Ivan LjubiÄ

List of Publications by Year
in descending order

28	578	623734 14	610901 24
papers	citations	h-index	g-index

28	28	28	829
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Study of the Mechanism and Kinetics of Gas-Phase Ozone Additions to Ethene, Fluoroethene, and Chloroethene:Â A Multireference Approach. Journal of Physical Chemistry A, 2002, 106, 4745-4757.	2.5	81
2	Unraveling the Mechanisms of Nonradiative Deactivation in Model Peptides Following Photoexcitation of a Phenylalanine Residue. Journal of the American Chemical Society, 2012, 134, 20340-20351.	13.7	66
3	A multifaceted approach to hydrogen storage. Physical Chemistry Chemical Physics, 2011, 13, 16955.	2.8	64
4	A surprisingly complex aqueous chemistry of the simplest amino acid. A pulse radiolysis and theoretical study on H/D kinetic isotope effects in the reaction of glycine anions with hydroxyl radicals. Physical Chemistry Chemical Physics, 2009, 11, 2256.	2.8	30
5	Non-radiative relaxation of UV photoexcited phenylalanine residues: probing the role of conical intersections by chemical substitution. Physical Chemistry Chemical Physics, 2014, 16, 2285.	2.8	28
6	CASSCF/CASPT2 and TD-DFT Study of Valence and Rydberg Electronic Transitions in Fluorene, Carbazole, Dibenzofuran, and Dibenzothiophene. Journal of Physical Chemistry A, 2011, 115, 4840-4850.	2.5	27
7	Photoinduced Dynamics of Formic Acid Monomers and Dimers: The Role of the Double Hydrogen Bond. Journal of Physical Chemistry A, 2012, 116, 11467-11475.	2.5	26
8	Characterisation of the electronic structure of some stable nitroxyl radicals using variable energy photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 10734-10742.	2.8	25
9	Signature of the Conformational Preferences of Small Peptides:â€‰ a Theoretical Investigation. Journal of Physical Chemistry A, 2007, 111, 8650-8658.	2.5	21
10	An experimental NEXAFS and computational TDDFT and Î”DFT study of the gas-phase core excitation spectra of nitroxide free radical TEMPO and its analogues. Physical Chemistry Chemical Physics, 2016, 18, 10207-10217.	2.8	21
11	Towards understanding a mechanism for reversible hydrogen storage: theoretical study of transition metal catalysed dehydrogenation of sodium alanate. Physical Chemistry Chemical Physics, 2010, 12, 4012.	2.8	20
12	Systematic CASPT2 analysis of the geometry and force field of ozone with extrapolation to the infinite basis set. Chemical Physics Letters, 2004, 385, 214-219.	2.6	16
13	Theoretical Study of Structure, Vibrational Frequencies, and Electronic Spectra of Polychlorinated Dibenzo-p-dioxins. Journal of Physical Chemistry A, 2006, 110, 4524-4534.	2.5	16
14	Fluorocarbonyl oxide: CASSCF/CASPT2 study of structure, cis effect and unimolecular decomposition paths. Chemical Physics, 2005, 309, 157-165.	1.9	15
15	Reliability of Density Functional and Perturbation Theories for Calculating Core-Ionization Spectra of Free Radicals. Journal of Chemical Theory and Computation, 2014, 10, 2333-2343.	5.3	14
16	The study of the electronic structure of some N-heterocyclic carbenes (NHCs) by variable energy photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 10656-10667.	2.8	13
17	Dibenzo-p-dioxin. An ab Initio CASSCF/CASPT2 Study of the Ï€â^—Ï€* and nâ^—Ï€* Valence Excited States. Journal of Physical Chemistry A, 2005, 109, 8209-8217.	2.5	12
18	Ozonolysis of Fluoroethene:Â Theoretical Study of Unimolecular Decomposition Paths of Primary and Secondary Fluorozonide. Journal of Physical Chemistry A, 2005, 109, 2381-2393.	2.5	12

#	Article	IF	Citations
19	Theoretical Study of Structure, Vibrational Frequencies, and Electronic Spectra of Dibenzofuran and Its Polychlorinated Derivatives. Journal of Physical Chemistry A, 2007, 111, 1339-1350.	2.5	11
20	Characterisation of the electronic structure of galvinoxyl free radical by variable energy UPS, XPS and NEXAFS spectroscopy. Physical Chemistry Chemical Physics, 2018, 20, 2480-2491.	2.8	11
21	Synthesis and characterization of three novel molybdenum(VI) complexes: Mononuclear [MoO2(C6H4(O)CHNCH(COO)CH2C(O)NH2)], [MoO2(C19H19N2O5)(CH3OH)]ClÂ·CH3OH and dinuclear [Mo2O4(C6H4(O)CHNCH(COO)CH2C(O)NH2)2]. Polyhedron, 2009, 28, 562-568.	2.2	10
22	Reactions of 2-Propanol Radical with Halogenated Organics in Aqueous Solution: Theoretical Evidence for Proton-Coupled Electron Transfer and Competing Mechanisms. Journal of Physical Chemistry B, 2016, 120, 11810-11820.	2.6	9
23	Comparing the performances of various density functionals for modelling the mechanisms and kinetics of bimolecular free radical reactions in aqueous solution. Physical Chemistry Chemical Physics, 2019, 21, 23425-23440.	2.8	7
24	An efficient buffer-mediated control between free radical substitution and proton-coupled electron transfer: dehalogenation of iodoethane by the Î±-hydroxyethyl radical in aqueous solution. Physical Chemistry Chemical Physics, 2013, 15, 18001.	2.8	6
25	Proton-coupled electron transfer is the dominant mechanism of reduction of haloacetates by the Î±-hydroxyethyl radical in aqueous media. Physical Chemistry Chemical Physics, 2018, 20, 19829-19840.	2.8	5
26	Vibrationally resolved valence and core photoionization and photoexcitation spectra of an electron-deficient trivalent boron compound: the case of catecholborane. Physical Chemistry Chemical Physics, 2020, 22, 25396-25407.	2.8	5
27	Kinetics of chain reaction driven by proton-coupled electron transfer: Î±-hydroxyethyl radical and bromoacetate in buffered aqueous solutions. Physical Chemistry Chemical Physics, 2021, 23, 10429-10439.	2.8	5
28	Frontier orbitals stability of nitroxyl organic radicals probed by means of inner shell resonantly enhanced valence band photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2022, , .	2.8	2