Ekaterina I Izgorodina

List of Publications by Year in Descending Order

95 papers	5,507 citations	39 h-index	73 g-index
99 ext. papers	5,979 ext. citations	5.4 avg, IF	5.97 L-index

#	Paper	IF	Citations
95	A DLPNO-CCSD(T) benchmarking study of intermolecular interactions of ionic liquids. *Journal of Computational Chemistry*, **2022**, 43, 106-120	3.5	1
94	Establishing the accuracy of density functional approaches for the description of noncovalent interactions in ionic liquids. *Physical Chemistry Chemical Physics*, **2021**, 23, 25558-25564	3.6	2
93	Experimental Evidence of Long-Lived Electric Fields of Ionic Liquid Bilayers. *Journal of the American Chemical Society*, **2021**, 143, 17431-17440	16.4	7
92	Prediction of lattice energy of benzene crystals: A robust theoretical approach. *Journal of Computational Chemistry*, **2021**, 42, 248-260	3.5	6
91	Electrochemical characterization and thermodynamic analysis of TEMPO derivatives in ionic liquids. *Physical Chemistry Chemical Physics*, **2021**, 23, 10205-10217	3.6	3
90	Isomers of Alkali Metal (Methylbenzyl)allylamides: A Theoretical Perspective. *ACS Omega*, **2020**, 5, 9448-9457	3.5	1
89	Ordered Solvents and Ionic Liquids Can Be Harnessed for Electrostatic Catalysis. *Journal of the American Chemical Society*, **2020**, 142, 12826-12833	16.4	22
88	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	3.4	3
87	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	8.3	8
86	A Systematic Study of DFT Performance for Geometry Optimizations of Ionic Liquid Clusters. *Journal of Chemical Theory and Computation*, **2020**, 16, 6735-6753	6.4	12
85	The effect of descriptor choice in machine learning models for ionic liquid melting point prediction. *Journal of Chemical Physics*, **2020**, 153, 104101	3.9	14
84	Investigation of cation binding and sensing by new crown ether core substituted naphthalene diimide systems. *New Journal of Chemistry*, **2019**, 43, 2011-2018	3.6	8
83	Toward Improved Performance of All-Organic Nitroxide Radical Batteries with Ionic Liquids: A Theoretical Perspective. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 5367-5375	8.3	14
82	Increased stability of nitroxide radicals in ionic liquids: more than a viscosity effect. *Physical Chemistry Chemical Physics*, **2019**, 21, 2882-2888	3.6	13
81	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	3.9	3
80	An Study of the Structure and Energetics of Hydrogen Bonding in Ionic Liquids. *Frontiers in Chemistry*, **2019**, 7, 208	5	33
79	Raman spectroscopy as a tool for tracking cyclopropane fatty acids in genetically engineered Saccharomyces cerevisiae. *Analyst, The*, **2019**, 144, 901-912	5	12

