

Zdzisław Xl;law Latajka

List of Publications by Year in descending order

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304602

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69
all docs

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docs citations

69
times ranked

1130
citing authors

#	ARTICLE	IF	CITATIONS
1	Application of density functional methods for the study of hydrogen-bonded systems: The hydrogen fluoride dimer. <i>Journal of Chemical Physics</i> , 1994, 101, 9793-9799.	1.2	138
2	Density functional theory applied to proton-transfer systems. A numerical test. <i>Chemical Physics Letters</i> , 1993, 208, 364-368.	1.2	89
3	Density Functional Study of Hydrogen-Bonded Systems: The Water-Carbon Monoxide Complex. <i>Journal of Physical Chemistry A</i> , 1997, 101, 5004-5009.	1.1	84
4	Critical assessment of density functional methods for study of proton transfer processes. (HF) ₂ . <i>Chemical Physics Letters</i> , 1995, 234, 159-164.	1.2	82
5	Basis sets for molecular interactions. 2. Application to H ₃ N-HF, H ₃ N-HOH, H ₂ O-HF, (NH ₃) ₂ , and H ₃ CH-OH ₂ . <i>Journal of Computational Chemistry</i> , 1987, 8, 674-682.	1.5	70
6	Basis sets for molecular interactions. 1. Construction and tests on (HF) ₂ and (H ₂ O) ₂ . <i>Journal of Computational Chemistry</i> , 1987, 8, 663-673.	1.5	61
7	Matrix isolation FTIR and ab initio study of complexes between formic acid and nitrogen. <i>Chemical Physics</i> , 1994, 189, 245-260.	0.9	53
8	Structure, energetics and vibrational spectra of dimers, trimers, and tetramers of HX (X = Cl, Br, I). <i>Chemical Physics</i> , 1997, 216, 37-52.	0.9	51
9	Proton transfer in the ground and first excited triplet states of malonaldehyde. <i>The Journal of Physical Chemistry</i> , 1992, 96, 9764-9767.	2.9	48
10	Structure, energetics, and vibrational spectrum of ammonia...water. <i>The Journal of Physical Chemistry</i> , 1990, 94, 217-221.	2.9	47
11	On the multiple B-N bonding in boron compounds using the topological analysis of electron localization function (ELF). <i>New Journal of Chemistry</i> , 2011, 35, 89-96.	1.4	40
12	On the Intramolecular Hydrogen Bond in Solution: Car-Parrinello and Path Integral Molecular Dynamics Perspective. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3505-3513.	2.3	32
13	High Kinetic Stability of HXeBr upon Interaction with Carbon Dioxide: HXeBr-CO ₂ Complex in a Xenon Matrix and HXeBr in a Carbon Dioxide Matrix. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4510-4517.	1.1	32
14	2-(Hydroxyimino)propanohydroxamic acid, a new effective ligand for aluminium. <i>Dalton Transactions RSC</i> , 2000, , 4201-4208.	2.3	31
15	Basis set superposition error in proton transfer potentials. <i>Chemical Physics Letters</i> , 1992, 196, 384-389.	1.2	27
16	Correlation between interaction energy and shift of the carbonyl stretching frequency. <i>Chemical Physics Letters</i> , 1990, 174, 179-184.	1.2	26
17	Dihydrogen-bonded complexes of xenon dihydride with water: Ab initio calculations and topological analysis of electron localisation function (ELF). <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 5521-5527.	1.3	26
18	Kinetics of proton transfer in (H ₃ C...CH ₃) ⁻ . <i>The Journal of Physical Chemistry</i> , 1987, 91, 724-730.	2.9	25

