Vyacheslav S Bryantsev

List of Publications by Year
in descending order

115 papers	7,292 citations	57631 44 h-index	56606 83 g-index
120 all docs	120 docs citations	120 times ranked	7514 citing authors

#	Article	IF	Citations
1	Calculation of Solvation Free Energies of Charged Solutes Using Mixed Cluster/Continuum Models. Journal of Physical Chemistry B, 2008, 112, 9709-9719.	1.2	567
2	Anionâ€“arene adducts: Câ€“H hydrogen bonding, anionâ€“Ï€ interaction, and carbon bonding motifs. Chemical Communications, 2008, , 2417.	2.2	361
3	Evaluation of B3LYP, X3LYP, and M06-Class Density Functionals for Predicting the Binding Energies of Neutral, Protonated, and Deprotonated Water Clusters. Journal of Chemical Theory and Computation, 2009, 5, 1016-1026.	2.3	326
4	Predicting Solvent Stability in Aprotic Electrolyte Liâ€“Air Batteries: Nucleophilic Substitution by the Superoxide Anion Radical (O₂^{â€¢â€“}). Journal of Physical Chemistry A, 2011, 115, 12399-12409.	1.1	320
5	A Rechargeable Liâ€“O₂ Battery Using a Lithium Nitrate/N,N-Dimethylacetamide Electrolyte. Journal of the American Chemical Society, 2013, 135, 2076-2079.	6.6	308
6	Structural Criteria for the Design of Anion Receptors:â€‰ The Interaction of Halides with Electron-Deficient Arenes. Journal of the American Chemical Society, 2007, 129, 48-58.	6.6	301
7	Bio-inspired nano-traps for uranium extraction from seawater and recovery from nuclear waste. Nature Communications, 2018, 9, 1644.	5.8	300
8	PAMAM Dendrimers Undergo pH Responsive Conformational Changes without Swelling. Journal of the American Chemical Society, 2009, 131, 2798-2799.	6.6	249
9	The Identification of Stable Solvents for Nonaqueous Rechargeable Li-Air Batteries. Journal of the Electrochemical Society, 2013, 160, A160-A171.	1.3	181
10	Computational Study of the Mechanisms of Superoxide-Induced Decomposition of Organic Carbonate-Based Electrolytes. Journal of Physical Chemistry Letters, 2011, 2, 379-383.	2.1	179
11	Are Câˆ’H Groups Significant Hydrogen Bonding Sites in Anion Receptors? Benzene Complexes with Cl-, NO3-, and ClO4-. Journal of the American Chemical Society, 2005, 127, 8282-8283.	6.6	157
12	Development and Validation of a ReaxFF Reactive Force Field for Cu Cation/Water Interactions and Copper Metal/Metal Oxide/Metal Hydroxide Condensed Phases. Journal of Physical Chemistry A, 2010, 114, 9507-9514.	1.1	156
13	Predicting Autoxidation Stability of Ether- and Amide-Based Electrolyte Solvents for Liâ€“Air Batteries. Journal of Physical Chemistry A, 2012, 116, 7128-7138.	1.1	146
14	pKa Calculations of Aliphatic Amines, Diamines, and Aminoamides via Density Functional Theory with a Poissonâˆ’Boltzmann Continuum Solvent Model. Journal of Physical Chemistry A, 2007, 111, 4422-4430.	1.1	131
15	Influence of Substituents on the Strength of Aryl Câˆ’HÂ·Â·Â·Anion Hydrogen Bonds. Organic Letters, 2005, 7, 5031-5034.	2.4	124
16	XAFS investigation of polyamidoxime-bound uranyl contests the paradigm from small molecule studies. Energy and Environmental Science, 2016, 9, 448-453.	15.6	115
17	Experimental and Computational Analysis of the Solventâ€Dependent O₂/Li⁺â€O₂^{âˆ’} Redox Couple: Standard Potentials, Coupling Strength, and Implications for Lithiumâ€“Oxygen Batteries. Angewandte Chemie - International Edition, 2016, 55, 3129-3134.	7.2	111
18	Computational Study of Copper(II) Complexation and Hydrolysis in Aqueous Solutions Using Mixed Cluster/Continuum Models. Journal of Physical Chemistry A, 2009, 113, 9559-9567.	1.1	110

