Peter B Karadakov

List of Publications by Year
in descending order

105	2,616	201674	223800
papers	citations	27 h-index	46 g-index

107	107	107	2114
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Magnetic shielding paints an accurate and easy-to-visualize portrait of aromaticity. Chemical Communications, 2021, 57, 9504-9513.	4.1	10
2	Spin-Coupled Generalized Valence Bond Theory: New Perspectives on the Electronic Structure of Molecules and Chemical Bonds. Journal of Physical Chemistry A, 2021, 125, 2021-2050.	2.5	26
3	Role of Dynamical Electron Correlation in the Differences in Bonding between CaAlH3 and MgAlH3. Journal of Physical Chemistry A, 2021, 125, 3912-3919.	2.5	0
4	Mechanism of dye solubilization and de-aggregation by urea. Dyes and Pigments, 2021, 193, 109530.	3.7	4
5	Magnetic Shielding Study of Bonding and Aromaticity in Corannulene and Coronene. Chemistry, 2021, 3, 861-872.	2.2	15
6	Aromaticity reversals and their effect on bonding in the low-lying electronic states of cyclooctatetraene. Physical Chemistry Chemical Physics, 2021, 23, 24750-24756.	2.8	5
7	Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another. Journal of Chemical Education, 2021, 98, 3617-3620.	2.3	12
8	Can Antiâ€Aufbau DFT Calculations Estimate Singlet Excited State Aromaticity? Correspondence on â€œDibenzoarsepins: Planarization of 8Ï€â€Electron System in the Lowest Singlet Excited Stateâ€• Angewandte Chemie, 2020, 132, 9312-9314.	2.0	1
9	Excited-State Aromaticity Reversals in MÃ¶bius Annulenes. Journal of Physical Chemistry A, 2020, 124, 9611-9616.	2.5	13
10	Controlling the S₁ Energy Profile by Tuning Excited-State Aromaticity. Journal of the American Chemical Society, 2020, 142, 14985-14992.	13.7	48
11	Detailed Visualization of Aromaticity Using Isotropic Magnetic Shielding. Angewandte Chemie, 2020, 132, 19437-19443.	2.0	4
12	Norcorrole: Aromaticity and Antiaromaticity in Contest. Organic Letters, 2020, 22, 8676-8680.	4.6	15
13	Nuclear Magnetic Resonance and Computational Study of trans-(Î¼2:Î·2,Î·2-1,3-Butadiene)bis(trichloroplatinate(II)). Organometallics, 2020, 39, 4723-4734.	2.3	0
14	Are Multicentre Bond Indices and Related Quantities Reliable Predictors of Excited-State Aromaticity?. Molecules, 2020, 25, 4791.	3.8	4
15	Can Antiâ€Aufbau DFT Calculations Estimate Singlet Excited State Aromaticity? Correspondence on â€œDibenzoarsepins: Planarization of 8Ï€â€Electron System in the Lowest Singlet Excited Stateâ€• Angewandte Chemie - International Edition, 2020, 59, 9228-9230.	13.8	13
16	Detailed Visualization of Aromaticity Using Isotropic Magnetic Shielding. Angewandte Chemie - International Edition, 2020, 59, 19275-19281.	13.8	22
17	Nature of the chemical bonding in D_{3h} [MH₃M]⁺ cations (M = Be, Mg). International Journal of Quantum Chemistry, 2020, 120, e26183.	2.0	3
18	Is the S₂N₂ ring a singlet diradical? Critical analysis of alternative valence bond descriptions. International Journal of Quantum Chemistry, 2019, 119, e25845.	2.0	8

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19	The critical role played by water in controlling Pd catalyst speciation in arylcyanation reactions. Reaction Chemistry and Engineering, 2019, 4, 122-130.	3.7	8
20	Demonstration of Baird's rule complementarity in the singlet state with implications for excited-state intramolecular proton transfer. Physical Chemistry Chemical Physics, 2019, 21, 11608-11614.	2.8	34
21	Statistical Thermodynamics Unveils How Ions Influence an Aqueous Dielsâ€Alder Reaction. ChemPhysChem, 2019, 20, 1538-1544.	2.1	4
