LÃ¡szlÃ³ von SzentpÃ¡ly

List of Publications by Year
in descending order

45 papers	2,095 citations	361413 20 h-index	243625 44 g-index
47 all docs	47 docs citations	47 times ranked	1814 citing authors

#	Article	IF	Citations
1	Understanding the Uniqueness of 2p Elements in Periodic Tables. Chemistry - A European Journal, 2020, 26, 15558-15564.	3.3	31
2	Why and When Is Electrophilicity Minimized? New Theorems and Guiding Rules. Journal of Physical Chemistry A, 2020, 124, 10897-10908.	2.5	54
3	Theorems and rules connecting bond energy and bond order with electronegativity equalization and hardness maximization. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	12
4	Correspondence on â€œCore Electron Topologies in Chemical Compounds: Case Study of Carbon versus Siliconâ€• Angewandte Chemie, 2019, 131, 10512-10515.	2.0	3
5	Correspondence on â€œCore Electron Topologies in Chemical Compounds: Case Study of Carbon versus Siliconâ€• Angewandte Chemie - International Edition, 2019, 58, 10404-10407.	13.8	2
6	Eliminating symmetry problems in electronegativity equalization and correcting selfâ€interaction errors in conceptual DFT. Journal of Computational Chemistry, 2018, 39, 1949-1969.	3.3	12
7	Hardness maximization or equalization? New insights and quantitative relations between hardness increase and bond dissociation energy. Journal of Molecular Modeling, 2017, 23, 217.	1.8	18
8	Comment on â€œA new equation based on ionization energies and electron affinities of atoms for calculating of group electronegativityâ€•by S. Kaya and C. Kaya [Comput. Theoret. Chem. 1052 (2015) 42â€“46]. Computational and Theoretical Chemistry, 2016, 1083, 72-74.	2.5	3
9	Symmetry Laws Improve Electronegativity Equalization by Orders of Magnitude and Call for a Paradigm Shift in Conceptual Density Functional Theory. Journal of Physical Chemistry A, 2015, 119, 1715-1722.	2.5	19
10	Physical Basis and Limitations of Equalization Rules and Principles: Valence-State Electronegativity and Valence-Pair-Affinity versus Operational Chemical Potential. Quantum Matter, 2015, 4, 47-55.	0.2	9
11	Chemical Potential of Molecules Contrasted to Averaged Atomic Electronegativities: Alarming Differences and Their Theoretical Rationalization. Journal of Physical Chemistry A, 2013, 117, 200-206.	2.5	20
12	Reply to â€œComment on 'Ruling Out Any Electrophilicity Equalization Principle'â€• Journal of Physical Chemistry A, 2012, 116, 792-795.	2.5	9
13	Ruling Out Any Electrophilicity Equalization Principle. Journal of Physical Chemistry A, 2011, 115, 8528-8531.	2.5	25
14	Universal Method to Calculate the Stability, Electronegativity, and Hardness of Dianions. Journal of Physical Chemistry A, 2010, 114, 10891-10896.	2.5	16
15	Atom-Based Thermochemistry: Predictions of the Sublimation Enthalpies of Group 12 Chalcogenides and the Formation Enthalpies of their Polonides. Journal of Physical Chemistry A, 2008, 112, 12695-12701.	2.5	22
16	Atom-Based Thermochemistry: Crystal Atomization and Sublimation Enthalpies in Linear Relationships to Molecular Atomization Enthalpy. Journal of the American Chemical Society, 2008, 130, 5962-5973.	13.7	11
17	Bornâ^'Haberâ^'Fajans Cycle Generalized:Â Linear Energy Relation between Molecules, Crystals, and Metals. Journal of the American Chemical Society, 2006, 128, 12314-12321.	13.7	29
18	Valence-State Atoms in Molecules. 7. Influence of Polarization and Bond-Charge on Spectroscopic Constants of Diatomic Molecules. Journal of Physical Chemistry A, 2004, 108, 595-606.	2.5	20