#	Article	IF	Citations
19	Origin of the unusually strong and selective binding of vanadium by polyamidoximes in seawater. Nature Communications, 2017, 8, 1560.	5.8	110
20	Anion Coordination in Metalâ˜'Organic Frameworks Functionalized with Urea Hydrogen-Bonding Groups. Crystal Growth and Design, 2006, 6, 555-563.	1.4	101
21	Lithium Nitrate As Regenerable SEI Stabilizing Agent for Rechargeable Li/O₂ Batteries. Journal of Physical Chemistry Letters, 2013, 4, 3760-3765.	2.1	97
22	Hydration of Copper(II): New Insights from Density Functional Theory and the COSMO Solvation Model. Journal of Physical Chemistry A, 2008, 112, 9104-9112.	1.1	96
23	ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries. Journal of the Electrochemical Society, 2014, 161, E3009-E3014.	1.3	88
24	Siderophore-inspired chelator hijacks uranium from aqueous medium. Nature Communications, 2019, 10, 819.	5.8	84
25	Predicting Stability Constants for Uranyl Complexes Using Density Functional Theory. Inorganic Chemistry, 2015, 54, 3995-4001.	1.9	83
26	De Novo Structure-Based Design of Bisurea Hosts for Tetrahedral Oxoanion Guests. Journal of the American Chemical Society, 2006, 128, 2035-2042.	6.6	77
27	Stability of Lithium Superoxide LiO₂ in the Gas Phase: Computational Study of Dimerization and Disproportionation Reactions. Journal of Physical Chemistry A, 2010, 114, 8165-8169.	1.1	76
28	Outer-Sphere Water Clusters Tune the Lanthanide Selectivity of Diglycolamides. ACS Central Science, 2018, 4, 739-747.	5.3	69
29	Investigation of Fluorinated Amides for Solidâ€"Electrolyte Interphase Stabilization in Liâ€"O₂ Batteries Using Amide-Based Electrolytes. Journal of Physical Chemistry C, 2013, 117, 11977-11988.	1.5	68
30	â€œStrainingâ€•to Separate the Rare Earths: How the Lanthanide Contraction Impacts Chelation by Diglycolamide Ligands. Inorganic Chemistry, 2017, 56, 1152-1160.	1.9	68
31	Bis-lactam-1,10-phenanthroline (BLPhen), a New Type of Preorganized Mixed N,O-Donor Ligand That Separates Am(III) over Eu(III) with Exceptionally High Efficiency. Inorganic Chemistry, 2017, 56, 5911-5917.	1.9	64
32	CO2 Capture via Crystalline Hydrogen-Bonded Bicarbonate Dimers. CheM, 2019, 5, 719-730.	5.8	64
33	Conformational Analysis and Rotational Barriers of Alkyl- and Phenyl-Substituted Urea Derivatives. Journal of Physical Chemistry A, 2005, 109, 832-842.	1.1	61
34	Trefoil-Shaped Outer-Sphere Ion Clusters Mediate Lanthanide(III) Ion Transport with Diglycolamide Ligands. Journal of the American Chemical Society, 2017, 139, 17350-17358.	6.6	60
35	Synergistic Effect of Oxygen and LiNO₃on the Interfacial Stability of Lithium Metal in a Li/O₂Battery. Journal of the Electrochemical Society, 2013, 160, A1544-A1550.	1.3	58
36	Theoretical prediction of Am(<scp>iii</scp>)/Eu(<scp>iii</scp>) selectivity to aid the design of actinide-lanthanide separation agents. Dalton Transactions, 2015, 44, 7935-7942.	1.6	58

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37	Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride. Journal of Physical Chemistry A, 2010, 114, 3556-3568.	1.1	55
38	Acidity of the Amidoxime Functional Group in Aqueous Solution: A Combined Experimental and Computational Study. Journal of Physical Chemistry B, 2015, 119, 3567-3576.	1.2	54
39	First-Principles Integrated Adsorption Modeling for Selective Capture of Uranium from Seawater by Polyamidoxime Sorbent Materials. ACS Applied Materials & Interfaces, 2018, 10, 12580-12593.	4.0	53