22	Magnetic Shielding, Aromaticity, Antiaromaticity and Bonding in the Lowâ€Lying Electronic States of S₂N₂. Chemistry - A European Journal, 2018, 24, 16791-16803.	3.3	19
23	Does the Electronic Structure of MÃ¶bius Annulenes Follow Heilbronner's Ideas?. ChemPhysChem, 2018, 19, 3186-3190.	2.1	6
24	Modern valence-bond descriptions of polycyclic fused aromatic compounds involving cyclopropenyl rings. Computational and Theoretical Chemistry, 2017, 1116, 32-39.	2.5	2
25	Magnetic Shielding Studies of C₂ and C₂H₂ Support Higher than Triple Bond Multiplicity in C₂. Chemistry - A European Journal, 2017, 23, 12949-12954.	3.3	21
26	Modern Valence-Bond Description of Homoaromaticity. Journal of Physical Chemistry A, 2016, 120, 8769-8779.	2.5	5
27	Magnetic Shielding, Aromaticity, Antiaromaticity, and Bonding in the Low-Lying Electronic States of Benzene and Cyclobutadiene. Journal of Organic Chemistry, 2016, 81, 11346-11352.	3.2	67
28	Mesomorphism and Photophysics of Some Metallomesogens Based on Hexasubstituted 2,2â€²:6â€², 2â€²â€²â€²â€²-Terpyridines. Chemistry - A European Journal, 2016, 22, 8215-8233.	3.3	31
29	Do large polycyclic aromatic hydrocarbons and graphene bend? How popular theoretical methods complicate finding the answer to this question. Chemical Physics Letters, 2016, 646, 190-196.	2.6	14
30	Exploring Chemical Bonds through Variations in Magnetic Shielding. Journal of Chemical Theory and Computation, 2016, 12, 558-563.	5.3	29
31	Bonding in Singlet and Triplet Butalene: Insights from Spin-Coupled Theory. Journal of Physical Chemistry A, 2015, 119, 2169-2175.	2.5	5
32	Shielding in and around Oxazole, Imidazole, and Thiazole: How Does the Second Heteroatom Affect Aromaticity and Bonding?. Journal of Organic Chemistry, 2015, 80, 7150-7157.	3.2	50
33	Bonding in benzodicyclobutadiene isomers: insights from modern valence bond theory. Molecular Physics, 2014, 112, 2840-2852.	1.7	3
34	Competition and cooperation: hydrogen and halogen bonding in co-crystals involving 4-iodotetrafluorobenzoic acid, 4-iodotetrafluorophenol and 4-bromotetrafluorophenol. CrystEngComm, 2014, 16, 4254-4264.	2.6	32
35	Halogenâ€and Hydrogenâ€Bonded Salts and Coâ€crystals Formed from 4â€Haloâ€2,3,5,6â€tetrafluorophenol and Cyclic Secondary and Tertiary Amines: Orthogonal and Nonâ€orthogonal Halogen and Hydrogen Bonding, and Synthetic Analogues of Halogenâ€Bonded Biological Systems. Chemistry - A European Journal, 2014, 20, 6721-6732.	3.3	43
36	Modern valence-bond description of aromatic annulene ions. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	4

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37	Electrophilic bromination of substituted stilbenes and stilbazoles: a quantum-chemical investigation. Physical Chemistry Chemical Physics, 2014, 16, 2576.	2.8	3
38	Chemical Bonding and Aromaticity in Furan, Pyrrole, and Thiophene: A Magnetic Shielding Study. Journal of Organic Chemistry, 2013, 78, 8037-8043.	3.2	105
39	Magnetic Shielding in and around Benzene and Cyclobutadiene: A Source of Information about Aromaticity, Antiaromaticity, and Chemical Bonding. Journal of Physical Chemistry A, 2013, 117, 518-523.	2.5	50
40	Halogen-bonded liquid crystals of 4-alkoxystilbazoles with molecular iodine: a very short halogen bond and unusual mesophase stability. Chemical Communications, 2013, 49, 3946.	4.1	47
41	Improved convergence of Hartreeâ€“Fock style excited-state wavefunctions using second-order optimisation with an exact Hessian. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	26
42	Spin-Coupled Theory for â€˜N Electrons in M Orbitalsâ€™ Active Spaces. Journal of Physical Chemistry A, 2012, 116, 7238-7244.	2.5	31