78	Cluster approach to the prediction of thermodynamic and transport properties of ionic liquids. *Journal of Chemical Physics*, **2018**, 148, 193832	3.9	9
77	Anisotropic Thermal and Guest-Induced Responses of an Ultramicroporous Framework with Rigid Linkers. *Chemistry - A European Journal*, **2018**, 24, 4774-4779	4.8	2
76	Cellulose-dissolving protic ionic liquids as low cost catalysts for direct transesterification reactions of cellulose. *Green Chemistry*, **2018**, 20, 1412-1422	10	45
75	Spectroscopic Studies on Photoinduced Reactions of the Anticancer Prodrug, trans,trans,trans-[Pt(N) (OH) (py)]. *Chemistry - A European Journal*, **2018**, 24, 5790-5803	4.8	22
74	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	4.8	
73	Contrasting Synergistic Heterobimetallic (Na-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	4.8	5
72	Is it possible to control kinetic rates of radical polymerisation in ionic liquids?. *Chemical Communications*, **2018**, 54, 11226-11243	5.8	8
71	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	3.6	31
70	Structural changes in coordination polymers in response to small changes in steric bulk (H vs. Me): an experimental and theoretical study. *CrystEngComm*, **2018**, 20, 4115-4126	3.3	9
69	Quantum Chemical Methods for the Prediction of Energetic, Physical, and Spectroscopic Properties of Ionic Liquids. *Chemical Reviews*, **2017**, 117, 6696-6754	68.1	137
68	Generalized spin-ratio scaled MP2 method for accurate prediction of intermolecular interactions for neutral and ionic species. *Journal of Chemical Physics*, **2017**, 146, 064108	3.9	26
67	A spectroscopic investigation into the binding of novel platinum(IV) and platium(II) anticancer drugs with DNA. *Vibrational Spectroscopy*, **2017**, 92, 82-95	2.1	9
66	Difference in chemical bonding between lithium and sodium salts: influence of covalency on their solubility. *Physical Chemistry Chemical Physics*, **2017**, 19, 17366-17372	3.6	15
65	Trends in Two- and Three-Body Effects in Multiscale Clusters of Ionic Liquids. *Journal of Physical Chemistry B*, **2017**, 121, 577-588	3.4	15
64	Application of spin-ratio scaled MP2 for the prediction of intermolecular interactions in chemical systems. *Physical Chemistry Chemical Physics*, **2017**, 19, 28936-28942	3.6	16
63	An improved model for malaria pigment and ħematin: Fe(OEP)picrate. *Journal of Raman Spectroscopy*, **2017**, 48, 1148-1157	2.3	1
62	Prediction of H NMR chemical shifts for clusters of imidazolium-based ionic liquids. *Physical Chemistry Chemical Physics*, **2017**, 19, 17411-17425	3.6	28
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, 5983-92	5.1	17

60	Mechanisms of low temperature capture and regeneration of CO2 using diamino protic ionic liquids. *Physical Chemistry Chemical Physics*, **2016**, 18, 1140-9	3.6	36
59	Unusual Products from Oxidation of Naphthalene Diimides. *Asian Journal of Organic Chemistry*, **2016**, 5, 490-493	3	8
58	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, 2553-68	6.4	13
57	Active space and basis set effects in CASPT2 models of the 1,3-butadiene-ethene cycloaddition and the 1,3-butadiene dimerization. *International Journal of Quantum Chemistry*, **2015**, 115, 989-1001	2.1	3
56	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, 3610-6	6.4	14
55	Physical Absorption Of CO2 in Protic and Aprotic Ionic Liquids: An Interaction Perspective. *Journal of Physical Chemistry B*, **2015**, 119, 11748-59	3.4	40
54	Two-coordinate hydrido-germylenes. *Chemical Communications*, **2015**, 51, 6854-7	5.8	29
53	Importance of dispersion forces for prediction of thermodynamic and transport properties of some common ionic liquids. *Physical Chemistry Chemical Physics*, **2014**, 16, 7209-21	3.6	85
52	New SCS- and SOS-MP2 Coefficients Fitted to Semi-Coulombic Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 3111-22	6.4	24
51	Anion□Anion Interactions in the Crystal Packing of Functionalized Methanide Anions: An Experimental and Computational Study. *Crystal Growth and Design*, **2014**, 14, 1922-1932	3.5	21
50	A Redox Switchable Dihydrobenzo[b]pyrazine Push-Pull System. *Asian Journal of Organic Chemistry*, **2014**, 3, 619-623	3	9
49	Ab initio prediction of proton NMR chemical shifts in imidazolium ionic liquids. *Journal of Physical Chemistry B*, **2013**, 117, 3186-97	3.4	54
48	Experimental and theoretical studies of tetramethoxy-p-benzoquinone: infrared spectra, structural and lithium insertion properties. *RSC Advances*, **2013**, 3, 19081	3.7	20
47	Diamino protic ionic liquids for CO2 capture. *Physical Chemistry Chemical Physics*, **2013**, 15, 19994-9	3.6	65
46	Assessment of Kohn-Sham density functional theory and M□ller-Plesset perturbation theory for ionic liquids. *Physical Chemistry Chemical Physics*, **2013**, 15, 13664-75	3.6	85
45	Assessment of atomic partial charge schemes for polarisation and charge transfer effects in ionic liquids. *Physical Chemistry Chemical Physics*, **2013**, 15, 1632-46	3.6	83
44	Large-scale ab initio calculations of archetypical ionic liquids. *Chemical Communications*, **2012**, 48, 1493-5	5.8	39
43	The interplay between hydrogen bonding and □□stacking interactions in the crystal packing of N1-thyminyl derivatives, and implications for the photo-chemical [2□+ 2□]-cycloaddition of thyminyl compounds. *Photochemical and Photobiological Sciences*, **2012**, 11, 1938-51	4.2	8

