David Danovich

List of Publications by Year
in descending order

117 papers	6,332 citations	57758 44 h-index	71685 76 g-index
129 all docs	129 docs citations	129 times ranked	4520 citing authors

#	Article	IF	Citations
1	Two-State Reactivity in Organometallic Gas-Phase Ion Chemistry. Helvetica Chimica Acta, 1995, 78, 1393-1407.	1.6	319
2	Charge-shift bonding and its manifestations in chemistry. Nature Chemistry, 2009, 1, 443-449.	13.6	303
3	Structure and reactivity/selectivity control by oriented-external electric fields. Chemical Society Reviews, 2018, 47, 5125-5145.	38.1	292
4	A Different Story of Ï€-DelocalizationThe Distortivity of Ï€-Electrons and Its Chemical Manifestationsâ€. Chemical Reviews, 2001, 101, 1501-1540.	47.7	267
5	Spinâ^'Orbit Coupling in the Oxidative Activation of Hâ^'H by FeO+. Selection Rules and Reactivity Effects. Journal of the American Chemical Society, 1997, 119, 1773-1786.	13.7	243
6	Charge-Shift Bondingâ€"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, 6358-6371.	3.3	234
7	On The Nature of the Halogen Bond. Journal of Chemical Theory and Computation, 2014, 10, 3726-3737.	5.3	232
8	Dihydrogen contacts in alkanes are subtle but not faint. Nature Chemistry, 2011, 3, 323-330.	13.6	231
9	Quadruple bonding in C2 and analogous eight-valence electron species. Nature Chemistry, 2012, 4, 195-200.	13.6	198
10	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.	13.7	195
11	The â€œRebound Controversyâ€• An Overview and Theoretical Modeling of the Rebound Step in Câ^'H Hydroxylation by Cytochrome P450. European Journal of Inorganic Chemistry, 2004, 2004, 207-226.	2.0	156
12	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.	13.7	141
13	Oriented-External Electric Fields Create Absolute Enantioselectivity in Dielsâ€"Alder Reactions: Importance of the Molecular Dipole Moment. Journal of the American Chemical Society, 2018, 140, 13350-13359.	13.7	113
14	Understanding the Nature of the CHÂ·Â·Â·HC Interactions in Alkanes. Journal of Chemical Theory and Computation, 2013, 9, 1977-1991.	5.3	112
15	External electric field effects on chemical structure and reactivity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1438.	14.6	104
16	Chemistry is about energy and its changes: A critique of bond-length/bond-strength correlations. Coordination Chemistry Reviews, 2017, 344, 355-362.	18.8	99
17	Origins of the Exalted b2uFrequency in the First Excited State of Benzene. Journal of the American Chemical Society, 1996, 118, 666-671.	13.7	91
18	Chargeâ€Shift Bonding: A New and Unique Form of Bonding. Angewandte Chemie - International Edition, 2020, 59, 984-1001.	13.8	84

