroatoms (S, Se, and Te) on the aromaticity of heterocirculenes. New Journal of Chemistry, 2019, 43, 12178-12190.	2.8	10
57	Ab Initio Study of Electronic States of Astrophysically Important Molecules. Russian Physics Journal, 2016, 59, 536-543.	0.4	9
58	Substituent-sensitive fluorescence of sequentially N-alkylated tetrabenzotetraaza [8] circulenes. New Journal of Chemistry, 2017, 41, 7621-7625.	2.8	9
59	Reactions of 1â€Arylbenziodoxolones with Azide Anion: Experimental and Computational Study of Substituent Effects. European Journal of Organic Chemistry, 2018, 2018, 640-647.	2.4	9
60	Single-layer polymeric tetraoxa[8]circulene modified by s-block metals: toward stable spin qubits and novel superconductors. Nanoscale, 2021, 13, 4799-4811.	5.6	9
61	Magnetically induced ring currents in metallocenothiaporphyrins. Physical Chemistry Chemical Physics, 2022, 24, 1666-1674.	2.8	9
62	Gas-Phase Peroxyl Radical Recombination Reactions: AÂComputational Study of Formation and Decomposition of Tetroxides. Journal of Physical Chemistry A, 2022, 126, 4046-4056.	2.5	9
63	The first example of a one-step synthesis of 2′-O-acetyl aryl-d-glucopyranosides. Carbohydrate Research, 2015, 409, 36-40.	2.3	8
64	Franck-Condon factors and vibronic patterns of singlet-triplet transitions of 16O3 molecule falling near the dissociation threshold and above. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 273, 107834.	2.3	8
65	So Close, Yet so Different: How One Donor Atom Changes Significantly the Photophysical Properties of Mononuclear Cu(l) Complexes. Inorganic Chemistry, 2022, 61, 11629-11638.	4.0	8
66	A new look at acid catalyzed deacetylation of carbohydrates: A regioselective synthesis and reactivity of 2-O-acetyl aryl glycopyranosides. Carbohydrate Research, 2018, 458-459, 60-66.	2.3	7
67	Positional Isomers of Isocyanoazulenes as Axial Ligands Coordinated to Ruthenium(II) Tetraphenylporphyrin: Fine-Tuning Redox and Optical Profiles. Inorganic Chemistry, 2019, 58, 9316-9325.	4.0	7
68	Dianthracenylazatrioxa[8]circulene: Synthesis, Characterization and Application in OLEDs. Chemistry - A European Journal, 2021, 27, 11609-11617.	3.3	7
69	Influence of perhalophenyl groups in the TADF mechanism of diphosphino gold(<scp>i</scp>) complexes. Journal of Materials Chemistry C, 2022, 10, 4894-4904.	5.5	7
70	Odd-Number Cyclo[<i>n</i>]Carbons Sustaining Alternating Aromaticity. Journal of Physical Chemistry A, 2022, 126, 2445-2452.	2.5	7
71	Vibronic absorption spectra of the angular fused bisindolo- and biscarbazoloanthracene blue fluorophores for OLED applications. Chemical Physics, 2018, 513, 105-111.	1.9	6
72	Deacetylation of per-acetatylated glycopyranosides: An overall pattern for acidic catalyzis. Chemical Physics Letters, 2019, 723, 123-127.	2.6	6

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73	Less is more: On the effect of benzannulation on solid-state emission of difluoroborates. Journal of Materials Chemistry $C,0,1$.	5.5	6
74	Energy transfer, pre-reactive complex formation and recombination reactions during the collision of peroxy radicals. Physical Chemistry Chemical Physics, 2022, 24, 10033-10043.	2.8	6
75	Theoretical investigation of fluorescence properties of EDTA and DTPA substituted tetraphenylporphyrin molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 99, 122-125.	3.9	5
76	Computational and experimental studies of the electronic excitation spectra of EDTA and DTPA substituted tetraphenylporphyrins and their Lu complexes. Journal of Molecular Modeling, 2013, 19, 4631-4637.	1.8	5