40	Efficient Separation of Light Lanthanides(III) by Using Bisâ€Ł actam Phenanthroline Ligands. Chemistry - A European Journal, 2019, 25, 6326-6331.	1.7	51
41	Predicting the stability of aprotic solvents in Li-air batteries: pKa calculations of aliphatic Câ€“H acids in dimethyl sulfoxide. Chemical Physics Letters, 2013, 558, 42-47.	1.2	49
42	Elucidating Ionic Correlations Beyond Simple Charge Alternation in Molten MgCl₂â€“KCl Mixtures. Journal of Physical Chemistry Letters, 2019, 10, 7603-7610.	2.1	49
43	Adsorption mechanism of alkyl hydroxamic acid onto bastnÃsite: Fundamental steps toward rational collector design for rare earth elements. Journal of Colloid and Interface Science, 2019, 553, 210-219.	5.0	47
44	Quantum Chemical Analysis of the Thermodynamics of 2D Cluster Formation of Oddn-Alcohols at the Air/Water Interface. Journal of Physical Chemistry B, 2002, 106, 11285-11294.	1.2	46
45	Computer-Aided Molecular Design of Bis-phosphine Oxide Lanthanide Extractants. Inorganic Chemistry, 2016, 55, 5787-5803.	1.9	46
46	Two-Electron Three-Centered Bond in Side-On (Î·²) Uranyl(V) Superoxo Complexes. Journal of Physical Chemistry A, 2008, 112, 5777-5780.	1.1	44
47	Conformational Preferences and Internal Rotation in Alkyl- and Phenyl-Substituted Thiourea Derivatives. Journal of Physical Chemistry A, 2006, 110, 4678-4688.	1.1	43
48	Spatial Engineering Direct Cooperativity between Binding Sites for Uranium Sequestration. Advanced Science, 2021, 8, 2001573.	5.6	43
49	Highly Preorganized Ligand 1,10-Phenanthroline-2,9-dicarboxylic Acid for the Selective Recovery of Uranium from Seawater in the Presence of Competing Vanadium Species. Inorganic Chemistry, 2016, 55, 10818-10829.	1.9	42
50	Calculation of solvation free energies of Li+ and O2 â^' ions and neutral lithiumâ€“oxygen compounds in acetonitrile using mixed cluster/continuum models. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	41
51	Synthesis of Naphthalimidedioxime Ligand-Containing Fibers for Uranium Adsorption from Seawater. Industrial & Engineering Chemistry Research, 2016, 55, 4161-4169.	1.8	40
52	Aqueous Sulfate Separation by Sequestration of [(SO₄)₂(H₂O)₄]^{4â^'} Clusters within Highly Insoluble Imineâ€Linked Bisâ€Guanidinium Crystals. Chemistry - A European Journal, 2016, 22, 1997-2003.	1.7	39
53	Structure Activity Relationship Approach toward the Improved Separation of Rare-Earth Elements Using Diglycolamides. Inorganic Chemistry, 2020, 59, 17620-17630.	1.9	39
54	Temperature Dependence of Short and Intermediate Range Order in Molten MgCl₂ and Its Mixture with KCl. Journal of Physical Chemistry B, 2020, 124, 2892-2899.	1.2	38

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55	Quantum Chemical Analysis of Thermodynamics of the Two-Dimensional Cluster Formation at the Air/Water Interface. Journal of Physical Chemistry B, 2002, 106, 121-131.	1.2	37
56	Addition of H₂O and O₂ to Acetone and Dimethylsulfoxide Ligated Uranyl(V) Dioxocations. Journal of Physical Chemistry A, 2009, 113, 2350-2358.	1.1	36
57	Amidoximes as ligand functionalities for braided polymeric materials for the recovery of uranium from seawater. Polyhedron, 2016, 109, 81-91.	1.0	33
58	A Computational Approach to Predicting Ligand Selectivity for the Sizeâ€Based Separation of Trivalent Lanthanides. European Journal of Inorganic Chemistry, 2016, 2016, 3474-3479.	1.0	31