42	Electrochemical properties of crystallized dilithium squarate: insight from dispersion-corrected density functional theory. *Physical Chemistry Chemical Physics*, **2012**, 14, 11398-412	3.6	22
41	Theoretical Approaches to Ionic Liquids: From Past History to Future Directions **2012**, 181-230		2
40	Low overpotential water oxidation to hydrogen peroxide on a MnOx catalyst. *Energy and Environmental Science*, **2012**, 5, 9496	35.4	114
39	Protic pharmaceutical ionic liquids and solids: aspects of protonics. *Faraday Discussions*, **2012**, 154, 335-52; discussion 439-64, 465-71	3.6	110
38	Towards large-scale, fully ab initio calculations of ionic liquids. *Physical Chemistry Chemical Physics*, **2011**, 13, 4189-207	3.6	115
37	A supramolecular twist to the structures of bis(polyfluorophenyl)mercurials. *CrystEngComm*, **2011**, 13, 88-92	3.3	4
36	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, 14688-97	3.4	94
35	Nature of hydrogen bonding in charged hydrogen-bonded complexes and imidazolium-based ionic liquids. *Journal of Physical Chemistry B*, **2011**, 115, 14659-67	3.4	114
34	First Principles Prediction of The Propagation Rate Coefficients of Acrylic and Vinyl Esters: Are We There Yet?. *Macromolecules*, **2010**, 43, 553-560	5.5	59
33	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	3.8	71
32	Theoretical and experimental insights into the mechanism of the nucleophilic addition of water and methanol to dicyanonitrosomethanide. *Journal of Physical Chemistry B*, **2010**, 114, 16517-27	3.4	21
31	Ionicity and proton transfer in protic ionic liquids. *Physical Chemistry Chemical Physics*, **2010**, 12, 10341-7	3.6	200
30	Aluminium speciation in 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide/AlCl3 mixtures. *Chemistry - A European Journal*, **2009**, 15, 3435-47	4.8	62
29	Ion-pair binding energies of ionic liquids: can DFT compete with ab initio-based methods?. *Journal of Physical Chemistry A*, **2009**, 113, 7064-72	2.8	153
28	The Madelung Constant of Organic Salts. *Crystal Growth and Design*, **2009**, 9, 4834-4839	3.5	55
27	On the concept of ionicity in ionic liquids. *Physical Chemistry Chemical Physics*, **2009**, 11, 4962-7	3.6	545
26	On the components of the dielectric constants of ionic liquids: ionic polarization?. *Physical Chemistry Chemical Physics*, **2009**, 11, 2452-8	3.6	141
25	The role of exchange in systematic DFT errors for some organic reactions. *Physical Chemistry Chemical Physics*, **2009**, 11, 1138-42	3.6	57