43	Quantum Chemical Investigation of Attractive Non-Covalent Interactions between Halomethanes and Rare Gases. Journal of Physical Chemistry A, 2012, 116, 10621-10628.	2.5	24
44	Halogen Bonding Interaction between Fluorohalides and Isocyanides. Journal of Physical Chemistry A, 2011, 115, 11079-11086.	2.5	20
45	Experimental and Theoretical Study of Halogen-Bonded Complexes of DMAP with Di- and Triiodofluorobenzenes. A Complex with a Very Short NÂ·Â·Â·I Halogen Bond. Crystal Growth and Design, 2010, 10, 3710-3720.	3.0	82
46	Modern valence bond description of the electronic mechanism of a [1,3] sigmatropic rearrangement linking bicyclo[3.2.0]heptâ€2â€ene and bicyclo[2.2.1]heptâ€2â€ene (norbornene). International Journal of Quantum Chemistry, 2009, 109, 1807-1811.	2.0	5
47	Comparison between the performances of the spinâ€projected Hartreeâ€“Fock, generalized valenceâ€bond, and spinâ€coupled approaches. International Journal of Quantum Chemistry, 2009, 109, 2447-2455.	2.0	6
48	Spin-coupled descriptions of organic reactivity. International Reviews in Physical Chemistry, 2009, 28, 169-206.	2.3	25
49	Ground- and Excited-State Aromaticity and Antiaromaticity in Benzene and Cyclobutadiene. Journal of Physical Chemistry A, 2008, 112, 7303-7309.	2.5	205
50	Spin-Coupled Description of Aromaticity in the Retro Dielsâ^'Alder Reaction of Norbornene. Journal of Physical Chemistry A, 2008, 112, 12823-12828.	2.5	9
51	Aromaticity and Antiaromaticity in the Low-Lying Electronic States of Cyclooctatetraene. Journal of Physical Chemistry A, 2008, 112, 12707-12713.	2.5	144
52	Mesomorphic 1,2,4-triazine-4-oxides in the synthesis of new heterocyclic liquid crystals. Journal of Materials Chemistry, 2008, 18, 1703.	6.7	21
53	A variationally stable compact Hartreeâ€“Fock-style wavefunction for a non-degenerate first excited state. Molecular Physics, 2007, 105, 2363-2373.	1.7	8
54	The unusual electronic mechanism of the [1,5] hydrogen shift in (Z)-1,3-pentadiene predicted by modern valence bond theory. Faraday Discussions, 2007, 135, 285-297.	3.2	10

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55	Modern Valence-Bond-Like Representations of SelectedD6hâ€œAromaticâ€•Rings. Journal of Physical Chemistry A, 2006, 110, 7913-7917.	2.5	7
56	The spin-coupled picture of clamped benzenes. Molecular Physics, 2006, 104, 677-680.	1.7	6
57	A spin-coupled study of the Claisen rearrangement of allyl vinyl ether. Theoretical Chemistry Accounts, 2006, 115, 212-220.	1.4	18
58	Spin-Coupled Study of the Electronic Mechanism of the Hetero-Dielsâ^'Alder Reaction of Acrolein and Ethene. Journal of Physical Chemistry A, 2005, 109, 231-235.	2.5	10
59	Spin-coupled study of addition reactions of singlet dihalocarbenes with ethene. International Journal of Quantum Chemistry, 2004, 98, 465-472.	2.0	12
60	Modern Valence Bond Description of the Electronic Mechanisms of SN2 Identity Reactions. Journal of Physical Chemistry A, 2004, 108, 914-920.	2.5	14
61	Aromatic vs Diradical Character in the Transition States of the Cope Rearrangements of 1,5-Hexadiene and Its Cyano Derivatives. Journal of Physical Chemistry A, 2004, 108, 194-202.	2.5	25
62	Calculation of NMR Chemical Shifts in Carbohydrates with ONIOM:â€‰ A Study of the Conformers of Î²-d-Glucopyranose. Journal of Physical Chemistry A, 2003, 107, 292-300.	2.5	22
63	Modern Valence-Bond Description of Chemical Reaction Mechanisms:â€‰ The 1,3-Dipolar Addition of Methyl Azide to Ethene. Journal of Physical Chemistry A, 2003, 107, 2548-2559.	2.5	10