59	Theoretical Study of Oxovanadium(IV) Complexation with Formamidoximate: Implications for the Design of Uranyl-Selective Adsorbents. Industrial & Engineering Chemistry Research, 2016, 55, 4231-4240.	1.8	31
60	Experimental and Computational Analysis of the Solventâ€Dependent O₂/Li⁺â€O₂^{â¯} Redox Couple: Standard Potentials, Coupling Strength, and Implications for Lithiumâ€“Oxygen Batteries. Angewandte Chemie, 2016, 128, 3181-3186.	1.6	30
61	A comparative study of surface energies and water adsorption on Ce-bastnÃsite, La-bastnÃsite, and calcite via density functional theory and water adsorption calorimetry. Physical Chemistry Chemical Physics, 2017, 19, 7820-7832.	1.3	30
62	Quantum chemical semi-empirical approach to the thermodynamic characteristics of oligomers and large aggregates of alcohols at the water/air interface. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2002, 209, 1-14.	2.3	28
63	Crystal Structures, Surface Stability, and Water Adsorption Energies of La-BastnÃsite via Density Functional Theory and Experimental Studies. Journal of Physical Chemistry C, 2016, 120, 16767-16781.	1.5	28
64	Quantum Chemical Semiempirical Approach to the Structural and Thermodynamic Characteristics of Fluoroalkanols at the Air/Water Interface. Journal of Physical Chemistry B, 2005, 109, 454-462.	1.2	27
65	Theoretical study of the coordination behavior of formate and formamidoximate with dioxovanadium(<scp>v</scp>) cation: implications for selectivity towards uranyl. Physical Chemistry Chemical Physics, 2015, 17, 31715-31726.	1.3	27
66	Radiometric evaluation of diglycolamide resins for the chromatographic separation of actinium from fission product lanthanides. Talanta, 2017, 175, 318-324.	2.9	24
67	Connections between the Speciation and Solubility of Ni(II) and Co(II) in Molten ZnCl₂. Journal of Physical Chemistry B, 2020, 124, 1253-1258.	1.2	24
68	N-methylacetamide as an Electrolyte Solvent for Rechargeable Li-O2 Batteries: Unexpected Stability at the O2 electrode. ECS Electrochemistry Letters, 2013, 3, A11-A14.	1.9	23
69	Assessing ligand selectivity for uranium over vanadium ions to aid in the discovery of superior adsorbents for extraction of UO₂²⁺ from seawater. Dalton Transactions, 2016, 45, 10744-10751.	1.6	23
70	Quantifying the binding strength of salicylaldoximeâ€“uranyl complexes relative to competing salicylaldoximeâ€“transition metal ion complexes in aqueous solution: a combined experimental and computational study. Dalton Transactions, 2016, 45, 9051-9064.	1.6	23
71	Influence of a Heterocyclic Nitrogen-Donor Group on the Coordination of Trivalent Actinides and Lanthanides by Aminopolycarboxylate Complexants. Inorganic Chemistry, 2018, 57, 1373-1385.	1.9	23
72	Dialing in Direct Air Capture of CO₂ by Crystal Engineering of Bisiminoguanidines. ChemSusChem, 2020, 13, 6381-6390.	3.6	23

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73	Unraveling Local Structure of Molten Salts via X-ray Scattering, Raman Spectroscopy, and Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 5971-5982.	1.2	23
74	Structure and dynamics of the molten alkali-chloride salts from an X-ray, simulation, and rate theory perspective. Physical Chemistry Chemical Physics, 2020, 22, 22900-22917.	1.3	22
75	Molecular Recognition at Mineral Interfaces: Implications for the Beneficiation of Rare Earth Ores. ACS Applied Materials & Interfaces, 2020, 12, 16327-16341.	4.0	20
76	A Holistic Approach for Elucidating Local Structure, Dynamics, and Speciation in Molten Salts with High Structural Disorder. Journal of the American Chemical Society, 2021, 143, 15298-15308.	6.6	20
