Ekaterina I Izgorodina

List of Publications by Year
in descending order

95 papers	6,417 citations	70961 41 h-index	64668 79 g-index
99 all docs	99 docs citations	99 times ranked	6323 citing authors

#	Article	IF	Citations
1	Ionic Liquids in Electrochemical Devices and Processes: Managing Interfacial Electrochemistry. Accounts of Chemical Research, 2007, 40, 1165-1173.	7.6	660
2	On the concept of ionicity in ionic liquids. Physical Chemistry Chemical Physics, 2009, 11, 4962.	1.3	645
3	Liquids intermediate between â€œmolecularâ€•and â€œionicâ€•liquids: Liquid Ion Pairs?. Chemical Communications, 2007, , 3817.	2.2	231
4	Ionicity and proton transfer in protic ionic liquids. Physical Chemistry Chemical Physics, 2010, 12, 10341.	1.3	229
5	Trends in Râˆ’X Bond Dissociation Energies (R = Me, Et,i-Pr,t-Bu; X = H, CH3, OCH3, OH, F):Â A Surprising Shortcoming of Density Functional Theory. Journal of Physical Chemistry A, 2005, 109, 7558-7566.	1.1	210
6	Electrochemistry at Negative Potentials in Bis(trifluoromethanesulfonyl)amide Ionic Liquids. Zeitschrift Fur Physikalische Chemie, 2006, 220, 1483-1498.	1.4	200
7	Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. Chemical Reviews, 2017, 117, 6696-6754.	23.0	181
8	On the components of the dielectric constants of ionic liquids: ionic polarization?. Physical Chemistry Chemical Physics, 2009, 11, 2452.	1.3	171
9	Ion-Pair Binding Energies of Ionic Liquids: Can DFT Compete with Ab Initio-Based Methods?. Journal of Physical Chemistry A, 2009, 113, 7064-7072.	1.1	163
10	Low overpotential water oxidation to hydrogen peroxide on a MnOx catalyst. Energy and Environmental Science, 2012, 5, 9496.	15.6	152
11	Should Contemporary Density Functional Theory Methods Be Used to Study the Thermodynamics of Radical Reactions?. Journal of Physical Chemistry A, 2007, 111, 10754-10768.	1.1	140
12	Accurate ab initio prediction of propagation rate coefficients in free-radical polymerization: Acrylonitrile and vinyl chloride. Chemical Physics, 2006, 324, 96-110.	0.9	136
13	Nature of Hydrogen Bonding in Charged Hydrogen-Bonded Complexes and Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 14659-14667.	1.2	132
14	Protic ionic liquids based on the dimeric and oligomeric anions: [(AcO)xHxâˆ’1]âˆ’. Physical Chemistry Chemical Physics, 2008, 10, 2972.	1.3	129
15	Protic pharmaceuticalionic liquids and solids: Aspects of protonics. Faraday Discussions, 2012, 154, 335-352.	1.6	129
16	Computational Studies of RAFT Polymerizationâ€“Mechanistic Insights and Practical Applications. Macromolecular Rapid Communications, 2006, 27, 473-497.	2.0	122
17	Towards large-scale, fully ab initio calculations of ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 4189.	1.3	121
18	Importance of dispersion forces for prediction of thermodynamic and transport properties of some common ionic liquids. Physical Chemistry Chemical Physics, 2014, 16, 7209-7221.	1.3	102