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19	Quantum Chemical Study of the Bimolecular Complex of HONO. Journal of Physical Chemistry A, 1999, 103, 6234-6239.	1.1	25
20	Quantum chemical calculations on FXeSiF. Chemical Physics Letters, 2001, 348, 147-154.	1.2	25
21	Basis set superposition errors and counterpoise corrections for some basis sets evaluated for a few X...M dimers. The Journal of Physical Chemistry, 1990, 94, 2267-2273.	2.9	23
22	Infrared matrix isolation and theoretical studies of SO ₂ -HNO ₃ and SO ₂ -HONO systems. Chemical Physics, 1998, 228, 17-29.	0.9	23
23	Car-Parrinello and path integral molecular dynamics study of the hydrogen bond in the chloroacetic acid dimer system. Journal of Chemical Physics, 2007, 127, 064304.	1.2	22
24	Spectroscopic and Computational Characterization of the HCO ⁺ -H ₂ O Complex. Journal of Physical Chemistry A, 2013, 117, 4385-4393.	1.1	22
25	Density functional studies of hydrogen-bonded systems. Chemical Physics, 2001, 263, 221-230.	0.9	20
26	Reaction of atomic hydrogen with formic acid. Physical Chemistry Chemical Physics, 2014, 16, 5993.	1.3	20
27	The proton position in amine-HX (X = Br, I) complexes. Chemical Physics, 1992, 166, 85-96.	0.9	19
28	Complexes between formic acid and carbon monoxide: an ab initio investigation. The Journal of Physical Chemistry, 1993, 97, 1152-1157.	2.9	19
29	Experimental and computational study of the HXe ⁺ -HY complexes (Y = Br and I). Journal of Chemical Physics, 2013, 138, 104314.	1.2	19
30	Proton Transfer Dynamics in Crystalline Maleic Acid from Molecular Dynamics Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1455-1461.	2.3	17
31	Kinetics and thermochemistry of the reversible gas phase reaction HONO+NH ₃ ⇌ H ₂ O+HONO studied by infrared diode laser spectroscopy. Chemical Physics Letters, 1994, 227, 6-12.	1.2	16
32	Density functional study of the H ₃ Ni-Cl ₂ system—the importance of Hartree-Fock exchange in density functional methods. Computational and Theoretical Chemistry, 1996, 371, 11-16.	1.5	16
33	Electron Localization Function Study on the Chemical Bonding in a Real Space for Tetrahedrane, Cubane, Adamantane, and Dodecahedrane and Their Perfluorinated Derivatives and Radical Anions. Journal of Physical Chemistry A, 2014, 118, 4147-4156.	1.1	15
34	Ab initio characterization of the xenon dihydride dimer (HXeH) ₂ . Chemical Physics Letters, 2003, 371, 295-303.	1.2	14
35	The protocovalent NO bond: Quantum chemical topology (QCT of ELF and ELI-D) study on the bonding in the nitrous acid HONO and its relevancy to the experiment. Chemical Physics Letters, 2008, 460, 559-562.	1.2	14
36	Electron localization function and electron localizability indicator applied to study the bonding in the peroxyxynitrous acid HOONO. Journal of Computational Chemistry, 2011, 32, 1528-1540.	1.5	14