24	Photo- and solvatochromic properties of nitrobenzospiropyran in ionic liquids containing the [NTf2]- anion. *Physical Chemistry Chemical Physics*, **2008**, 10, 5919-24	3.6	44
23	Protic ionic liquids based on the dimeric and oligomeric anions: [(AcO)xH(x-1)]-. *Physical Chemistry Chemical Physics*, **2008**, 10, 2972-8	3.6	115
22	How Accurate Are Approximate Methods for Evaluating Partition Functions for Hindered Internal Rotations?. *Journal of Physical Chemistry A*, **2008**, 112, 1956-1964	2.8	65
21	The Supramolecular Architecture of Arene Complexes of Bis(polyfluorophenyl)mercurials. *European Journal of Inorganic Chemistry*, **2008**, 2008, 4770-4780	2.3	15
20	Homoleptic 12-coordinate lanthanoids with eta(2)-nitroso ligands. *Dalton Transactions*, **2007**, 1371-3	4.3	38
19	Should contemporary density functional theory methods be used to study the thermodynamics of radical reactions?. *Journal of Physical Chemistry A*, **2007**, 111, 10754-68	2.8	131
18	Liquids intermediate between "molecular" and "ionic" liquids: liquid ion pairs?. *Chemical Communications*, **2007**, 3817-9	5.8	212
17	Ionic liquids in electrochemical devices and processes: managing interfacial electrochemistry. *Accounts of Chemical Research*, **2007**, 40, 1165-73	24.3	603
16	Towards a Better Understanding of Delocalized Charge in Ionic Liquid Anions. *Australian Journal of Chemistry*, **2007**, 60, 15	1.2	71
15	Energy-directed tree search: an efficient systematic algorithm for finding the lowest energy conformation of molecules. *Physical Chemistry Chemical Physics*, **2007**, 9, 2507-16	3.6	46
14	Accurate ab initio prediction of propagation rate coefficients in free-radical polymerization: Acrylonitrile and vinyl chloride. *Chemical Physics*, **2006**, 324, 96-110	2.3	125
13	Computational Studies of RAFT Polymerization. Mechanistic Insights and Practical Applications. *Macromolecular Rapid Communications*, **2006**, 27, 473-497	4.8	115
12	Quantum Chemical Mapping of Initialization Processes in RAFT Polymerization. *Macromolecular Rapid Communications*, **2006**, 27, 1015-1022	4.8	64
11	Is the Addition-Fragmentation Step of the RAFT Polymerisation Process Chain Length Dependent?. *Macromolecular Theory and Simulations*, **2006**, 15, 394-403	1.5	39
10	Thioketone spin traps as mediating agents for free radical polymerization processes. *Chemical Communications*, **2006**, 835-7	5.8	49
9	Electrochemistry at Negative Potentials in Bis(trifluoromethanesulfonyl)amide Ionic Liquids. *Zeitschrift Fur Physikalische Chemie*, **2006**, 220, 1483-1498	3.1	167
8	Radical Addition to Thioketones: Computer-Aided Design of Spin Traps for Controlling Free-Radical Polymerization. *Journal of Chemical Theory and Computation*, **2006**, 2, 1632-45	6.4	26
7	Addition-Fragmentation Kinetics of Fluorodithioformates (F-RAFT) in Styrene, Vinyl Acetate, and Ethylene Polymerization: An Ab Initio Investigation. *Macromolecules*, **2006**, 39, 4585-4591	5.5	52

6	Reliable low-cost theoretical procedures for studying addition-fragmentation in RAFT polymerization. *Journal of Physical Chemistry A*, **2006**, 110, 2486-92	2.8	78
5	Trends in R-X bond dissociation energies (R = Me, Et, i-Pr, t-Bu; X = H, CH3, OCH3, OH, F): a surprising shortcoming of density functional theory. *Journal of Physical Chemistry A*, **2005**, 109, 7558-66	2.8	203
4	Calculation of 0□ excitation energies of organic molecules by CIS(D) quantum chemical methods. *Chemical Physics*, **2004**, 305, 223-230	2.3	89
3	Configuration interaction study of the excited states of CO adsorbed on a Pt97 cluster. *Chemical Physics*, **2003**, 291, 115-124	2.3	7
2	Use of exchange maximization to generate starting vectors for self-consistent field calculations on metal cluster/adsorbate systems. *Journal of Computational Chemistry*, **2002**, 23, 943-9	3.5	6
1	Quantum-Chemical Studies of RAFT Polymerization: Methodology, Structure-Reactivity Correlations and Kinetic Implications5-49		13