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19	Understanding the Effect of the C2 Proton in Promoting Low Viscosities and High Conductivities in Imidazolium-Based Ionic Liquids: Part I. Weakly Coordinating Anions. Journal of Physical Chemistry B, 2011, 115, 14688-14697.	1.2	101
20	Assessment of Kohnâ€“Sham density functional theory and MÃ¸llerâ€“Plesset perturbation theory for ionic liquids. Physical Chemistry Chemical Physics, 2013, 15, 13664.	1.3	98
21	Calculation of 0â€“0 excitation energies of organic molecules by CIS(D) quantum chemical methods. Chemical Physics, 2004, 305, 223-230.	0.9	91
22	Assessment of atomic partial charge schemes for polarisation and charge transfer effects in ionic liquids. Physical Chemistry Chemical Physics, 2013, 15, 1632-1646.	1.3	89
23	Reliable Low-Cost Theoretical Procedures for Studying Additionâ^'Fragmentation in RAFT Polymerization. Journal of Physical Chemistry A, 2006, 110, 2486-2492.	1.1	85
24	New Insights into the Relationship between Ion-Pair Binding Energy and Thermodynamic and Transport Properties of Ionic Liquids. Journal of Physical Chemistry C, 2010, 114, 20472-20478.	1.5	81
25	Towards a Better Understanding of 'Delocalized Charge' in Ionic Liquid Anions. Australian Journal of Chemistry, 2007, 60, 15.	0.5	79
26	Diamino protic ionic liquids for CO2 capture. Physical Chemistry Chemical Physics, 2013, 15, 19994.	1.3	77
27	Aluminium Speciation in 1â€Butylâ€1â€Methylpyrrolidinium Bis(trifluoromethylsulfonyl)amide/AlCl‹sub›3‹/sub› Mixtures. Chemistry - A European Journal, 2009, 15, 3435-3447.	1.7	69
28	How Accurate Are Approximate Methods for Evaluating Partition Functions for Hindered Internal Rotations?. Journal of Physical Chemistry A, 2008, 112, 1956-1964.	1.1	68
29	Quantum Chemical Mapping of Initialization Processes in RAFT Polymerization. Macromolecular Rapid Communications, 2006, 27, 1015-1022.	2.0	67
30	First Principles Prediction of The Propagation Rate Coefficients of Acrylic and Vinyl Esters: Are We There Yet?. Macromolecules, 2010, 43, 553-560.	2.2	66
31	The Madelung Constant of Organic Salts. Crystal Growth and Design, 2009, 9, 4834-4839.	1.4	64
32	The role of exchange in systematic DFT errors for some organic reactions. Physical Chemistry Chemical Physics, 2009, 11, 1138.	1.3	60
33	Thioketone spin traps as mediating agents for free radical polymerization processes. Chemical Communications, 2006, , 835.	2.2	56
34	Ab Initio Prediction of Proton NMR Chemical Shifts in Imidazolium Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 3186-3197.	1.2	56
35	Addition-Fragmentation Kinetics of Fluorodithioformates (F-RAFT) in Styrene, Vinyl Acetate, and Ethylene Polymerization:Â An Ab Initio Investigation. Macromolecules, 2006, 39, 4585-4591.	2.2	55
36	Cellulose-dissolving protic ionic liquids as low cost catalysts for direct transesterification reactions of cellulose. Green Chemistry, 2018, 20, 1412-1422.	4.6	52

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37	Physical Absorption Of CO₂ in Protic and Aprotic Ionic Liquids: An Interaction Perspective. Journal of Physical Chemistry B, 2015, 119, 11748-11759.	1.2	50
38	Energy-directed tree search: an efficient systematic algorithm for finding the lowest energy conformation of molecules. Physical Chemistry Chemical Physics, 2007, 9, 2507.	1.3	49
39	An ab initio Study of the Structure and Energetics of Hydrogen Bonding in Ionic Liquids. Frontiers in Chemistry, 2019, 7, 208.	1.8	48
40	Photo- and solvatochromic properties of nitrobenzospiropyran in ionic liquids containing the [NTf2]â^' anion. Physical Chemistry Chemical Physics, 2008, 10, 5919.	1.3	46
41	Is the Addition-Fragmentation Step of the RAFT Polymerisation Process Chain Length Dependent?. Macromolecular Theory and Simulations, 2006, 15, 394-403.	0.6	44
42	Large-scale ab initio calculations of archetypical ionic liquids. Chemical Communications, 2012, 48, 1493-1495.	2.2	43
43	Mechanisms of low temperature capture and regeneration of CO₂ using diamino protic ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1140-1149.	1.3	42
44	Two-coordinate hydrido-germylenes. Chemical Communications, 2015, 51, 6854-6857.	2.2	41
45	Bulk properties of aqueous graphene oxide and reduced graphene oxide with surfactants and polymers: adsorption and stability. Physical Chemistry Chemical Physics, 2018, 20, 16801-16816.	1.3	41
46	Homoleptic 12-coordinate lanthanoids with Î·2-nitroso ligands. Dalton Transactions, 2007, , 1371-1373.	1.6	40
47	Reversible Reduction of the TEMPO Radical: One Step Closer to an All-Organic Redox Flow Battery. ACS Sustainable Chemistry and Engineering, 2020, 8, 17988-17996.	3.2	37
48	Ordered Solvents and Ionic Liquids Can Be Harnessed for Electrostatic Catalysis. Journal of the American Chemical Society, 2020, 142, 12826-12833.	6.6	37
49	Generalized spin-ratio scaled MP2 method for accurate prediction of intermolecular interactions for neutral and ionic species. Journal of Chemical Physics, 2017, 146, 064108.	1.2	34
50	Prediction of ¹H NMR chemical shifts for clusters of imidazolium-based ionic liquids. Physical Chemistry Chemical Physics, 2017, 19, 17411-17425.	1.3	33
51	A Systematic Study of DFT Performance for Geometry Optimizations of Ionic Liquid Clusters. Journal of Chemical Theory and Computation, 2020, 16, 6735-6753.	2.3	32
52	Spectroscopic Studies on Photoinduced Reactions of the Anticancer Prodrug, trans,trans,transâ€[Pt(N₃)₂(OH)₂(py)₂]. Chemistry - A European Journal, 2018, 24, 5790-5803.	1.7	31
53	Experimental Evidence of Long-Lived Electric Fields of Ionic Liquid Bilayers. Journal of the American Chemical Society, 2021, 143, 17431-17440.	6.6	31
54	New SCS- and SOS-MP2 Coefficients Fitted to Semi-Coulombic Systems. Journal of Chemical Theory and Computation, 2014, 10, 3111-3122.	2.3	29