77	Thermodynamic, Spectroscopic, and Computational Studies of f-Element Complexation by N-Hydroxyethyl-diethylenetriamine-N,Nâ€²,Nâ€³,Nâ€³-tetraacetic Acid. Inorganic Chemistry, 2017, 56, 1722-1733.	1.9	19
78	Comparison of fixed charge and polarizable models for predicting the structural, thermodynamic, and transport properties of molten alkali chlorides. Journal of Chemical Physics, 2020, 153, 214502.	1.2	19
79	High Concentration Lithium Nitrate/Dimethylacetamide Electrolytes for Lithium/Oxygen Cells. Journal of the Electrochemical Society, 2016, 163, A2673-A2678.	1.3	18
80	Capping the calix: how toluene completes cesium(<scp>i</scp>) coordination with calix[4]pyrrole. Chemical Communications, 2017, 53, 5610-5613.	2.2	18
81	Absolute Molecular Orientation of Isopropanol at Ceria (100) Surfaces: Insight into Catalytic Selectivity from the Interfacial Structure. Journal of Physical Chemistry C, 2017, 121, 14137-14146.	1.5	18
82	Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. International Journal of Quantum Chemistry, 2018, 118, e25516.	1.0	17
83	Predicting the Electrochemical Behavior of Lithium Nitrite in Acetonitrile with Quantum Chemical Methods. Journal of the American Chemical Society, 2014, 136, 3087-3096.	6.6	16
84	Finding Order in the Disordered Hydration Shell of Rapidly Exchanging Water Molecules around the Heaviest Alkali Cs⁺ and Fr⁺. Journal of Physical Chemistry B, 2018, 122, 12067-12076.	1.2	16
85	Quantum Chemical Prediction of pK_a Values of Cationic Ion-Exchange Groups in Polymer Electrolyte Membranes. Journal of Physical Chemistry C, 2018, 122, 2490-2501.	1.5	14
86	Calculation of thermochemical properties of conjugated radicals. International Journal of Quantum Chemistry, 2004, 96, 123-135.	1.0	13
87	A Molecular-Scale Approach to Rare-Earth Beneficiation: Thinking Small to Avoid Large Losses. IScience, 2020, 23, 101435.	1.9	13
88	X-ray scattering reveals ion clustering of dilute chromium species in molten chloride medium. Chemical Science, 2021, 12, 8026-8035.	3.7	13
89	Bifunctional Ionic Covalent Organic Networks for Enhanced Simultaneous Removal of Chromium(VI) and Arsenic(V) Oxoanions via Synergetic Ion Exchange and Redox Process. Small, 2021, 17, e2104703.	5.2	13
90	Using the MMFF94 model to predict structures and energies for hydrogen-bonded ureaâ€“anion complexes. Computational and Theoretical Chemistry, 2005, 725, 177-182.	1.5	12

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91	Simple guanidinium motif for the selective binding and extraction of sulfate. Separation Science and Technology, 2018, 53, 1864-1873.	1.3	12
92	The Coordination Chemistry and Stoichiometry of Extracted Diglycolamide Complexes of Lanthanides in Extraction Chromatography Materials. Solvent Extraction and Ion Exchange, 2022, 40, 6-27.	0.8	11
93	Transition State for Aggregation and Reorganization of Normal Fatty Alcohols at the Air/Water Interface. Journal of Physical Chemistry B, 2004, 108, 8330-8337.	1.2	10
94	Synthesis and characterization of a novel aminopolycarboxylate complexant for efficient trivalent f-element differentiation: N-butyl-2-acetamide-diethylenetriamine-N,Nâ€²,Nâ€²â€²,Nâ€²â€²-tetraacetic acid. Dalton Transactions, 2018, 47, 1092-1105.	1.6	10
95	Mineralâ€“Water Interface Structure of Xenotime (YPO4) {100}. Journal of Physical Chemistry C, 2018, 122, 20232-20243.	1.5	10