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19	The Nature of the Fourth Bond in the Ground State of C₂: The Quadruple Bond Conundrum. Chemistry - A European Journal, 2014, 20, 6220-6232.	3.3	77
20	A Single Transition State Serves Two Mechanisms:ÂAn 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, 130-134.	13.7	76
21	Green's function methods for calculating ionization potentials, electron affinities, and excitation energies. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 377-387.	14.6	68
22	The First PersistentÎ²-Silyl-Substituted Vinyl Cation. Angewandte Chemie International Edition in English, 1991, 30, 1479-1482.	4.4	66
23	Catalysis of Methyl Transfer Reactions by Oriented External Electric Fields: Are Goldâ€“Thiolate Linkers Innocent?. Journal of the American Chemical Society, 2018, 140, 4354-4362.	13.7	66
24	Silynes (RCâ‰¡SiRâ€²) and Disilynes (RSiâ‰¡SiRâ€²): Why Are Less Bonds Worth Energetically More? The research is supported by an Israel Science Foundation (ISF) and a Niedersachsen grant (to S.S.), by a U.S.â€“Israel Binational Science Foundation (BSF) grant (to Y.A.) and by the Minerva Foundation. S.S. and F.O. thank the European Union for a Marie Curie Fellowship (Contract number: MCFI-1999-00145). S.S. and D.D. thank P. C. Hiberty for the helpful advice.. Angewandte Chemie - International Edition, 2001, 40, 4023.	13.8	65
25	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.	13.7	62
26	Spinâ^'Orbit Coupling Patterns Induced by Twist and Pyramidalization Modes in C2H4:Â A Quantitative Study and a Qualitative Analysis. Journal of Physical Chemistry A, 1998, 102, 5923-5936.	2.5	61
27	17O, 31P and 183W NMR spectra of paramagnetic complexes with the heteropolytungstate anion [Ln(PW11O39)2]11â^' and their co. Polyhedron, 1990, 9, 1249-1256.	2.2	60
28	The Nature of the Idealized Triple Bonds Between Principal Elements and the Ïƒ Origins of Trans-Bent Geometriesâ€"A Valence Bond Study. Journal of Chemical Theory and Computation, 2011, 7, 955-968.	5.3	59
29	The Quadruple Bonding in C₂ Reproduces the Properties of the Molecule. Chemistry - A European Journal, 2016, 22, 4116-4128.	3.3	59
30	The origins of the directionality of noncovalent intermolecular interactions[#]. Journal of Computational Chemistry, 2016, 37, 34-45.	3.3	59
31	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.	13.7	58
32	A tutorial for understanding chemical reactivity through the valence bond approach. Chemical Society Reviews, 2014, 43, 4968-4988.	38.1	58
33	Oriented External Electric Fields: Tweezers and Catalysts for Reactivity in Halogen-Bond Complexes. Journal of the American Chemical Society, 2019, 141, 7122-7136.	13.7	57
34	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.	13.7	56
35	A Response to the Critical Comments on â€œOne Molecule, Two Atoms, Three Views, Four Bonds?â€• Angewandte Chemie - International Edition, 2013, 52, 5926-5928.	13.8	55
36	Using Valence Bond Theory to Understand Electronic Excited States:Â Application to the Hidden Excited State (21Ag) of C2nH2n+2(n= 2â^'14) Polyenes. Journal of Physical Chemistry A, 2000, 104, 8744-8758.	2.5	53

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37	A different story of benzene. Computational and Theoretical Chemistry, 1997, 398-399, 155-167.	1.5	52
38	Does solvation cause symmetry breaking in the I3â^' ion in aqueous solution?. Journal of Chemical Physics, 1998, 109, 9928-9937.	3.0	52
39	Comparison of Câ^'Cl and Siâ^'Cl Bonds. A Valence Bond Study. The Journal of Physical Chemistry, 1996, 100, 5715-5720.	2.9	51
40	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.	5.3	50
41	Hydrogenâ€•and Halogenâ€Bonds between Ions of like Charges: Are They Antiâ€Electrostatic in Nature?. Journal of Computational Chemistry, 2018, 39, 481-487.	3.3	50
42	An Excursion from Normal to Inverted Cï£¿C Bonds Shows a Clear Demarcation between Covalent and Chargeâ€Shift Cï£¿C Bonds. ChemPhysChem, 2009, 10, 2658-2669.	2.1	46
43	Blended hydrogen atom abstraction and proton-coupled electron transfer mechanisms of closed-shell molecules. Chemical Science, 2012, 3, 1903.	7.4	46
44	Electron-transfer reactivity in the activation of organic fluorides by bare metal monocations. Chemical Physics Letters, 1997, 278, 391-397.	2.6	45
45	TITAN: A Code for Modeling and Generating Electric Fieldsâ€"Features and Applications to Enzymatic Reactivity. Journal of Computational Chemistry, 2020, 41, 74-82.	3.3	45
46	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.	0.9	42
47	The Self-Association of Graphane Is Driven by London Dispersion and Enhanced Orbital Interactions. Journal of Chemical Theory and Computation, 2015, 11, 1621-1630.	5.3	41
48	No-Pair Bonding in the High-Spin3State of Li2. A Valence Bond Study of Its Origins. Journal of the American Chemical Society, 1999, 121, 3165-3174.	13.7	38
49	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, 2410-2418.	5.3	37
50	Covalent vs Charge-Shift Nature of the Metalâ€"Metal Bond in Transition Metal Complexes: A Unified Understanding. Journal of the American Chemical Society, 2020, 142, 12277-12287.	13.7	37
51	Ferromagnetic Bonding:â€‰ Properties of High-Spin Lithium Clusters n+1Lin (n = 2â^'12) Devoid of Electron Pairs. Journal of Physical Chemistry A, 2002, 106, 4961-4969.	2.5	36
52	Ab initio calculations for small iodo clusters. Good performance of relativistic effective core potentials. Chemical Physics Letters, 1995, 233, 249-256.	2.6	35
53	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.	4.4	35
54	An Accurate Barrier for the Hydrogen Exchange Reaction from Valence Bond Theory: Is this Theory Coming of Age?. Chemistry - A European Journal, 2003, 9, 4540-4547.	3.3	34

