Rashid R Valiev

List of Publications by Year
in descending order

100 papers	2,470 citations	293460 24 h-index	252626 46 g-index
102 all docs	102 docs citations	102 times ranked	2943 citing authors

#	Article	IF	Citations
1	Influence of perhalophenyl groups in the TADF mechanism of diphosphino gold(<scp>i</scp>) complexes. Journal of Materials Chemistry C, 2022, 10, 4894-4904.	2.7	7
2	Integration of global ring currents using the AmpÃ¨reâ€“Maxwell law. Physical Chemistry Chemical Physics, 2022, 24, 624-628.	1.3	15
3	Magnetically induced ring currents in metallocenothiaporphyrins. Physical Chemistry Chemical Physics, 2022, 24, 1666-1674.	1.3	9
4	Non-intersecting ring currents in [12]infinitene. Physical Chemistry Chemical Physics, 2022, 24, 6404-6409.	1.3	23
5	Vibronic Spectra of Bifluorene and Terfluorene. Russian Physics Journal, 2022, 64, 2082-2088.	0.2	1
6	Energy transfer, pre-reactive complex formation and recombination reactions during the collision of peroxy radicals. Physical Chemistry Chemical Physics, 2022, 24, 10033-10043.	1.3	6
7	Odd-Number Cyclo[n]Carbons Sustaining Alternating Aromaticity. Journal of Physical Chemistry A, 2022, 126, 2445-2452.	1.1	7
8	Photo- and Electroluminescent Neutral Iridium(III) Complexes Bearing Imidoylamidinate Ligands. Inorganic Chemistry, 2022, 61, 8670-8684.	1.9	5
9	Gas-Phase Peroxyl Radical Recombination Reactions: AÂComputational Study of Formation and Decomposition of Tetroxides. Journal of Physical Chemistry A, 2022, 126, 4046-4056.	1.1	9
10	So Close, Yet so Different: How One Donor Atom Changes Significantly the Photophysical Properties of Mononuclear Cu(I) Complexes. Inorganic Chemistry, 2022, 61, 11629-11638.	1.9	8
11	Fast estimation of the internal conversion rate constant in photophysical applications. Physical Chemistry Chemical Physics, 2021, 23, 6344-6348.	1.3	16
12	Molecular mechanism for rapid autoxidation in Î±-pinene ozonolysis. Nature Communications, 2021, 12, 878.	5.8	47
13	Dianthracenylazatrioxa[8]circulene: Synthesis, Characterization and Application in OLEDs. Chemistry - A European Journal, 2021, 27, 11609-11617.	1.7	7
14	Plasmon-assisted MXene grafting: tuning of surface termination and stability enhancement. 2D Materials, 2021, 8, 045037.	2.0	19
15	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.	1.1	8
16	A hybrid molecular sensitizer for triplet fusion upconversion. Chemical Engineering Journal, 2021, 426, 131282.	6.6	5
17	Single-layer polymeric tetraoxa[8]circulene modified by s-block metals: toward stable spin qubits and novel superconductors. Nanoscale, 2021, 13, 4799-4811.	2.8	9
18	Computational Investigation of the Formation of Peroxide (ROOR) Accretion Products in the OH- and NO₃-Initiated Oxidation of Î±-Pinene. Journal of Physical Chemistry A, 2021, 125, 10632-10639.	1.1	13

