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	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
2	A Photoresponsive Receptor with a 10 ⁵ Magnitude of Reversible Anionâ€Binding Switching. Chemistry - A European Journal, 2022, , .	1.7	2
3	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
4	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
5	Anti-electrostatic hydrogen-bonded tellurate dimers captured and stabilized by crystallization of a bis-iminoguanidinium salt. Polyhedron, 2022, 223, 115990.	1.0	0
6	Spatial Engineering Direct Cooperativity between Binding Sites for Uranium Sequestration. Advanced Science, 2021, 8, 2001573.	5.6	43
7	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
8	X-ray scattering reveals ion clustering of dilute chromium species in molten chloride medium. Chemical Science, 2021, 12, 8026-8035.	3.7	13
9	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
10	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
11	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
12	Aminopolycarboxylates in trivalent f-element separations. Fundamental Theories of Physics, 2021, 60, 1-162.	0.1	2
13	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
14	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
15	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
16	A Molecular-Scale Approach to Rare-Earth Beneficiation: Thinking Small to Avoid Large Losses. IScience, 2020, 23, 101435.	1.9	13
17	Dialing in Direct Air Capture of CO₂ by Crystal Engineering of Bisiminoguanidines. ChemSusChem, 2020, 13, 6381-6390.	3.6	23
18	Structure Activity Relationship Approach toward the Improved Separation of Rare-Earth Elements Using Diglycolamides. Inorganic Chemistry, 2020, 59, 17620-17630.	1.9	39

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19	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
20	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
21	Molecular Recognition at Mineral Interfaces: Implications for the Beneficiation of Rare Earth Ores. ACS Applied Materials & Interfaces, 2020, 12, 16327-16341.	4.0	20
22	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
23	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
24	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
25	CO2 Capture via Crystalline Hydrogen-Bonded Bicarbonate Dimers. CheM, 2019, 5, 719-730.	5.8	64
26	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
27	Efficient Separation of Light Lanthanides(III) by Using Bisâ€Lactam Phenanthroline Ligands. Chemistry - A European Journal, 2019, 25, 6326-6331.	1.7	51
28	Siderophore-inspired chelator hijacks uranium from aqueous medium. Nature Communications, 2019, 10, 819.	5.8	84
29	Enhancing selectivity of cation exchange with anion receptors. Chemical Communications, 2019, 55, 3590-3593.	2.2	8
30	Elucidating Ionic Correlations Beyond Simple Charge Alternation in Molten MgCl₂â€“KCl Mixtures. Journal of Physical Chemistry Letters, 2019, 10, 7603-7610.	2.1	49
31	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
32	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
33	Bio-inspired nano-traps for uranium extraction from seawater and recovery from nuclear waste. Nature Communications, 2018, 9, 1644.	5.8	300
34	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
35	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
36	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

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37	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
38	Simple guanidinium motif for the selective binding and extraction of sulfate. Separation Science and Technology, 2018, 53, 1864-1873.	1.3	12
39	Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. International Journal of Quantum Chemistry, 2018, 118, e25516.	1.0	17
40	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
41	Mineralâ€“Water Interface Structure of Xenotime (YPO4) {100}. Journal of Physical Chemistry C, 2018, 122, 20232-20243.	1.5	10
42	Outer-Sphere Water Clusters Tune the Lanthanide Selectivity of Diglycolamides. ACS Central Science, 2018, 4, 739-747.	5.3	69
43	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
44	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
45	Capping the calix: how toluene completes cesium(<scp>i</scp>) coordination with calix[4]pyrrole. Chemical Communications, 2017, 53, 5610-5613.	2.2	18
46	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
47	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
48	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
49	Radiometric evaluation of diglycolamide resins for the chromatographic separation of actinium from fission product lanthanides. Talanta, 2017, 175, 318-324.	2.9	24
50	Origin of the unusually strong and selective binding of vanadium by polyamidoximes in seawater. Nature Communications, 2017, 8, 1560.	5.8	110
51	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
52	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
53	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
54	High Concentration Lithium Nitrate/Dimethylacetamide Electrolytes for Lithium/Oxygen Cells. Journal of the Electrochemical Society, 2016, 163, A2673-A2678.	1.3	18