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37	Proton-transfer dynamics in the (HCO ₃) ⁺ ₂ dimer of KHCO ₃ from Carâ€Parrinello and path-integrals molecular dynamics calculations. Acta Crystallographica Section B: Structural Science, 2010, 66, 222-228.	1.8	13
38	Quantum chemical topology study on the electronic structure of <i>cis</i> - and <i>trans</i> -FONO. Journal of Chemical Physics, 2010, 133, 034304.	1.2	13
39	On the multiple BO bonding using the topological analysis of Electron Localisation Function (ELF). Computational and Theoretical Chemistry, 2015, 1053, 130-141.	1.1	13
40	The dimerization shift of the OH-stretching fundamentals of the water dimer. Chemical Physics Letters, 1994, 217, 436-442.	1.2	12
41	Dynamical Nonplanarity of Benzene. Evidences from the Carâ€Parrinello Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2011, 2, 2881-2884.	2.1	12
42	Density functional study of the Xe2H3 ⁺ cation. Chemical Physics, 1999, 247, 215-224.	0.9	11
43	Proton distribution in KHCO ₃ from abinitio molecular dynamics simulation. Chemical Physics Letters, 2009, 476, 223-226.	1.2	11
44	Theoretical study of the H ₂ Oâ€CO hydrogen-bonded ternary complexes. Chemical Physics Letters, 1994, 222, 33-39.	1.2	10
45	Theoretical study of the geometry of GeH ₃ and electronic structure of SiH ₃ and GeH ₃ . Computational and Theoretical Chemistry, 1987, 150, 189-197.	1.5	9
46	Spectroscopic and theoretical studies of the OCOâ€HF complex in pressurized gases. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 3473-3479.	1.7	9
47	A mechanism of the 1,3â€dipolar cycloaddition between the hydrogen nitril HNO ₂ and acetylene HCCH: The electron localization function study on evolution of the chemical bonds. International Journal of Quantum Chemistry, 2011, 111, 2378-2389.	1.0	9
48	CNDO/2 molecular orbital calculations of dewar structures of pyridine. Journal of Molecular Structure, 1974, 21, 299-303.	1.8	8
49	Structural analysis and sheep pituitary receptor binding of GnRH and its complexes with metal ions. Journal of Inorganic Biochemistry, 2003, 94, 28-35.	1.5	8
50	Electron localization function (ELF) study on intramolecular delocalization of the electron density in the H ₂ X, H ₂ CX and XO ₂ (X=O, S, Se, Te) molecules: Role of the atomic core and lone pair. Journal of Molecular Structure, 2007, 844-845, 278-285.	1.8	7
51	The structure and chemical bonding in the N ₂ â€CuX and N ₂ â€XCu (X = F, Cl, Br) systems studied by means of the molecular orbital and Quantum Chemical Topology methods. Journal of Computational Chemistry, 2008, 29, 2677-2692.	1.5	7
52	Protocovalent Nâ€O bonding in methyl nitrite (CH ₃ ONO) and ethyl nitrite (C ₂ H ₅ ONO). Topological analysis of the electron localization function (ELF) and electron localizability indicator (ELI-D) functions. Chemical Physics Letters, 2010, 493, 392-398.	1.2	7
53	Site-site function and successive reaction counterpoise calculation of basis set superposition error for proton transfer. Computational and Theoretical Chemistry, 1995, 342, 153-159.	1.5	6
54	<i>Ab Initio</i> and Quantum Chemical Topology studies on the isomerization of HONO ₂ . Effect of the basis set in QCT. Journal of Computational Chemistry, 2010, 31, 2555-2567.	1.5	6

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55	Rotation around the glycosidic bond as driving force of proton transfer in protonated 2'-deoxyriboadenosine monophosphate (dAMP). <i>Chemical Physics Letters</i> , 2010, 490, 221-225.	1.2	6
56	Oxygen bound iodine (O ⁺ I): The Electron Localization Function (ELF) study on bonding in cis- and trans-IONO. <i>Chemical Physics Letters</i> , 2011, 506, 15-21.	1.2	6
57	Entropy versus aromaticity in the conformational dynamics of aromatic rings. <i>Journal of Molecular Modeling</i> , 2013, 19, 4073-4077.	0.8	5
58	Effects of Xenon Insertion into Hydrogen Bromide. Comparison of the Electronic Structure of the HBr $\cdot\cdot\cdot$ CO ₂ and HXeBr $\cdot\cdot\cdot$ CO ₂ Complexes Using Quantum Chemical Topology Methods: Electron Localization Function, Atoms in Molecules and Symmetry Adapted Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3980-3989.	1.1	5
59	Introduction: Special issue devoted in memory of Professor Oleg V. Shishkin. <i>Structural Chemistry</i> , 2016, 27, 1-1.	1.0	4
60	Direction of Protein Biosynthesis as a Reflection of the Prebiotic Environment. <i>Journal of Theoretical Biology</i> , 1997, 189, 151-158.	0.8	3
61	Tuning of character of the N ⁺ O bond in HONO from covalent to protocovalent by different types of intramolecular interactions. <i>Journal of Chemical Physics</i> , 2013, 139, 124308.	1.2	3
62	About the Aromaticity of <i>symm</i> -Triaminotrinitrobenzene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2244-2251.	1.1	2
63	On the structure of the 3B1 excited state of water. <i>Computational and Theoretical Chemistry</i> , 1995, 334, 127-136.	1.5	1
64	FONO: A difficult case for theory. The ELF and ELI-D topological studies on the chemical bonding using correlated wavefunctions. <i>Journal of Chemical Physics</i> , 2013, 138, 134313.	1.2	1
65	Impact of Deuteration and Temperature on Furan Ring Dynamics. <i>Molecules</i> , 2021, 26, 2889.	1.7	0
66	Computational Mechanochemistry. , 2016, , 233-243.		0