77	Theoretical Investigation of the Structural and Spectroscopic Properties of Anthracene Dimers. Russian Physics Journal, 2014, 57, 95-99.	0.4	5
78	Ab initio investigation of electric and magnetic dipole electronic transitions in the complex of oxygen with benzene. Journal of Molecular Modeling, 2016, 22, 214.	1.8	5
79	Experimental and theoretical study of photo- and electroluminescence of divinyldiphenyl and divinylphenanthrene derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 59-64.	3.9	5
80	Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization. Dyes and Pigments, 2018, 151, 372-379.	3.7	5
81	The aromaticity of verdazyl radicals and their closed-shell charged species. New Journal of Chemistry, 2018, 42, 19987-19994.	2.8	5
82	Computational study of aromaticity, 1H NMR spectra and intermolecular interactions of twisted thia-norhexaphyrin and its multiply annulated polypyrrolic derivatives. Physical Chemistry Chemical Physics, 2019, 21, 25334-25343.	2.8	5
83	A hybrid molecular sensitizer for triplet fusion upconversion. Chemical Engineering Journal, 2021, 426, 131282.	12.7	5
84	Photo- and Electroluminescent Neutral Iridium(III) Complexes Bearing Imidoylamidinate Ligands. Inorganic Chemistry, 2022, 61, 8670-8684.	4.0	5
85	Electronic absorption spectrum of monoaminosubstituted tetraphenylporphyrin with diethylenetriaminepenetaacetic acid for the substitute. Russian Physics Journal, 2012, 55, 378-382.	0.4	4
86	The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. New Journal of Chemistry, 2020, 44, 20643-20650.	2.8	4
87	Design, synthesis and evaluation of a new Mn $\hat{a}\in$ Contrast agent for MR imaging of myocardium based on the DTPA-phenylpentadecanoic acid complex. Chemical Physics Letters, 2016, 665, 111-116.	2.6	3
88	Electroluminescence of a Zinc Complex Exciplex with a Hole-Transporting Material. Russian Physics Journal, 2019, 62, 140-146.	0.4	3
89	Competition between the nonadiabatic electronic state-mixing and the Herzberg-Teller vibronic effects in fluorescence process of tetraoxa[8]circulene. Chemical Physics Letters, 2020, 738, 136914.	2.6	3
90	Photophysical properties of the triangular [Au(HNî€COH)] < sub>3 < /sub> complex and its dimer. Physical Chemistry Chemical Physics, 2020, 22, 10314-10321.	2.8	3

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91	General and Simple Method for the Synthesis of 3-nitroformazan Using Arenediazonium Tosylates. Current Organic Synthesis, 2016, 13, 623-628.	1.3	3
92	Stimulated Emission of Active Media in the Red Spectral Range. Russian Physics Journal, 2016, 59, 1-7.	0.4	2
93	Optimization of core–valence states of molecules. Molecular Physics, 2017, 115, 252-259.	1.7	2
94	Influence of Molecular Oxygen on Ortho-Para Conversion of Water Molecules. Russian Physics Journal, 2017, 60, 485-493.	0.4	2
95	Ab Initio Study of Phosphorescence of Hetero[8]Circulenes. Russian Physics Journal, 2019, 62, 406-410.	0.4	2
96	Photophysical Constants of the Tetraoxa[8]Circulene Molecule. Russian Physics Journal, 2019, 61, 1759-1763.	0.4	2
97	Complex Study of Electronic States and Spectra of 3-Nitroformazans. Russian Physics Journal, 2016, 59, 197-203.	0.4	1
98	Theoretical Study of Nonradiative Energy Transfer from Exciplex to Perovskites. Russian Physics Journal, 2020, 62, 1911-1916.	0.4	1
99	Vibronic Spectra of Bifluorene and Terfluorene. Russian Physics Journal, 2022, 64, 2082-2088.	0.4	1
100	Is either direct photolysis or photocatalysed H-shift of peroxyl radicals a competitive pathway in the troposphere?. Royal Society Open Science, 2020, 7, 200521.	2.4	0