96	Complexation of lanthanides and other metal ions by the polypyridyl ligand quaterpyridine: Relation between metal ion size, chelate ring size, and complex stability. Inorganica Chimica Acta, 2019, 488, 19-27.	1.2	10
97	Exploring Soft Donor Character of the N-2-Pyrazinylmethyl Group by Coordinating Trivalent Actinides and Lanthanides Using Aminopolycarboxylates. Inorganic Chemistry, 2020, 59, 138-150.	1.9	10
98	Hydration structure and water exchange kinetics at xenotimeâ€“water interfaces: implications for rare earth minerals separation. Physical Chemistry Chemical Physics, 2020, 22, 7719-7727.	1.3	10
99	A conformationally persistent pseudo-bicyclic guanidinium for anion coordination as stabilized by dual intramolecular hydrogen bonds. RSC Advances, 2015, 5, 107266-107269.	1.7	9
100	Enhancing selectivity of cation exchange with anion receptors. Chemical Communications, 2019, 55, 3590-3593.	2.2	8
101	Influence of a Preâ€organized Nâ€Donor Group on the Coordination of Trivalent Actinides and Lanthanides by an Aminopolycarboxylate Complexant. Chemistry - A European Journal, 2019, 25, 2545-2555.	1.7	8
102	Improving the theoretical description of Ln(<scp>iii</scp>)/An(<scp>iii</scp>) separation with phosphinic acid ligands: a benchmarking study of structure and selectivity. Physical Chemistry Chemical Physics, 2021, 23, 19558-19570.	1.3	6
103	Guanidinium-Based Ionic Covalent-Organic Nanosheets for Sequestration of Cr(VI) and As(V) Oxoanions in Water. ACS Applied Nano Materials, 2021, 4, 13319-13328.	2.4	6
104	Improving Rare-Earth Mineral Separation with Insights from Molecular Recognition: Functionalized Hydroxamic Acid Adsorption onto BastnÃsite and Calcite. Langmuir, 2022, 38, 5439-5453.	1.6	6
105	Two Ligands of Interest in Recovering Uranium from the Oceans: The Correct Formation Constants of the Uranyl(VI) Cation with 2,2â€²-Bipyridyl-6,6â€²-dicarboxylic Acid and 1,10-Phenanthroline-2,9-dicarboxylic Acid. Inorganic Chemistry, 2022, 61, 9960-9967.	1.9	6
106	Aggregation and re-organization of normal fatty alcohols at the air/water interface. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2004, 239, 135-140.	2.3	5
107	Spectroscopic characterization of neptunium(<scp>vi</scp>), plutonium(<scp>vi</scp>), americium(<scp>vi</scp>) and neptunium(<scp>v</scp>) encapsulated in uranyl nitrate hexahydrate. Physical Chemistry Chemical Physics, 2021, 23, 13228-13241.	1.3	2
108	Aminopolycarboxylates in trivalent f-element separations. Fundamental Theories of Physics, 2021, 60, 1-162.	0.1	2

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109	A Photoresponsive Receptor with a 10 ⁵ Magnitude of Reversible Anionâ€Binding Switching. Chemistry - A European Journal, 2022, , .	1.7	2
110	Comment on Using Cyclic Voltammetry to Determine a Standard Potential of a Reversible Redox Couple Involving Oxidation or Reduction of a Gas. Journal of the Electrochemical Society, 2013, 160, H818-H819.	1.3	1
111	Title is missing!. Russian Journal of Organic Chemistry, 2002, 38, 1244-1251.	0.3	0
112	Title is missing!. Russian Journal of Organic Chemistry, 2002, 38, 1588-1593.	0.3	0
113	Substituent Effects on Hyperfine Coupling Constants Analyzed in Terms of p-Bound Electron Perturbation Theory. Journal of Structural Chemistry, 2003, 44, 803-812.	0.3	0
114	Computer-Aided Design of Organic Host Architectures for Selective Chemosensors. , 2009, , 113-133.		0
115	Anti-electrostatic hydrogen-bonded tellurate dimers captured and stabilized by crystallization of a bis-iminoguanidinium salt. Polyhedron, 2022, 223, 115990.	1.0	0