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19	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.	1.2	3
20	Perhalophenyl Three-Coordinate Gold(I) Complexes as TADF Emitters: A Photophysical Study from Experimental and Computational Viewpoints. Inorganic Chemistry, 2020, 59, 14236-14244.	1.9	15
21	Application of a 2D Molybdenum Telluride in SERS Detection of Biorelevant Molecules. ACS Applied Materials & Interfaces, 2020, 12, 47774-47783.	4.0	25
22	The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids. New Journal of Chemistry, 2020, 44, 20643-20650.	1.4	4
23	Is either direct photolysis or photocatalysed H-shift of peroxyl radicals a competitive pathway in the troposphere?. Royal Society Open Science, 2020, 7, 200521.	1.1	0
24	When are Antiaromatic Molecules Paramagnetic?. Journal of Physical Chemistry C, 2020, 124, 21027-21035.	1.5	18
25	Comparing Reaction Routes for ³(ROÂ·Â·Â·ORâ€²) Intermediates Formed in Peroxy Radical Self- and Cross-Reactions. Journal of Physical Chemistry A, 2020, 124, 8305-8320.	1.1	24
26	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. Physical Chemistry Chemical Physics, 2020, 22, 22314-22323.	1.3	32
27	Aromaticity of Even-Number Cyclo[n]carbons (n = 6â€“100). Journal of Physical Chemistry A, 2020, 124, 10849-10855.	1.1	30
28	Can Plasmon Change Reaction Path? Decomposition of Unsymmetrical Iodonium Salts as an Organic Probe. Journal of Physical Chemistry Letters, 2020, 11, 5770-5776.	2.1	27
29	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.	7.8	21
30	Theoretical Study of Nonradiative Energy Transfer from Exciplex to Perovskites. Russian Physics Journal, 2020, 62, 1911-1916.	0.2	1
31	Photolysis of diatomic molecules as a source of atoms in planetary exospheres. Astronomy and Astrophysics, 2020, 633, A39.	2.1	24
32	Photophysical properties of the triangular [Au(HNî€COH)]₃ complex and its dimer. Physical Chemistry Chemical Physics, 2020, 22, 10314-10321.	1.3	3
33	The blue vibronically resolved electroluminescence of azatrioxa[8]circulene. Chemical Physics Letters, 2019, 732, 136667.	1.2	10
34	Calculating rate constants for intersystem crossing and internal conversion in the Franckâ€“Condon and Herzbergâ€“Teller approximations. Physical Chemistry Chemical Physics, 2019, 21, 18495-18500.	1.3	38
35	Intersystem Crossings Drive Atmospheric Gas-Phase Dimer Formation. Journal of Physical Chemistry A, 2019, 123, 6596-6604.	1.1	35
36	Ab Initio Study of Phosphorescence of Hetero[8]Circulenes. Russian Physics Journal, 2019, 62, 406-410.	0.2	2

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37	Impact of heteroatoms (S, Se, and Te) on the aromaticity of heterocirculenes. New Journal of Chemistry, 2019, 43, 12178-12190.	1.4	10
38	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. Journal of Physical Chemistry Letters, 2019, 10, 6701-6705.	2.1	103
39	Thermally activated delayed fluorescence in dibenzothiophene sulfone derivatives: Theory and experiment. Chemical Physics Letters, 2019, 717, 53-58.	1.2	11
40	Positional Isomers of Isocyanoazulenes as Axial Ligands Coordinated to Ruthenium(II) Tetraphenylporphyrin: Fine-Tuning Redox and Optical Profiles. Inorganic Chemistry, 2019, 58, 9316-9325.	1.9	7
41	2-Iodoxybenzoic acid ditriflate: the most powerful hypervalent iodine(<scp>v</scp>) oxidant. Chemical Communications, 2019, 55, 7760-7763.	2.2	23
42	Electroluminescence of a Zinc Complex Exciplex with a Hole-Transporting Material. Russian Physics Journal, 2019, 62, 140-146.	0.2	3
43	Deacetylation of per-acetatylated glycopyranosides: An overall pattern for acidic catalyzis. Chemical Physics Letters, 2019, 723, 123-127.	1.2	6
44	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.	1.3	19
45	Photophysical Constants of the Tetraoxa[8]Circulene Molecule. Russian Physics Journal, 2019, 61, 1759-1763.	0.2	2
46	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.	1.3	5
47	First-principles method for calculating the rate constants of internal-conversion and intersystem-crossing transitions. Physical Chemistry Chemical Physics, 2018, 20, 6121-6133.	1.3	79
48	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.	1.1	7
49	Verdazyl Radical Building Blocks: Synthesis, Structure, and Sonogashira Crossâ€Coupling Reactions. European Journal of Organic Chemistry, 2018, 2018, 4802-4811.	1.2	23
50	Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization. Dyes and Pigments, 2018, 151, 372-379.	2.0	5
51	Reactions of 1â€Arylbenziodoxolones with Azide Anion: Experimental and Computational Study of Substituent Effects. European Journal of Organic Chemistry, 2018, 2018, 640-647.	1.2	9
52	Photon Upconversion Kinetic Nanosystems and Their Optical Response. Laser and Photonics Reviews, 2018, 12, 1700144.	4.4	42
53	Relations between the aromaticity and magnetic dipole transitions in the electronic spectra of hetero[8]circulenes. Physical Chemistry Chemical Physics, 2018, 20, 30239-30246.	1.3	16
54	The aromaticity of verdazyl radicals and their closed-shell charged species. New Journal of Chemistry, 2018, 42, 19987-19994.	1.4	5