64	Modern Valence Bond Description of Gas-Phase Pericyclic Reactions. Theoretical and Computational Chemistry, 2002, 10, 41-53.	0.4	19
65	Calculations of magnetic shielding for the tin nucleus in a series of tetra-organotin compounds using density functional theory. Physical Chemistry Chemical Physics, 2002, 4, 5925-5932.	2.8	29
66	Electron correlation and basis set effects on the 17O and 1H nuclear magnetic shieldings in water clusters (H2O)n (n=2â€“5). Journal of Molecular Structure, 2002, 602-603, 293-301.	3.6	12
67	Modern Valence-Bond Description of Chemical Reaction Mechanisms:Â The 1,3-Dipolar Addition of Diazomethane to Ethene. Journal of Organic Chemistry, 2001, 66, 4285-4292.	3.2	25
68	Reply to Comment â€œElectronic Reorganization in 1,3-Dipolar Cycloaddition of Fulminic Acid to Acetyleneâ€• Journal of Physical Chemistry A, 2001, 105, 10946-10946.	2.5	8
69	3 Theoretical description of reaction mechanisms: reaction pathways and electronic structure rearrangements. Annual Reports on the Progress of Chemistry Section C, 2001, 97, 61-90.	4.4	2
70	ONIOM as an efficient tool for calculating NMR chemical shielding constants in large molecules. Chemical Physics Letters, 2000, 317, 589-596.	2.6	101
71	Spin-Coupled Model of the Bonding in First-Row Transition Metal Methylene Monocations. Journal of Physical Chemistry A, 2000, 104, 7091-7098.	2.5	10
72	Bent-bond versus separated-bond models: A spin-coupled survey for a few organic and inorganic systems. International Journal of Quantum Chemistry, 1999, 74, 223-229.	2.0	22

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73	The Effect of Electron Correlation on the 19F Chemical Shifts in Fluorobenzenes. ACS Symposium Series, 1999, , 115-125.	0.5	3
74	Bentâ€bond versus separatedâ€bond models: A spinâ€coupled survey for a few organic and inorganic systems. International Journal of Quantum Chemistry, 1999, 74, 223-229.	2.0	2
75	The spin-coupled description of phenylenedimethylidene. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3301-3305.	1.7	5
76	Modern valence-bond description of chemical reaction mechanisms: the 1,3-dipolar addition of fulminic acid to ethyne. Theoretical Chemistry Accounts, 1998, 100, 222-229.	1.4	39
77	Spin-coupled description of fluorocyclophosphazenes (NPF2)3, (NPF2)4, (NPF2)5. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1541-1545.	1.7	2
78	Modern Valence-Bond Description of Chemical Reaction Mechanisms:Â Dielsâ^'Alder Reaction. Journal of the American Chemical Society, 1998, 120, 3975-3981.	13.7	45
79	Antiferromagnetic Spin Couplings in Cyclobutadiene Chains. Journal of Physical Chemistry B, 1997, 101, 6688-6691.	2.6	14
80	Chemical bonding in oxofluorides of hypercoordinate sulfur. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2247-2254.	1.7	46
81	Study of the electronic states of the allyl radical using spin-coupled valence bond theory. Journal of Chemical Physics, 1997, 106, 3663-3672.	3.0	26
82	Spin-Coupled Valence Bond Study of the Reaction between Benzene and a Methyl Cation. Journal of Physical Chemistry A, 1997, 101, 2886-2892.	2.5	16
83	The electronic structure of borabenzene: Combination of an aromatic ?-sextet and a reactive ?-framework. International Journal of Quantum Chemistry, 1997, 63, 441-449.	2.0	26
84	Modern valence bond representations of CASSCF wavefunctions. Theoretica Chimica Acta, 1996, 93, 343-366.	0.8	143
85	Chemical bonding in oxohalides of hypercoordinate nitrogen and phosphorus. International Journal of Quantum Chemistry, 1996, 60, 393-400.	2.0	19