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55	Valence Bond Theory Reveals Hidden Delocalized Diradical Character of Polyenes. Journal of the American Chemical Society, 2017, 139, 9302-9316.	13.7	33
56	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.	13.8	32
57	Nature of the Three-Electron Bond. Journal of Physical Chemistry A, 2018, 122, 1873-1885.	2.5	31
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.	13.7	30
59	â€œNo-Pair Bondingâ€•in High-Spin Lithium Clusters:Ân+1Lin(n= 2â^'6). Journal of Physical Chemistry A, 2000, 104, 11223-11231.	2.5	30
60	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.	13.7	29
61	Ferromagnetic bonding in high-spin alkali-metal clusters. How does sodium compare to lithium?. Physical Chemistry Chemical Physics, 2003, 5, 158-164.	2.8	27
62	The ICN-INC system: experiment and quantum chemical calculations. Chemical Physics Letters, 1994, 225, 391-397.	2.6	26
63	A Response to a Comment by G. Frenking and M. Hermann on: â€œThe Quadruple Bonding in C₂ Reproduces the Properties of the Moleculeâ€• Chemistry - A European Journal, 2016, 22, 18977-18980.	3.3	26
64	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.	13.7	26
65	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. Angewandte Chemie - International Edition, 2019, 58, 12332-12338.	13.8	25
66	Valence Bond Theoryâ€”Its Birth, Struggles with Molecular Orbital Theory, Its Present State and Future Prospects. Molecules, 2021, 26, 1624.	3.8	25
67	Electron-transfer reactivity in the activation of organic fluorides by bare metal monocations. Chemical Physics Letters, 1997, 273, 164-170.	2.6	24
68	Ferromagnetic Bonding:Â High Spin Copper Clusters (n+1Cun;n= 2â^'14) Devoid of Electron Pairs but Possessing Strong Bondingâ€. Journal of Physical Chemistry A, 2006, 110, 8510-8518.	2.5	24
69	Chargeâ€Shift Bonding: A New and Unique Form of Bonding. Angewandte Chemie, 2020, 132, 996-1013.	2.0	24
70	New Landscape of Electron-Pair Bonding: Covalent, Ionic, and Charge-Shift Bonds. Structure and Bonding, 2015, , 169-211.	1.0	23
71	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.	0.9	22
72	Formation of Carbonâ€“Carbon Triply Bonded Molecules from Two Free Carbyne Radicals via a Conical Intersection. Journal of Physical Chemistry Letters, 2013, 4, 58-64.	4.6	22

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73	The Ground and Excited States of Polyenyl Radicals C2nâˆ’1H2n+1 (n=2â€“13): A Valence Bond Study. ChemPhysChem, 2004, 5, 515-528.	2.1	21
74	Spinâ€“Orbit Coupling and Outer-Core Correlation Effects in Ir- and Pt-Catalyzed Câ€“H Activation. Journal of Chemical Theory and Computation, 2012, 8, 1641-1645.	5.3	21
75	Bonding with Parallel Spins: High-Spin Clusters of Monovalent Metal Atoms. Accounts of Chemical Research, 2014, 47, 417-426.	15.6	20
76	Computational prediction of the ISC rate for triplet norbornene. Chemical Physics Letters, 2000, 322, 358-362.	2.6	19
77	Protonated Alcohols Are Examples of Complete Charge-Shift Bonds. Journal of Organic Chemistry, 2014, 79, 9998-10001.	3.2	19
78	To hybridize or not to hybridize? This is the dilemma. Computational and Theoretical Chemistry, 2017, 1116, 242-249.	2.5	18
79	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.	2.3	17
80	No-Pair Bonding in Coinage Metal Dimers. Journal of Physical Chemistry A, 2008, 112, 12995-13001.	2.5	17
81	Photoinduced Proton Transfer in a Pyridine Based Polymer Gel. Journal of Physical Chemistry B, 2010, 114, 10728-10733.	2.6	17
82	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.	2.5	17
83	Attraction between electrophilic caps: A counterintuitive case of noncovalent interactions. Journal of Computational Chemistry, 2019, 40, 1015-1022.	3.3	17
84	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.	0.9	15
85	Inner-sphere electron transfer in metal-cation chemistry. International Journal of Mass Spectrometry, 2000, 200, 163-173.	1.5	15
86	An electrochemical aromatic chlorination, comparison with electrophilic reaction. Journal of Electroanalytical Chemistry, 2001, 499, 39-47.	3.8	14
87	Bound Triplet Pairs in the Highest Spin States of Coinage Metal Clusters. Journal of Chemical Theory and Computation, 2010, 6, 1479-1489.	5.3	14
88	Halogen Bonds in Novel Polyhalogen Monoanions. Chemistry - A European Journal, 2017, 23, 8719-8728.	3.3	14
89	Comment on â€œRabbit-ears hybrids, VSEPR sterics, and other orbital anachronismsâ€• A reply to a criticism. Chemistry Education Research and Practice, 2015, 16, 689-693.	2.5	13
90	Nature of the Trigger Linkage in Explosive Materials Is a Charge-Shift Bond. Journal of Organic Chemistry, 2021, 86, 15588-15596.	3.2	13