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55	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
56	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
57	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
58	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
59	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 - International Edition, 2016, 55, 3129-3134.	7.2	111
60	XAFS investigation of polyamidoxime-bound uranyl contests the paradigm from small molecule studies. Energy and Environmental Science, 2016, 9, 448-453.	15.6	115
61	Computer-Aided Molecular Design of Bis-phosphine Oxide Lanthanide Extractants. Inorganic Chemistry, 2016, 55, 5787-5803.	1.9	46
62	Amidoximes as ligand functionalities for braided polymeric materials for the recovery of uranium from seawater. Polyhedron, 2016, 109, 81-91.	1.0	33
63	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
64	Synthesis of Naphthalimidedioxime Ligand-Containing Fibers for Uranium Adsorption from Seawater. Industrial & Engineering Chemistry Research, 2016, 55, 4161-4169.	1.8	40
65	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
66	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
67	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
68	Predicting Stability Constants for Uranyl Complexes Using Density Functional Theory. Inorganic Chemistry, 2015, 54, 3995-4001.	1.9	83
69	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
70	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
71	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
72	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

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73	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
74	Lithium Nitrate As Regenerable SEI Stabilizing Agent for Rechargeable Li/O₂ Batteries. Journal of Physical Chemistry Letters, 2013, 4, 3760-3765.	2.1	97
75	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
76	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
77	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
78	The Identification of Stable Solvents for Nonaqueous Rechargeable Li-Air Batteries. Journal of the Electrochemical Society, 2013, 160, A160-A171.	1.3	181
79	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
80	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
81	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
82	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
83	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
84	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
85	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
86	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
87	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
88	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
89	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
90	PAMAM Dendrimers Undergo pH Responsive Conformational Changes without Swelling. Journal of the American Chemical Society, 2009, 131, 2798-2799.	6.6	249

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91	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
92	Computer-Aided Design of Organic Host Architectures for Selective Chemosensors. , 2009, , 113-133.		0
93	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
94	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
95	Anionâ€“arene adducts: Câ€“H hydrogen bonding, anionâ€“Ï€ interaction, and carbon bonding motifs. Chemical Communications, 2008, , 2417.	2.2	361
96	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
97	pKa Calculations of Aliphatic Amines, Diamines, and Aminoamides via Density Functional Theory with a Poissonâ^'Boltzmann Continuum Solvent Model. Journal of Physical Chemistry A, 2007, 111, 4422-4430.	1.1	131
98	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
99	Conformational Preferences and Internal Rotation in Alkyl- and Phenyl-Substituted Thiourea Derivatives. Journal of Physical Chemistry A, 2006, 110, 4678-4688.	1.1	43
100	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
101	Anion Coordination in Metalâ^'Organic Frameworks Functionalized with Urea Hydrogen-Bonding Groups. Crystal Growth and Design, 2006, 6, 555-563.	1.4	101
102	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
103	Are Câ^'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
104	Influence of Substituents on the Strength of Aryl Câ^'HÂ·Â·Â·Anion Hydrogen Bonds. Organic Letters, 2005, 7, 5031-5034.	2.4	124
105	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
106	Conformational Analysis and Rotational Barriers of Alkyl- and Phenyl-Substituted Urea Derivatives. Journal of Physical Chemistry A, 2005, 109, 832-842.	1.1	61
107	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
108	Calculation of thermochemical properties of conjugated radicals. International Journal of Quantum Chemistry, 2004, 96, 123-135.	1.0	13

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109	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
110	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
111	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
112	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
113	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
114	Title is missing!. Russian Journal of Organic Chemistry, 2002, 38, 1244-1251.	0.3	0
115	Title is missing!. Russian Journal of Organic Chemistry, 2002, 38, 1588-1593.	0.3	0