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55	Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins. Physical Chemistry Chemical Physics, 2018, 20, 17705-17713.	1.3	21
56	Vibronic absorption spectra of the angular fused bisindolo- and biscarbazoloanthracene blue fluorophores for OLED applications. Chemical Physics, 2018, 513, 105-111.	0.9	6
57	Computational Studies of Aromatic and Photophysical Properties of Expanded Porphyrins. Journal of Physical Chemistry A, 2018, 122, 4756-4767.	1.1	41
58	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. New Journal of Chemistry, 2017, 41, 2717-2723.	1.4	16
59	Dye-sensitized lanthanide-doped upconversion nanoparticles. Chemical Society Reviews, 2017, 46, 4150-4167.	18.7	281
60	Substituent-sensitive fluorescence of sequentially N-alkylated tetrabenzotetraaza[8]circulenes. New Journal of Chemistry, 2017, 41, 7621-7625.	1.4	9
61	Optimization of coreâ€“valence states of molecules. Molecular Physics, 2017, 115, 252-259.	0.8	2
62	Closed-shell paramagnetic porphyrinoids. Chemical Communications, 2017, 53, 9866-9869.	2.2	40
63	Optical and magnetic properties of antiaromatic porphyrinoids. Physical Chemistry Chemical Physics, 2017, 19, 25979-25988.	1.3	19
64	Photolysis of metal oxides as a source of atoms in planetary exospheres. Planetary and Space Science, 2017, 145, 38-48.	0.9	12
65	Influence of Molecular Oxygen on Ortho-Para Conversion of Water Molecules. Russian Physics Journal, 2017, 60, 485-493.	0.2	2
66	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.	2.0	5
67	Ab initio investigation of electric and magnetic dipole electronic transitions in the complex of oxygen with benzene. Journal of Molecular Modeling, 2016, 22, 214.	0.8	5
68	Ab Initio Study of Electronic States of Astrophysically Important Molecules. Russian Physics Journal, 2016, 59, 536-543.	0.2	9
69	Efficient Broadband Upconversion of Nearâ€Infrared Light in Dyeâ€Sensitized Core/Shell Nanocrystals. Advanced Optical Materials, 2016, 4, 1760-1766.	3.6	104
70	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	1.3	54
71	Design, synthesis and evaluation of a new Mn â€“ Contrast agent for MR imaging of myocardium based on the DTPA-phenylpentadecanoic acid complex. Chemical Physics Letters, 2016, 665, 111-116.	1.2	3
72	Stimulated Emission of Active Media in the Red Spectral Range. Russian Physics Journal, 2016, 59, 1-7.	0.2	2

