David Danovich

List of Publications by Citations

119	4,950	40	67
papers	citations	h-index	g-index
129	5,595	8.8	5.83
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
119	Two-State Reactivity in Organometallic Gas-Phase Ion Chemistry. *Helvetica Chimica Acta*, **1995**, 78, 1393-1407	2	270
118	Charge-shift bonding and its manifestations in chemistry. *Nature Chemistry*, **2009**, 1, 443-9	17.6	258
117	Spin□Orbit Coupling in the Oxidative Activation of H□H by FeO+. Selection Rules and Reactivity Effects. *Journal of the American Chemical Society*, **1997**, 119, 1773-1786	16.4	222
116	A different story of pi-delocalization--the distortivity of pi-electrons and its chemical manifestations. *Chemical Reviews*, **2001**, 101, 1501-39	68.1	222
115	Dihydrogen contacts in alkanes are subtle but not faint. *Nature Chemistry*, **2011**, 3, 323-30	17.6	199
114	Charge-shift bonding--a class of electron-pair bonds that emerges from valence bond theory and is supported by the electron localization function approach. *Chemistry - A European Journal*, **2005**, 11, 6358-71	4.8	195
113	On The Nature of the Halogen Bond. *Journal of Chemical Theory and Computation*, **2014**, 10, 3726-37	6.4	194
112	Structure and reactivity/selectivity control by oriented-external electric fields. *Chemical Society Reviews*, **2018**, 47, 5125-5145	58.5	170
111	Quadruple bonding in C2 and analogous eight-valence electron species. *Nature Chemistry*, **2012**, 4, 195-200	17.6	164
110	The □Rebound Controversy□An Overview and Theoretical Modeling of the Rebound Step in C□H Hydroxylation by Cytochrome P450. *European Journal of Inorganic Chemistry*, **2004**, 2004, 207-226	2.3	138
109	Why Does Benzene Possess a D6h Symmetry? A Quasiclassical State Approach for Probing .pi.-Bonding and Delocalization Energies. *Journal of the American Chemical Society*, **1995**, 117, 7760-7768	16.4	121
108	Understanding the Nature of the CH□□HC Interactions in Alkanes. *Journal of Chemical Theory and Computation*, **2013**, 9, 1977-91	6.4	90
107	Origins of the Exalted b2u Frequency in the First Excited State of Benzene. *Journal of the American Chemical Society*, **1996**, 118, 666-671	16.4	77
106	Electric-Field Mediated Chemistry: Uncovering and Exploiting the Potential of (Oriented) Electric Fields to Exert Chemical Catalysis and Reaction Control. *Journal of the American Chemical Society*, **2020**, 142, 12551-12562	16.4	75
105	Oriented-External Electric Fields Create Absolute Enantioselectivity in Diels-Alder Reactions: Importance of the Molecular Dipole Moment. *Journal of the American Chemical Society*, **2018**, 140, 13350-13359	16.4	75
104	A single transition state serves two mechanisms: an ab initio classical trajectory study of the electron transfer and substitution mechanisms in reactions of ketyl radical anions with alkyl halides. *Journal of the American Chemical Society*, **2001**, 123, 130-4	16.4	67
103	The nature of the fourth bond in the ground state of C2: the quadruple bond conundrum. *Chemistry - A European Journal*, **2014**, 20, 6220-32	4.8	60

102	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. *Coordination Chemistry Reviews*, **2017**, 344, 355-362	23.2	58
101	Green's function methods for calculating ionization potentials, electron affinities, and excitation energies. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 377-387	7.9	57
100	Spin□Orbit Coupling Patterns Induced by Twist and Pyramidalization Modes in C2H4:´A Quantitative Study and a Qualitative Analysis. *Journal of Physical Chemistry A*, **1998**, 102, 5923-5936	2.8	56
99	What Is Physically Wrong with the Description of Odd-Electron Bonding by Hartree-Fock Theory? A Simple Nonempirical Remedy. *Journal of the American Chemical Society*, **1995**, 117, 9003-9011	16.4	54