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19	Hard Bends Soft:â€‰ Bond Angle and Bending Force Constant Predictions for Dihalides, Dihydrides, and Dilithides of Groups 2 and 12. Journal of Physical Chemistry A, 2002, 106, 11945-11949.	2.5	37
20	Valence-State Atoms in Molecules. 6. Universal Ionicâ''Covalent Potential Energy Curves. Journal of Physical Chemistry A, 2001, 105, 9467-9477.	2.5	22
21	Modeling the charge dependence of total energy and its relevance to electrophilicity. International Journal of Quantum Chemistry, 2000, 76, 222-234.	2.0	45
22	Modeling the charge dependence of total energy and its relevance to electrophilicity. , 2000, 76, 222.		1
23	Valence State Atoms in Molecules. 5. Universal Scaling of the Inner Branch of Fifty RKR Potential Energy Curves. Comparison of the Valence State, Morse, and Rydberg Curves. Journal of Physical Chemistry A, 1999, 103, 9313-9322.	2.5	29
24	Valence States in Molecules. 3. Transferable Vibrational Force Constants from Homonuclear Data. Journal of Physical Chemistry A, 1998, 102, 10912-10915.	2.5	36
25	Fullab InitioConformational Spectrum of Î±,Î±â€˜-Diaminoacetone. Journal of Physical Chemistry A, 1997, 101, 3032-3037.	2.5	4
26	Valence states and a universal potential energy curve for covalent and ionic bonds. Chemical Physics Letters, 1995, 245, 209-214.	2.6	39
27	Modeling intercalatedPAH metabolites: Explanation for the bay region methyl effect. International Journal of Quantum Chemistry, 1995, 56, 191-199.	2.0	2
28	Computer simulation studies on Î²â€quinol clathrates with various gases. Interdependence of host and guest molecules. Journal of Chemical Physics, 1994, 101, 683-692.	3.0	7
29	A â€œslow-coolingâ€•Monte Carlo conformational space study of 18-crown-6 and its alkali metal cation complexes. Computational and Theoretical Chemistry, 1994, 308, 125-140.	1.5	7
30	Consistent point-charges at the 18-crown-6 atoms from correlated ab initio calculations. Computational and Theoretical Chemistry, 1994, 305, 249-260.	1.5	11
31	Electronic absorption and fluorescence spectra and excited singlet-state dipole moments of biologically important pyrimidines. Structural Chemistry, 1992, 3, 277-289.	2.0	36
32	Studies on electronegativity equalization. Computational and Theoretical Chemistry, 1991, 233, 71-81.	1.5	75
33	Which double-octet ABC molecules are bent? CI calculations on CaF2, and a softness criterion to predict bending. Chemical Physics Letters, 1990, 170, 555-560.	2.6	63
34	Pseudopotential and multiple scattering xÎ± calculations of nuclear quadrupole coupling constants and other properties of diatomic halogen molecules and their monoanions and monocations. Computational and Theoretical Chemistry, 1989, 184, 87-101.	1.5	15
35	Free electron PMO:F-omega model with variable electronegativity and self-interaction correction: application to ionic reaction intermediates. Computational and Theoretical Chemistry, 1989, 187, 139-160.	1.5	1
36	The MCS model of chemical initiation of cancer: ppp calculations on methylated and N-heteroaromatic polycycles. Computational and Theoretical Chemistry, 1987, 151, 245-257.	1.5	12

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37	Experimental and theoretical dipole moments of purines in their ground and lowest excited singlet states. Journal of Molecular Structure, 1987, 156, 119-135.	3.6	52
38	Dipole moments of indoles in their ground and the first excited singlet states. Computational and Theoretical Chemistry, 1986, 135, 105-116.	1.5	34
39	Carcinogenesis by polycyclic aromatic hydrocarbons: a multilinear regression on new type PMO indexes. Journal of the American Chemical Society, 1984, 106, 6021-6028.	13.7	60
40	A proper account of core-polarization with pseudopotentials: single valence-electron alkali compounds. Chemical Physics Letters, 1982, 89, 418-422.	2.6	898
41	Pseudopotential calculations on Rb+2, Cs+2, RbH+, CsH+ and the mixed alkali dimer ions. Chemical Physics Letters, 1982, 93, 555-559.	2.6	253
42	Potential curves for the alkali dimers and their cations: A new spectroscopic rule and its predictions. Chemical Physics Letters, 1982, 88, 321-324.	2.6	26
43	Electrophilic aromatic substitution: a free-electron approach. Chemical Physics Letters, 1981, 77, 352-358.	2.6	7
44	Inorganic and biological ti-electron systems computed with a pocket calculator. Journal of Molecular Structure, 1980, 60, 391-395.	3.6	2
45	Correlation of free-electron molecular orbital energies with Ï€ ionization energies of aromatic hydrocarbons. Chemical Physics Letters, 1979, 67, 63-68.	2.6	6