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55	The effect of descriptor choice in machine learning models for ionic liquid melting point prediction. Journal of Chemical Physics, 2020, 153, 104101.	1.2	29
56	Radical Addition to Thioketones:â€‰ Computer-Aided Design of Spin Traps for Controlling Free-Radical Polymerization. Journal of Chemical Theory and Computation, 2006, 2, 1632-1645.	2.3	27
57	Toward Improved Performance of All-Organic Nitroxide Radical Batteries with Ionic Liquids: A Theoretical Perspective. ACS Sustainable Chemistry and Engineering, 2019, 7, 5367-5375.	3.2	27
58	Anionâ€“Anion Interactions in the Crystal Packing of Functionalized Methanide Anions: An Experimental and Computational Study. Crystal Growth and Design, 2014, 14, 1922-1932.	1.4	25
59	Electrochemical properties of crystallized dilithium squarate: insight from dispersion-corrected density functional theory. Physical Chemistry Chemical Physics, 2012, 14, 11398.	1.3	23
60	Theoretical and Experimental Insights into the Mechanism of the Nucleophilic Addition of Water and Methanol to Dicyanonitrosomethanide. Journal of Physical Chemistry B, 2010, 114, 16517-16527.	1.2	22
61	Comprehensive Vibrational Spectroscopic Investigation of trans,trans,trans-[Pt(N₃)₂(OH)₂(py)₂], a Pt(IV) Diazido Anticancer Prodrug Candidate. Inorganic Chemistry, 2016, 55, 5983-5992.	1.9	22
62	Difference in chemical bonding between lithium and sodium salts: influence of covalency on their solubility. Physical Chemistry Chemical Physics, 2017, 19, 17366-17372.	1.3	22
63	Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties. RSC Advances, 2013, 3, 19081.	1.7	21
64	Application of spin-ratio scaled MP2 for the prediction of intermolecular interactions in chemical systems. Physical Chemistry Chemical Physics, 2017, 19, 28936-28942.	1.3	21
65	Comparison of the Effective Fragment Potential Method with Symmetry-Adapted Perturbation Theory in the Calculation of Intermolecular Energies for Ionic Liquids. Journal of Chemical Theory and Computation, 2016, 12, 2553-2568.	2.3	19
66	Trends in Two- and Three-Body Effects in Multiscale Clusters of Ionic Liquids. Journal of Physical Chemistry B, 2017, 121, 577-588.	1.2	19
67	Increased stability of nitroxide radicals in ionic liquids: more than a viscosity effect. Physical Chemistry Chemical Physics, 2019, 21, 2882-2888.	1.3	18
68	The Supramolecular Architecture of Arene Complexes of Bis(polyfluorophenyl)mercurials. European Journal of Inorganic Chemistry, 2008, 2008, 4770-4780.	1.0	17
69	Raman spectroscopy as a tool for tracking cyclopropane fatty acids in genetically engineeredSaccharomyces cerevisiae. Analyst, The, 2019, 144, 901-912.	1.7	17
70	Novel SCS-IL-MP2 and SOS-IL-MP2 Methods for Accurate Energetics of Large-Scale Ionic Liquid Clusters. Journal of Chemical Theory and Computation, 2015, 11, 3610-3616.	2.3	15
71	Is it possible to control kinetic rates of radical polymerisation in ionic liquids?. Chemical Communications, 2018, 54, 11226-11243.	2.2	14
72	Electrochemical characterization and thermodynamic analysis of TEMPO derivatives in ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 10205-10217.	1.3	13