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91	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.	2.5	12
92	Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another. Journal of Chemical Education, 2021, 98, 3617-3620.	2.3	12
93	Ionization energies of azines from green's function method in semiempirical AM1 approximation. Computational and Theoretical Chemistry, 1989, 188, 159-166.	1.5	11
94	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.	2.5	11
95	AM1 outer valence green's function ionization energies of the azoles. Computational and Theoretical Chemistry, 1989, 187, 297-306.	1.5	10
96	Theoretical study of the radiationless decay channels of triplet state norbornene. Chemical Physics Letters, 1998, 287, 601-607.	2.6	10
97	Response to the Comment by J. Grunenberg on â€œThe Nature of the Fourth Bond in the Ground State of C₂: The Quadruple Bond Conundrumâ€²â€². Chemistry - A European Journal, 2015, 21, 17127-17128.	3.3	10
98	On the Nature of Bonding in Parallel Spins in Monovalent Metal Clusters. Annual Review of Physical Chemistry, 2016, 67, 419-439.	10.8	10
99	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.	0.9	9
100	NDDO semiempirical approximations coupled with Green's function techniqueâ€”a reliable approach for calculating ionization potentials. Computational and Theoretical Chemistry, 1997, 401, 235-252.	1.5	9
101	Continuous Symmetry Measures of Density Maps. Journal of Physical Chemistry C, 2010, 114, 20342-20349.	3.1	8
102	A Conversation on New Types of Chemical Bonds. Israel Journal of Chemistry, 2022, 62, .	2.3	8
103	On the nature of the chemical bond in valence bond theory. Journal of Chemical Physics, 2022, 157, .	3.0	8
104	The Lise Meitner-Minerva Center for Computational Quantum Chemistry: 18 Years of Israeli-German Collaboration. Israel Journal of Chemistry, 2015, 55, 1167-1176.	2.3	6
105	Acidity of the methyne group of poly(4-vinylpyridine) leads to side-chain protonation in pyridine. New Journal of Chemistry, 2015, 39, 5920-5922.	2.8	6
106	Tuning the Ground State Symmetry of Acetylenyl Radicals. ACS Central Science, 2015, 1, 270-278.	11.3	5
107	Orbitals and the Interpretation of Photoelectron Spectroscopy and (e,2e) Ionization Experiments. Angewandte Chemie, 2019, 131, 12460-12466.	2.0	3
108	The ICN-INC system: experiment and quantum chemical calculations. Chemical Physics Letters, 1994, 231, 124.	2.6	2

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109	4-Isopropylpyridine Hydroperoxide Crystals Resulting from the Aerobic Oxidation of a 4-Isopropylpyridine/4-Propylpyridine Mixture. Journal of Physical Chemistry B, 2009, 113, 4555-4559.	2.6	2
110	Comment on â€œDecoding real space bonding descriptors in valence bond languageâ€•by A. MartÃn PendÃ¡s and E. Francisco, Phys. Chem. Chem. Phys., 2018, 20, 12368. Physical Chemistry Chemical Physics, 2019, 21, 8170-8174.	2.8	2
111	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.	2.5	2
112	Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Applications and Insights. , 2013, , 1-57.		1
113	Valence Bond Diagrams and Chemical Reactivity. , 2024, , 683-711.		1
114	A Tutorial on XMVB. , 2024, , 276-310.		1
115	Green's function method for photoelectron spectroscopy calculations based on MNDO and AM1 semiempirical approximations. Journal of Structural Chemistry, 1989, 30, 474-477.	1.0	0
116	The â€œRebound Controversyâ€• An Overview and Theoretical Modeling of the Rebound Step in Câ€”H Hydroxylation by Cytochrome P450. ChemInform, 2004, 35, no.	0.0	0
117	Blue-Violet Photoluminescence of 4-Isopropyl-pyridine Hydroxide Crystals. Journal of Physical Chemistry A, 2014, 118, 3061-3067.	2.5	0