98	17O, 31P and 183W NMR spectra of paramagnetic complexes with the heteropolytungstate anion [Ln(PW11O39)2]11□and their co. *Polyhedron*, **1990**, 9, 1249-1256	2.7	54
97	Silynes (RC?SiR') and Disilynes (RSi?SiR'): Why Are Less Bonds Worth Energetically More?. *Angewandte Chemie - International Edition*, **2001**, 40, 4023-4026	16.4	53
96	The First Persistent β-Silyl-Substituted Vinyl Cation. *Angewandte Chemie International Edition in English*, **1991**, 30, 1479-1482		53
95	Charge-Shift Bonding: A New and Unique Form of Bonding. *Angewandte Chemie - International Edition*, **2020**, 59, 984-1001	16.4	53
94	The Nature of the Idealized Triple Bonds Between Principal Elements and the □Origins of Trans-Bent Geometries-A Valence Bond Study. *Journal of Chemical Theory and Computation*, **2011**, 7, 955-68	6.4	49
93	The origins of the directionality of noncovalent intermolecular interactions. *Journal of Computational Chemistry*, **2016**, 37, 34-45	3.5	49
92	A response to the critical comments on "One molecule, two atoms, three views, four bonds?". *Angewandte Chemie - International Edition*, **2013**, 52, 5926-8	16.4	48
91	Dissociative Electron Transfer, Substitution, and Borderline Mechanisms in Reactions of Ketyl Radical Anions. Differences and Difficulties in Their Reaction Paths. *Journal of the American Chemical Society*, **1997**, 119, 9237-9245	16.4	48
90	Comparison of C□Cl and Si□Cl Bonds. A Valence Bond Study. *The Journal of Physical Chemistry*, **1996**, 100, 5715-5720		48
89	Using Valence Bond Theory to Understand Electronic Excited States: Application to the Hidden Excited State (21Ag) of C2nH2n+2 (n = 2□4) Polyenes. *Journal of Physical Chemistry A*, **2000**, 104, 8744-8758	2.8	47
88	A different story of benzene. *Computational and Theoretical Chemistry*, **1997**, 398-399, 155-167		46
87	A tutorial for understanding chemical reactivity through the valence bond approach. *Chemical Society Reviews*, **2014**, 43, 4968-88	58.5	45
86	Does solvation cause symmetry breaking in the I3□ion in aqueous solution?. *Journal of Chemical Physics*, **1998**, 109, 9928-9937	3.9	45
85	Catalysis of Methyl Transfer Reactions by Oriented External Electric Fields: Are Gold-Thiolate Linkers Innocent?. *Journal of the American Chemical Society*, **2018**, 140, 4354-4362	16.4	44

84	Blended hydrogen atom abstraction and proton-coupled electron transfer mechanisms of closed-shell molecules. *Chemical Science*, **2012**, 3, 1903	9.4	43
83	Hydrogen- and Halogen-Bonds between Ions of like Charges: Are They Anti-Electrostatic in Nature?. *Journal of Computational Chemistry*, **2018**, 39, 481-487	3.5	42
82	External electric field effects on chemical structure and reactivity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1438	7.9	42
81	Electron-transfer reactivity in the activation of organic fluorides by bare metal monocations. *Chemical Physics Letters*, **1997**, 278, 391-397	2.5	41
80	The Quadruple Bonding in C2 Reproduces the Properties of the Molecule. *Chemistry - A European Journal*, **2016**, 22, 4116-28	4.8	41
79	A Unified Theory for the Blue- and Red-Shifting Phenomena in Hydrogen and Halogen Bonds. *Journal of Chemical Theory and Computation*, **2017**, 13, 1626-1637	6.4	40
78	Ionization potentials of porphyrins and phthalocyanines. A comparative benchmark study of fast improvements of Koopman's Theorem. *Journal of the Chemical Society Perkin Transactions II*, **1999**, 1653-1662		37
77	The Self-Association of Graphane Is Driven by London Dispersion and Enhanced Orbital Interactions. *Journal of Chemical Theory and Computation*, **2015**, 11, 1621-30	6.4	36
76	Oriented External Electric Fields: Tweezers and Catalysts for Reactivity in Halogen-Bond Complexes. *Journal of the American Chemical Society*, **2019**, 141, 7122-7136	16.4	34
