Elena E Zvereva

List of Publications by Year in descending order

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35 papers	1,337 citations	471371 17 h-index	377752 34 g-index
35 all docs	35 docs citations	35 times ranked	1949 citing authors

#	Article	IF	Citations
1	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
2	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. Physical Chemistry Chemical Physics, 2020, 22, 15496-15508.	1.3	14
3	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
4	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
5	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
6	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
7	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
8	Interface identification of the solid electrolyte interphase on graphite. Carbon, 2017, 111, 789-795.	5.4	15
9	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
10	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
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	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
13	Synthesis and Some Properties of Transition Metal Complexes Based on the Octathiophophetane Ammonium Salts. Heteroatom Chemistry, 2014, 25, 434-441.	0.4	1
14	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
15	The Mechanism of Citryl-Coenzyme A Formation Catalyzed by Citrate Synthase. Journal of Physical Chemistry B, 2014, 118, 4505-4513.	1.2	12
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	Ab Initio and DFT Predictions of Infrared Intensities and Raman Activities. Journal of Physical Chemistry A, 2011, 115, 63-69.	1.1	132
27	Synthesis, IR/Raman, and quantum-chemical structural analysis of new octathiotetraphosphetane ammonium salts. Heteroatom Chemistry, 2011, 22, 24-30.	0.4	10
28	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
29	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
30	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
31	Phosphonium ionic liquids based on bulky phosphines: synthesis, structure and properties. Dalton Transactions, 2010, 39, 5564.	1.6	39
32	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
33	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
34	Revisiting Ether-Derivatized Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2007, 111, 10095-10108.	1.2	121
35	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