Elena E Zvereva

List of Publications by Year
in descending order

35	1,337	471371 17	377752 34
papers	citations	h-index	g-index

35	35	35	1949
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Application of Density Functional Theory and Vibrational Spectroscopy Toward the Rational Design of Ionic Liquids. Journal of Physical Chemistry A, 2007, 111, 352-370.	1.1	238
2	Molecular Structure, Vibrational Spectra, and Hydrogen Bonding of the Ionic Liquid 1-Ethyl-3-methyl-1H-imidazolium Tetrafluoroborate. Helvetica Chimica Acta, 2004, 87, 2556-2565.	1.0	197
3	Ab Initio and DFT Predictions of Infrared Intensities and Raman Activities. Journal of Physical Chemistry A, 2011, 115, 63-69.	1.1	132
4	How Strong Is Hydrogen Bonding in Ionic Liquids? Combined X-ray Crystallographic, Infrared/Raman Spectroscopic, and Density Functional Theory Study. Journal of Physical Chemistry B, 2013, 117, 9094-9105.	1.2	130
5	Revisiting Ether-Derivatized Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2007, 111, 10095-10108.	1.2	121
6	A remarkable anion effect on palladium nanoparticle formation and stabilization in hydroxyl-functionalized ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 6026.	1.3	59
7	Phosphonium ionic liquids based on bulky phosphines: synthesis, structure and properties. Dalton Transactions, 2010, 39, 5564.	1.6	39
8	Quantification of Conventional and Nonconventional Charge-Assisted Hydrogen Bonds in the Condensed and Gas Phases. Journal of Physical Chemistry Letters, 2015, 6, 4431-4436.	2.1	39
9	Complex Formation of dâ€Metal Ions at the Interface of Tb^{III}â€Doped Silica Nanoparticles as a Basis of Substrateâ€Responsive Tb^{III}â€Centered Luminescence. ChemPhysChem, 2012, 13, 3357-3364.	1.0	35
10	Is There a Simple Way to Reliable Simulations of Infrared Spectra of Organic Compounds?. Journal of Physical Chemistry A, 2013, 117, 6664-6670.	1.1	33
11	Conjugation in and Optical Properties of 1-R-1,2-Diphospholes and 1-R-Phospholes. Journal of Physical Chemistry A, 2014, 118, 12168-12177.	1.1	30
12	Rationalization of Solvation and Stabilization of Palladium Nanoparticles in Imidazoliumâ€Based Ionic Liquids by DFT and Vibrational Spectroscopy. ChemPhysChem, 2012, 13, 1781-1790.	1.0	27
13	Fast Quantum Chemical Simulations of Infrared Spectra of Organic Compounds with the B97-3c Composite Method. Journal of Physical Chemistry A, 2019, 123, 3802-3808.	1.1	26
14	Application of Time-Dependent Density Functional Theory and Optical Spectroscopy toward the Rational Design of Novel 3,4,5-Triaryl-1-R-1,2-diphospholes. Journal of Physical Chemistry A, 2013, 117, 6827-6834.	1.1	24
15	Solvation of Palladium Clusters in an Ionic Liquid: A QM/MM Molecular Dynamics Study. Journal of Physical Chemistry C, 2016, 120, 4596-4604.	1.5	23
16	Solvation and stabilization of palladium nanoparticles in phosphonium-based ionic liquids: a combined infrared spectroscopic and density functional theory study. Physical Chemistry Chemical Physics, 2014, 16, 20672-20680.	1.3	22
17	Water transverse relaxation rates in aqueous dispersions of superparamagnetic iron oxide nanoclusters with diverse hydrophilic coating. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2014, 443, 450-458.	2.3	17
18	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 2570-2585.	2.3	16

#	Article	IF	Citations
19	A simple physical model for the simultaneous rationalisation of melting points and heat capacities of ionic liquids. Physical Chemistry Chemical Physics, 2010, 12, 13780.	1.3	15
20	Interface identification of the solid electrolyte interphase on graphite. Carbon, 2017, 111, 789-795.	5.4	15
21	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. Physical Chemistry Chemical Physics, 2020, 22, 15496-15508.	1.3	14
22	The Mechanism of Citryl-Coenzyme A Formation Catalyzed by Citrate Synthase. Journal of Physical Chemistry B, 2014, 118, 4505-4513.	1.2	12
23	The role of London dispersion interactions in strong and moderate intermolecular hydrogen bonds in the crystal and in the gas phase. Chemical Physics Letters, 2017, 672, 124-127.	1.2	11
24	Synthesis, IR/Raman, and quantum-chemical structural analysis of new octathiotetraphosphetane ammonium salts. Heteroatom Chemistry, 2011, 22, 24-30.	0.4	10
25	Decyl(Tri-Tert-Butyl)Phosphonium Tetrafluoroborate/Palladium Acetate: An Effective Catalyst for Cross-Coupling Reaction of Arylbromides with Phenylacetylene in Copper-Free Conditions. Phosphorus, Sulfur and Silicon and the Related Elements, 2013, 188, 168-170.	0.8	10
26	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. Photochemical and Photobiological Sciences, 2018, 17, 323-331.	1.6	10
27	IR and NMR spectra, intramolecular hydrogen bonding and conformations of mercaptothiacalix[4]arene molecules and their para-tert-butyl-derivative. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2008, 60, 281-291.	1.6	7
28	What quantum chemical simulations tell us about the infrared spectra, structure and interionic interactions of a bulk ionic liquid. Physical Chemistry Chemical Physics, 2022, 24, 7349-7355.	1.3	6
29	New Method for the Preparation of Octathiotetraphosphetanes on the Basis of Elemental Phosphorus and Sulfur: Structure and Properties. Phosphorus, Sulfur and Silicon and the Related Elements, 2011, 186, 852-853.	0.8	5
30	Leaching from Palladium Nanoparticles in an Ionic Liquid Leads to the Formation of Ionic Monometallic Species. Journal of Physical Chemistry Letters, 2017, 8, 3452-3456.	2.1	5
31	Coordination Features of P,S-Ligands Based on the Phosphorus Derivatives with I and Viii Group Metals. Phosphorus, Sulfur and Silicon and the Related Elements, 2013, 188, 490-492.	0.8	4
32	IR and NMR spectra, intramolecular hydrogen bonding and conformations of para-tert-butyl-aminothiacalix[4]arene in solid state and chloroform solution. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 872-879.	2.0	2
33	Guest-induced conformation shift of p-sulphonatothiacalix[4]arene in the solid state and solution manipulated by [Zn(dipy)₃]²⁺. Supramolecular Chemistry, 2010, 22, 203-211.	1.5	2
34	Synthesis and Some Properties of Transition Metal Complexes Based on the Octathiophophetane Ammonium Salts. Heteroatom Chemistry, 2014, 25, 434-441.	0.4	1
35	Corrigendum to â€œWater transverse relaxation rates in aqueous dispersions of superparamagnetic iron oxide nanoclusters with diverse hydrophilic coatingâ€•[Colloids Surf. A: Physicochem. Eng. Asp. 443 (2014) 450â€“458]. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2014, 453, 176.	2.3	0