Padeleimon Karafiloglou

List of Publications by Year
in descending order

37	898	361413	454955
papers	citations	20 h-index	30 g-index

37	37	37	459
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Bridge Between MO And VB: The VB Description Of Functional Groups Inside Molecules By Means Of Poly-Electron Population Analysis. , 2024, , 625-641.		0
2	To Be or Not to Be: Demystifying the 2ndâ€Quantized Picture of Complex Electronic Configuration Patterns in Chemistry with Natural Polyâ€Electron Population Analysis. Journal of Computational Chemistry, 2019, 40, 1509-1520.	3.3	7
3	Ab initio quantum transport in AB-stacked bilayer penta-silicene using atomic orbitals. RSC Advances, 2018, 8, 34041-34046.	3.6	3
4	Natural bond orbitals: Local sets showing minimal intra-pair correlations and minimal unpaired electron populations. Computational and Theoretical Chemistry, 2017, 1100, 1-12.	2.5	18
5	Unpaired electrons, spin polarization, and bond orders in radicals from the 2â€RDM in orbital spaces: Basic notions and testing calculations. International Journal of Quantum Chemistry, 2014, 114, 696-707.	2.0	5
6	Unpaired electrons at the secondâ€order reduced density matrix level: Covalent bonding, and coulomb and fermi correlations in closed shell systems. International Journal of Quantum Chemistry, 2013, 113, 1775-1786.	2.0	9
7	Investigating sigma bonds in an electric field from the Paulingâ€™s perspective: the behavior of Clâ€“X and Hâ€“X (XÂ=ÂC, Si) bonds. Theoretical Chemistry Accounts, 2010, 126, 213-222.	1.4	25
8	Control of delocalization and structural changes by means of an electric field. Journal of Computational Chemistry, 2006, 27, 1883-1891.	3.3	25
9	Aspects of three-electron two-centre, four-electron three-centre and six-electron five-centre bonding in cycloimmonium ylides. Computational and Theoretical Chemistry, 2005, 729, 155-161.	1.5	11
10	Order of Coulomb and Fermi pairs: application in a Ï€-system. Chemical Physics Letters, 2004, 389, 400-404.	2.6	32
11	Comparing electron (de)localization in the through benzene and anthracene charge transfer. Chemical Physics, 2003, 289, 231-242.	1.9	26
12	UNDERSTANDING DELOCALIZATION AND HYPERCONJUGATION IN TERMS OF (COVALENT AND IONIC) RESONANCE STRUCTURES. Chemistry Education Research and Practice, 2002, 3, 119-127.	2.5	10
13	Looking at Chemical Bonding from Coulomb and Exchange Correlations in NAOs. Journal of Physical Chemistry A, 2001, 105, 4524-4534.	2.5	32
14	A method to calculate the weights of nbo electronic structures from Moffitt's theorem. Journal of Computational Chemistry, 2001, 22, 306-315.	3.3	37
15	Explicit calculation of Coulomb correlation in bond orbitals. Chemical Physics Letters, 2001, 345, 201-206.	2.6	14
16	Local description of the through phenyl transfer of a negative charge within resonance theory: topological effects in xylylene radical anions. Chemical Physics, 1999, 250, 1-12.	1.9	12
17	Quasi-linear dependence of one- and two- electron densities in natural bond orbitals. Chemical Physics Letters, 1999, 315, 446-448.	2.6	13
18	Interaction of two charge centres through bipyridines: is the â€œchemicalâ€•mechanism possible in a favourable electron transfer?. Computational and Theoretical Chemistry, 1998, 428, 221-229.	1.5	10

#	Article	IF	Citations
19	Electron Pair (De)Coupling in Aniline Radical Cation and Its Implications for Organic â€œMixed Valenceâ€• Systems. Journal of Physical Chemistry A, 1998, 102, 8004-8012.	2.5	39
20	Common features of various mechanisms of electron transfer across a 4,4â€²-bipyridine bridge: a theoretical evaluation of resonance structures of the transition state. Chemical Physics, 1997, 214, 171-182.	1.9	14
21	Calculation of the Weights of Resonance Structures of Molecules in Solution. The Journal of Physical Chemistry, 1995, 99, 6461-6467.	2.9	32
22	Natural polyelectron population analysis. International Journal of Quantum Chemistry, 1994, 52, 1127-1144.	2.0	36
23	Examination of the Hund rule in closed-shell systems: Investigation of spin correlation effects. International Journal of Quantum Chemistry, 1993, 47, 191-211.	2.0	17
24	Investigating the possibility of simultaneously finding an electron-hole and an electron-pair in a molecule: Delocalization, competition of ionic vs. covalent character, and related effects in push-pull ethylenes. International Journal of Quantum Chemistry, 1992, 44, 337-362.	2.0	27
25	Understanding molecular orbital wave functions in terms of resonance structures. Journal of Chemical Education, 1991, 68, 583.	2.3	52
26	Chemical structures from multi-electron density operators. Chemical Physics, 1990, 140, 373-383.	1.9	43
27	Electron-pair distributions in the carbon-carbon double bond: effects of a push-pull substitution. The Journal of Physical Chemistry, 1990, 94, 2763-2767.	2.9	31
28	An efficient calculation of the weights of non-orthogonal determinantal functions from the decomposition of MO wavefunctions. Computational and Theoretical Chemistry, 1989, 184, 213-219.	1.5	13
29	The double (or dynamic) spin polarization in Ï€ diradicals. Journal of Chemical Education, 1989, 66, 816.	2.3	49
30	How to obtain a mixed local-non-local molecular wavefunction. Chemical Physics, 1988, 127, 41-51.	1.9	23
31	A general p-electron (Mulliken-like) population analysis. Chemical Physics, 1988, 128, 373-381.	1.9	37
32	Ab initio calculation of the ferromagnetic interaction in a copper-vanadyl oxide (CuIIVIIO) heterodinuclear system. Journal of the American Chemical Society, 1988, 110, 5676-5680.	13.7	47
33	Valence bond analysis of molecular orbital wavefunctions: The ionicity of the B1Ï*f*u+ state of H2. Computational and Theoretical Chemistry, 1988, 180, 31-36.	1.5	11
34	The effect of electronic correlation on molecular wavefunctions. Chemical Physics, 1986, 104, 383-398.	1.9	51
35	Through bond interaction of two radical centers: Analysis of the spin polarization and related mechanisms in linear Ï€ diradicals. Journal of Chemical Physics, 1985, 82, 3728-3740.	3.0	45
36	AnalyticalMO study of the singlet-triplet coupling in xylylenes. International Journal of Quantum Chemistry, 1984, 25, 293-308.	2.0	18

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37	The valence bond description of xylylenes. Theoretica Chimica Acta, 1982, 61, 171-177.	0.8	24