75	An excursion from normal to inverted C-C bonds shows a clear demarcation between covalent and charge-shift C-C bonds. *ChemPhysChem*, **2009**, 10, 2658-69	3.2	34
74	Das erste persistente Silyl-substituierte Vinyl-Kation. *Angewandte Chemie*, **1991**, 103, 1546-1549	3.6	34
73	Electrophilic Aromatic Substitution Reactions: Mechanistic Landscape, Electrostatic and Electric-Field Control of Reaction Rates, and Mechanistic Crossovers. *Journal of the American Chemical Society*, **2019**, 141, 9719-9730	16.4	32
72	Charge-Shift Bonding Emerges as a Distinct Electron-Pair Bonding Family from Both Valence Bond and Molecular Orbital Theories. *Journal of Chemical Theory and Computation*, **2014**, 10, 2410-8	6.4	32
71	Ferromagnetic Bonding: Properties of High-Spin Lithium Clusters n+1Lin (n = 2–12) Devoid of Electron Pairs. *Journal of Physical Chemistry A*, **2002**, 106, 4961-4969	2.8	32
70	No-Pair Bonding in the High-Spin 3 State of Li2. A Valence Bond Study of Its Origins. *Journal of the American Chemical Society*, **1999**, 121, 3165-3174	16.4	32
69	Ab initio calculations for small iodo clusters. Good performance of relativistic effective core potentials. *Chemical Physics Letters*, **1995**, 233, 249-256	2.5	31
68	An accurate barrier for the hydrogen exchange reaction from valence bond theory: is this theory coming of age?. *Chemistry - A European Journal*, **2003**, 9, 4540-7	4.8	28
67	No-Pair Bonding in High-Spin Lithium Clusters: n+1Lin (n = 2–8). *Journal of Physical Chemistry A*, **2000**, 104, 11223-11231	2.8	28

66	Towards the Definition of the Maximum Allowable Tightness of an Electron Transfer Transition State in the Reactions of Radical Anions and Alkyl Halides. *Angewandte Chemie International Edition in English*, **1996**, 35, 1098-1100		28
65	Synthesis and X-ray Molecular Structure of the First Stable Organic Radical Lacking Resonance Stabilization. *Journal of the American Chemical Society*, **1999**, 121, 8118-8119	16.4	27
64	The Twin-Excited State as a Probe for the Transition State in Concerted Unimolecular Reactions: The Semibullvalene Rearrangement. *Angewandte Chemie - International Edition*, **1998**, 37, 1394-1397	16.4	26
63	Ferromagnetic bonding in high-spin alkali-metal clusters. How does sodium compare to lithium?. *Physical Chemistry Chemical Physics*, **2003**, 5, 158-164	3.6	26
62	TITAN: A Code for Modeling and Generating Electric Fields-Features and Applications to Enzymatic Reactivity. *Journal of Computational Chemistry*, **2020**, 41, 74-82	3.5	26
61	Ferromagnetic bonding: high spin copper clusters (n+1)Cu(n); n = 2-14) devoid of electron pairs but possessing strong bonding. *Journal of Physical Chemistry A*, **2006**, 110, 8510-8	2.8	24
60	Valence Bond Theory Reveals Hidden Delocalized Diradical Character of Polyenes. *Journal of the American Chemical Society*, **2017**, 139, 9302-9316	16.4	23
59	Electron-transfer reactivity in the activation of organic fluorides by bare metal monocations. *Chemical Physics Letters*, **1997**, 273, 164-170	2.5	23
58	Reactivity Paradigms: Transition State Structure, Mechanisms of Barrier Formation, and Stereospecificity of Nucleophilic Substitutions on .sigma.-Cation Radicals. *Journal of the American Chemical Society*, **1995**, 117, 3205-3222	16.4	23
57	The ICN-INC system: experiment and quantum chemical calculations. *Chemical Physics Letters*, **1994**, 225, 391-397	2.5	23
56	Nature of the Three-Electron Bond. *Journal of Physical Chemistry A*, **2018**, 122, 1873-1885	2.8	21
55	Spin-Orbit Coupling and Outer-Core Correlation Effects in Ir- and Pt-Catalyzed C-H Activation. *Journal of Chemical Theory and Computation*, **2012**, 8, 1641-5	6.4	21