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73	Prediction of lattice energy of benzene crystals: A robust theoretical approach. Journal of Computational Chemistry, 2021, 42, 248-260.	1.5	12
74	A Redox Switchable Dihydrobenzo[b]pyrazine Pushâ€Pull System. Asian Journal of Organic Chemistry, 2014, 3, 619-623.	1.3	11
75	Cluster approach to the prediction of thermodynamic and transport properties of ionic liquids. Journal of Chemical Physics, 2018, 148, 193832.	1.2	11
76	Structural changes in coordination polymers in response to small changes in steric bulk (H vs.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.3	11
77	Investigation of cation binding and sensing by new crown ether core substituted naphthalene diimide systems. New Journal of Chemistry, 2019, 43, 2011-2018.	1.4	11
78	Unusual Products from Oxidation of Naphthalene Diimides. Asian Journal of Organic Chemistry, 2016, 5, 490-493.	1.3	10
79	A spectroscopic investigation into the binding of novel platinum(IV) and platium(II) anticancer drugs with DNA. Vibrational Spectroscopy, 2017, 92, 82-95.	1.2	10
80	The interplay between hydrogen bonding and Ï€-Ï€ stacking interactions in the crystal packing of N1-thyminyl derivatives, and implications for the photo-chemical [2Ï€ + 2Ï€]-cycloaddition of thyminyl compounds. Photochemical and Photobiological Sciences, 2012, 11, 1938-1951.	1.6	9
81	Configuration interaction study of the excited states of CO adsorbed on a Pt97 cluster. Chemical Physics, 2003, 291, 115-124.	0.9	8
82	Contrasting Synergistic Heterobimetallic (Naâ€“Mg) and Homometallic (Na or Mg) Bases in Metallation Reactions of Dialkylphenylphosphines and Dialkylanilines: Lateral versus Ring Selectivities. Chemistry - A European Journal, 2018, 24, 15669-15677.	1.7	8
83	Use of exchange maximization to generate starting vectors for self-consistent field calculations on metal cluster/adsorbate systems. Journal of Computational Chemistry, 2002, 23, 943-949.	1.5	6
84	A <scp>DLPNOâ€CCSD</scp>(T) benchmarking study of intermolecular interactions of ionic liquids. Journal of Computational Chemistry, 2022, 43, 106-120.	1.5	6
85	A supramolecular twist to the structures of bis(polyfluorophenyl)mercurials. CrystEngComm, 2011, 13, 88-92.	1.3	5
86	Influence of DFT Functionals and Solvation Models on the Prediction of Far-Infrared Spectra of Pt-Based Anticancer Drugs: Why Do Different Complexes Require Different Levels of Theory?. ACS Omega, 2019, 4, 5254-5269.	1.6	5
87	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 25558-25564.	1.3	5
88	Behavior of counterpoise correction in manyâ€body molecular clusters of organic compounds: <scp>Hartreeâ€“Fock</scp> interaction energy perspective. Journal of Computational Chemistry, 2022, 43, 568-576.	1.5	5
89	Inclusion of More Physics Leads to Less Data: Learning the Interaction Energy as a Function of Electron Deformation Density with Limited Training Data. Journal of Chemical Theory and Computation, 2022, 18, 1607-1618.	2.3	5
90	Active space and basis set effects in <scp>CASPT</scp>2 models of the 1,3â€butadieneâ€ethene cycloaddition and the 1,3â€butadiene dimerization. International Journal of Quantum Chemistry, 2015, 115, 989-1001.	1.0	4

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91	Predicting Entropic Effects of Water Mixing with Ionic Liquids Containing Anions of Strong Hydrogen Bonding Ability: Role of the Cation. Journal of Physical Chemistry B, 2020, 124, 9182-9194.	1.2	4
92	Anisotropic Thermal and Guestâ€Induced Responses of an Ultramicroporous Framework with Rigid Linkers. Chemistry - A European Journal, 2018, 24, 4774-4779.	1.7	3
93	Isomers of Alkali Metal (Methylbenzyl)allylamides: A Theoretical Perspective. ACS Omega, 2020, 5, 9448-9457.	1.6	3
94	An improved model for malaria pigment and Î² â€hematin: Fe(OEP)picrate. Journal of Raman Spectroscopy, 2017, 48, 1148-1157.	1.2	1
95	Spectroscopic Studies on Photoinduced Reactions of the Anticancer Prodrug, trans,trans,trans -[Pt(N3)2 (OH)2 (py)2]. Chemistry - A European Journal, 2018, 24, 5679-5679.	1.7	0