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73	Complex Study of Electronic States and Spectra of 3-Nitroformazans. Russian Physics Journal, 2016, 59, 197-203.	0.2	1
74	Electroluminescence of Halogen Complexes with Monovalent Copper: OLED Devices and DFT Modeling. Russian Physics Journal, 2016, 58, 1205-1211.	0.2	14
75	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.	1.3	28
76	Aromaticity of the doubly charged [8]circulenes. Physical Chemistry Chemical Physics, 2016, 18, 8980-8992.	1.3	34
77	General and Simple Method for the Synthesis of 3-nitroformazan Using Arenediazonium Tosylates. Current Organic Synthesis, 2016, 13, 623-628.	0.7	3
78	Aromatic Pathways in Carbathiaporphyrins. Journal of Physical Chemistry A, 2015, 119, 1201-1207.	1.1	23
79	DFT simulation of the heteroannelated octatetraenes vibronic spectra with the Franckâ€“Condon and Herzbergâ€“Teller approaches including Duschinsky effect. Chemical Physics, 2015, 459, 65-71.	0.9	22
80	The first example of a one-step synthesis of 2â€²-O-acetyl aryl-d-glucopyranosides. Carbohydrate Research, 2015, 409, 36-40.	1.1	8
81	Predicting the degree of aromaticity of novel carbaporphyrinoids. Physical Chemistry Chemical Physics, 2015, 17, 14215-14222.	1.3	27
82	Computational and Experimental Investigation of the Optical Properties of the Chromene Dyes. Journal of Physical Chemistry A, 2015, 119, 1948-1956.	1.1	23
83	Aromaticity of the completely annelated tetraphenylenes: NICS and GIMIC characterization. Journal of Molecular Modeling, 2015, 21, 136.	0.8	34
84	Energy-Cascaded Upconversion in an Organic Dye-Sensitized Core/Shell Fluoride Nanocrystal. Nano Letters, 2015, 15, 7400-7407.	4.5	341
85	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.	2.0	33
86	Theoretical and experimental investigation of photophysical properties of Zn(DFP SAMQ)2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 137-140.	2.0	17
87	Ab initio simulation of pyrene spectra in water matrices. RSC Advances, 2014, 4, 42054-42065.	1.7	38
88	Theoretical Investigation of the Structural and Spectroscopic Properties of Anthracene Dimers. Russian Physics Journal, 2014, 57, 95-99.	0.2	5
89	Aromaticity of the planar hetero[8]circulenes and their doubly charged ions: NICS and GIMIC characterization. Physical Chemistry Chemical Physics, 2014, 16, 15367-15374.	1.3	69
90	The aromatic character of thienopyrrole-modified 20Ï€-electron porphyrinoids. Physical Chemistry Chemical Physics, 2014, 16, 11010.	1.3	26

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91	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.	0.8	5
92	The influence of benzene rings on aromatic pathways in the porphyrins. International Journal of Quantum Chemistry, 2013, 113, 2563-2567.	1.0	19
93	Insights into Magnetically Induced Current Pathways and Optical Properties of Isophlorins. Journal of Physical Chemistry A, 2013, 117, 9062-9068.	1.1	38
94	Lasing of pyrromethene 567 in solid matrices. Chemical Physics Letters, 2013, 588, 184-187.	1.2	19
95	Electronic absorption spectrum of monoaminosubstituted tetraphenylporphyrin with diethylenetriaminepenetaacetic acid for the substitute. Russian Physics Journal, 2012, 55, 378-382.	0.2	4
96	Theoretical investigation of fluorescence properties of EDTA and DTPA substituted tetraphenylporphyrin molecules. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 99, 122-125.	2.0	5
97	Computational studies of photophysical properties of porphin, tetraphenylporphyrin and tetrabenzoporphyrin. Physical Chemistry Chemical Physics, 2012, 14, 11508.	1.3	56
98	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.	2.0	12
99	Less is more: On the effect of benzannulation on solid-state emission of difluoroborates. Journal of Materials Chemistry C, 0, , .	2.7	6
100	Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds. Chemical Modelling, 0, , 1-42.	0.2	28