54	New Landscape of Electron-Pair Bonding: Covalent, Ionic, and Charge-Shift Bonds. *Structure and Bonding*, **2015**, 169-211	0.9	19
53	Covalent vs Charge-Shift Nature of the Metal-Metal Bond in Transition Metal Complexes: A Unified Understanding. *Journal of the American Chemical Society*, **2020**, 142, 12277-12287	16.4	19
52	Formation of Carbon-Carbon Triply Bonded Molecules from Two Free Carbyne Radicals via a Conical Intersection. *Journal of Physical Chemistry Letters*, **2013**, 4, 58-64	6.4	19
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50	Protonated alcohols are examples of complete charge-shift bonds. *Journal of Organic Chemistry*, **2014**, 79, 9998-10001	4.2	18
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48	Computational prediction of the ISC rate for triplet norbornene. *Chemical Physics Letters*, **2000**, 322, 358-362	2.5	18
47	A Response to a Comment by G. Frenking and M. Hermann on: "The Quadruple Bonding in C Reproduces the Properties of the Molecule". *Chemistry - A European Journal*, **2016**, 22, 18977-18980	4.8	17
46	No-pair bonding in coinage metal dimers. *Journal of Physical Chemistry A*, **2008**, 112, 12995-3001	2.8	16
45	A reliable and inexpensive method for calculating ionization potentials and electron affinities of radicals and molecules. *Journal of the Chemical Society Perkin Transactions II*, **1993**, 321		16
44	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. *Angewandte Chemie - International Edition*, **2019**, 58, 12332-12338	16.4	15
43	Photoinduced proton transfer in a pyridine based polymer gel. *Journal of Physical Chemistry B*, **2010** , 114, 10728-33	3.4	15
42	To hybridize or not to hybridize? This is the dilemma. *Computational and Theoretical Chemistry*, **2017**, 1116, 242-249	2	14
41	Cross Conjugation in Polyenes and Related Hydrocarbons: What Can Be Learned from Valence Bond Theory about Single-Molecule Conductance?. *Journal of the American Chemical Society*, **2019**, 141, 6030-6047	16.4	14
40	Bonding with parallel spins: high-spin clusters of monovalent metal atoms. *Accounts of Chemical Research*, **2014**, 47, 417-26	24.3	14
39	A Response to the Critical Comments on One Molecule, Two Atoms, Three Views, Four Bonds? *Angewandte Chemie*, **2013**, 125, 6040-6042	3.6	14
38	Ionization Energies of Linear and Cyclic Polysilanes. Application of the Green's Function Method Coupled with Semiempirical Molecular Orbital Calculations. *Organometallics*, **1996**, 15, 350-360	3.8	14
37	Inner-sphere electron transfer in metal-cation chemistry. *International Journal of Mass Spectrometry* , **2000**, 200, 163-173	1.9	13
36	Charge-Shift Bonding: A New and Unique Form of Bonding. *Angewandte Chemie*, **2020**, 132, 996-1013	3.6	13
35	Bound Triplet Pairs in the Highest Spin States of Coinage Metal Clusters. *Journal of Chemical Theory and Computation*, **2010**, 6, 1479-89	6.4	12
34	An electrochemical aromatic chlorination, comparison with electrophilic reaction. *Journal of Electroanalytical Chemistry*, **2001**, 499, 39-47	4.1	12
33	Ionization energies of triazines and tetrazines. Application of Green's function method coupled with semiempirical molecular orbital calculations. *Journal of the Chemical Society Perkin Transactions II*, **1991**, 1865		12
32	Attraction between electrophilic caps: A counterintuitive case of noncovalent interactions. *Journal of Computational Chemistry*, **2019**, 40, 1015-1022	3.5	12
31	A Theoretical Study of the Radiationless Decay Mechanism of Cyclic Alkenes in the Lowest Triplet State. *Journal of Physical Chemistry A*, **2000**, 104, 5366-5373	2.8	11

30	Valence Bond Theory-Its Birth, Struggles with Molecular Orbital Theory, Its Present State and Future Prospects. *Molecules*, **2021**, 26,	4.8	11