86	Modern valence-bond description of the electronic structure of benzocyclobutadiene. International Journal of Quantum Chemistry, 1996, 60, 545-552.	2.0	16
87	Modern valence bond representations of CASSCF wavefunctions. Theoretica Chimica Acta, 1996, 93, 343.	0.8	4
88	Modern valence-bond description of bonding in strained three-membered rings: cyclopropane, aziridine, ethene oxide, phosphirane and thiirane. Computational and Theoretical Chemistry, 1995, 341, 13-24.	1.5	10
89	The Electronic Structure of Cyclooctatetraene and the Modern Valence-Bond Understanding of Antiaromaticity. The Journal of Physical Chemistry, 1995, 99, 10186-10195.	2.9	39
90	SPINS: A collection of algorithms for symbolic generation and transformation of many-electron spin eigenfunctions. Theoretica Chimica Acta, 1995, 90, 51-73.	0.8	49

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91	Modern valence-bond description of the ground state of Li2 ?. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3751.	1.7	6
92	Bonding in YXXY dihalides and dihydrides of dioxygen and disulfur. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3357.	1.7	30
93	Aromatic electrophilic substitution. A modern valence bond study. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 4011.	1.7	11
94	Catalytic chemistry of furan and thiophene. Ab initio calculations, using the spin-coupled valence bond method, of the interaction of furan and thiophene with a positively charged centre. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 749.	1.7	7
95	Modern valence-bond description of (CH3)4Li4. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 3363.	1.7	6
96	Spin-coupled description of organic reaction pathways: the cycloaddition reaction of two ethene molecules. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1643.	1.7	10
97	Spin-Coupled Study of the Electronic Structure of Polyenyl Radicals C3H5-C9H11. Journal of the American Chemical Society, 1994, 116, 2075-2084.	13.7	18
98	Chemical Bonding to Hypercoordinate Second-Row Atoms: d Orbital Participation versus Democracy. Journal of the American Chemical Society, 1994, 116, 4414-4426.	13.7	98
99	The Nature of the Carbon-Carbon Bonds in Cyclopropane and Cyclobutane: A Comparison Based on Spin-Coupled Theory. Journal of the American Chemical Society, 1994, 116, 7714-7721.	13.7	23
100	Sequential cycloaddition-cycloreversion-cycloaddition-cope rearrangement with an annelated norbornadiene and electrophilic dienes. unusual [Ï€2s + Ï€2a + Ïƒ2a] transformation of a pentacyclo-[11.4.0.17,10.04,13.06,11]octadeca-3,8,14,17-tetraene.1. Tetrahedron, 1993, 49, 4699-4710.	1.9	8
101	The Lowest Singlet and Triplet States of oâ€Benzyne: Spinâ€Coupled Interpretation of the Electronic Structure at CAS SCF Equilibrium Geometries. Israel Journal of Chemistry, 1993, 33, 253-264.	2.3	27
102	Bent versus .sigma.-.pi. bonds in ethene and ethyne: the spin-coupled point of view. Journal of the American Chemical Society, 1993, 115, 6863-6869.	13.7	34
103	Coreâ€valence separation in the spinâ€coupled wave function: A fully variational treatment based on a secondâ€order constrained optimization procedure. Journal of Chemical Physics, 1992, 97, 7637-7655.	3.0	76
104	The unusual reaction of tetrachlorothiophene dioxide with an adduct of 5,6-bismethylenenorbornene and hexachloronorbornadiene. Journal of the Chemical Society Chemical Communications, 1991, , 1763.	2.0	3
105	Investigating IstvÃ¡n Mayer's â€œimprovedâ€•definitions of bond orders and free valence for correlated singletâ€state wave functions. International Journal of Quantum Chemistry, 0, , e26612.	2.0	1