29	The nature of bonding in metal-metal singly bonded coinage metal dimers: Cu 2 , Ag 2 and Au 2. *Computational and Theoretical Chemistry*, **2017**, 1116, 195-201	2	10
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26	Response to the Comment by J. Grunenberg on "The Nature of the Fourth Bond in the Ground State of C2: The Quadruple Bond Conundrum''. *Chemistry - A European Journal*, **2015**, 21, 17127-8	4.8	10
25	Theoretical study of the radiationless decay channels of triplet state norbornene. *Chemical Physics Letters*, **1998**, 287, 601-607	2.5	9
24	Electron transfer mechanistic manifold and variable transition state character. A theoretical investigation of model electron transfer processes between nucleophiles and ethane cation radical. *Journal of the Chemical Society Perkin Transactions II*, **1995**, 1525		8
23	Continuous Symmetry Measures of Density Maps *Journal of Physical Chemistry C*, **2010**, 114, 20342-20348	3.8	7
22	NDDO semiempirical approximations coupled with Green's function technique reliable approach for calculating ionization potentials. *Computational and Theoretical Chemistry*, **1997**, 401, 235-252		7
21	Ionization energies of azines from green's function method in semiempirical AM1 approximation. *Computational and Theoretical Chemistry*, **1989**, 188, 159-166		7
20	AM1 outer valence green's function ionization energies of the azoles. *Computational and Theoretical Chemistry*, **1989**, 187, 297-306		7
19	Captodative Substitution Enhances the Diradical Character of Compounds, Reduces Aromaticity, and Controls Single-Molecule Conductivity Patterns: A Valence Bond Study. *Journal of Physical Chemistry A*, **2019**, 123, 7133-7141	2.8	6
18	On the Nature of Bonding in Parallel Spins in Monovalent Metal Clusters. *Annual Review of Physical Chemistry*, **2016**, 67, 419-39	15.7	6
17	Acidity of the methyne group of poly(4-vinylpyridine) leads to side-chain protonation in pyridine. *New Journal of Chemistry*, **2015**, 39, 5920-5922	3.6	5
16	Tuning the Ground State Symmetry of Acetylenyl Radicals. *ACS Central Science*, **2015**, 1, 270-8	16.8	5
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13	A Conversation on New Types of Chemical Bonds. *Israel Journal of Chemistry*,	3.4	4

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10	Der angeregte Zwillingszustand als Sonde für den Übergangszustand in konzertierten unimolekularen Reaktionen: die Semibullvalen-Umlagerung. *Angewandte Chemie*, **1998**, 110, 1470-1473	3.6	2
9	The ICN-INC system: experiment and quantum chemical calculations. *Chemical Physics Letters*, **1994**, 231, 124	2.5	2
8	Nature of the Trigger Linkage in Explosive Materials Is a Charge-Shift Bond. *Journal of Organic Chemistry*, **2021**, 86, 15588-15596	4.2	2
7	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. *Angewandte Chemie*, **2019**, 131, 12460-12466	3.6	1
6	Insights into the Trends in the Acidity Strength of Organic and Inorganic Compounds: A Valence-Bond Perspective. *Journal of Physical Chemistry A*, **2019**, 123, 1851-1860	2.8	1
5	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights **2013**, 1-57		1
4	4-isopropylpyridine hydroperoxide crystals resulting from the aerobic oxidation of a 4-isopropylpyridine/4-propylpyridine mixture. *Journal of Physical Chemistry B*, **2009**, 113, 4555-9	3.4	1
3	Blue-violet photoluminescence of 4-isopropyl-pyridine hydroxide crystals. *Journal of Physical Chemistry A*, **2014**, 118, 3061-7	2.8	
2	Bound Triplet Pairs in the Highest Spin States of Monovalent Metal Clusters **2014**, 149-174		
1	Green's function method for photoelectron spectroscopy calculations based on MNDO and AM1 semiempirical approximations. *Journal of Structural Chemistry*, **1989**, 30, 474-477	0.9	