Thom H Dunning

List of Publications by Year
in descending order

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63 papers	57,394 citations	186265 28 h-index	118850 62 g-index
64 all docs	64 docs citations	64 times ranked	20798 citing authors

#	Article	IF	Citations
1	Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. Journal of Chemical Physics, 1989, 90, 1007-1023.	3.0	27,560
2	Electron affinities of the firstâ€row atoms revisited. Systematic basis sets and wave functions. Journal of Chemical Physics, 1992, 96, 6796-6806.	3.0	13,437
3	Gaussian basis sets for use in correlated molecular calculations. III. The atoms aluminum through argon. Journal of Chemical Physics, 1993, 98, 1358-1371.	3.0	8,623
4	Benchmark calculations with correlated molecular wave functions. IV. The classical barrier height of the H+H2â†'H2+H reaction. Journal of Chemical Physics, 1994, 100, 7410-7415.	3.0	1,636
5	Gaussian basis sets for use in correlated molecular calculations. X. The atoms aluminum through argon revisited. Journal of Chemical Physics, 2001, 114, 9244-9253.	3.0	1,463
6	Gaussian basis sets for use in correlated molecular calculations. IX. The atoms gallium through krypton. Journal of Chemical Physics, 1999, 110, 7667-7676.	3.0	1,309
7	Gaussian basis sets for use in correlated molecular calculations. VII. Valence, core-valence, and scalar relativistic basis sets for Li, Be, Na, and Mg. Theoretical Chemistry Accounts, 2011, 128, 69-82.	1.4	536
8	Generalized valence bond description of bonding in low-lying states of molecules. Accounts of Chemical Research, 1973, 6, 368-376.	15.6	467
9	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
10	Variational transition state theory and tunneling for a heavyâ€“lightâ€“heavy reaction using an ab initio potential energy surface. 37Cl+H(D) 35Clâ†'H(D) 37Cl+35Cl. Journal of Chemical Physics, 1983, 78, 4400-4413.	3.0	242
11	A theoretical study of the potential energy surface for OH+H2. Journal of Chemical Physics, 1980, 72, 1303-1311.	3.0	206
12	Benchmark calculations with correlated molecular wave functions. VIII. Bond energies and equilibrium geometries of the CHn and C2Hn (n=1â€“4) series. Journal of Chemical Physics, 1997, 106, 4119-4140.	3.0	116
13	Valence correlation in the s2dn, sdn+1, and dn+2 states of the firstâ€row transition metal atoms. Journal of Chemical Physics, 1981, 75, 3466-3476.	3.0	113
14	Theoretical studies of the reactions of HCN with atomic hydrogen. Journal of Chemical Physics, 1985, 82, 2280-2294.	3.0	102
15	SO2 revisited: Impact of tight d augmented correlation consistent basis sets on structure and energetics. Journal of Chemical Physics, 2003, 119, 11712-11714.	3.0	83
16	Theory of Hypervalency: Recoupled Pair Bonding in SF_n (n = 1â^'6). Journal of Physical Chemistry A, 2009, 113, 7915-7926.	2.5	81
17	Insights into the Perplexing Nature of the Bonding in C₂ from Generalized Valence Bond Calculations. Journal of Chemical Theory and Computation, 2014, 10, 195-201.	5.3	66
18	Theoretical characterization of the potential energy surface of the ground state of the HCO system. Journal of Chemical Physics, 1980, 73, 2304-2309.	3.0	65

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19	Theoretical characterization of negative ions. Calculation of the electron affinities of carbon, oxygen, and fluorine. Journal of Chemical Physics, 1982, 76, 6046-6056.	3.0	64
20	Reaction dynamics for O(3P)+H2 and D2. IV. Reduced dimensionality quantum and quasiclassical rate constants with an adiabatic incorporation of the bending motion. Journal of Chemical Physics, 1984, 81, 1739-1752.	3.0	49
21	The First Row Anomaly and Recoupled Pair Bonding in the Halides of the Late p-Block Elements. Accounts of Chemical Research, 2013, 46, 359-368.	15.6	47
22	Theoretical studies of the O+H2 reaction. Journal of Chemical Physics, 1980, 72, 2894-2896.	3.0	42
23	Bonding in ClF_n (n = 1â^'7) Molecules: Further Insight into the Electronic Structure of Hypervalent Molecules and Recoupled Pair Bonds. Journal of Physical Chemistry A, 2009, 113, 12645-12654.	2.5	42
24	A comparison between polar covalent bonding and hypervalent recoupled pair bonding in diatomic chalcogen halide species {O,S,Se} Ã— {F,Cl,Br}. Molecular Physics, 2009, 107, 991-998.	1.7	42
25	Insights into the Electronic Structure of Molecules from Generalized Valence Bond Theory. Journal of Physical Chemistry A, 2016, 120, 1763-1778.	2.5	42
26	Recoupled Pair Bonding in PF_n(n= 1â^'5)^{â€}. Journal of Physical Chemistry A, 2010, 114, 8845-8851.	2.5	41
27	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
28	Insights into the Electronic Structure of Ozone and Sulfur Dioxide from Generalized Valence Bond Theory: Bonding in O₃ and SO₂. Journal of Physical Chemistry A, 2015, 119, 7683-7694.	2.5	37
29	Bonding in SCl_n (n = 1â^'6): A Quantum Chemical Study. Journal of Physical Chemistry A, 2011, 115, 4757-4764.	2.5	26
30	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
31	Bonding and Isomerism in SF_{nâ^'1}Cl (n = 1â^'6): A Quantum Chemical Study. Journal of Physical Chemistry A, 2011, 115, 329-341.	2.5	25
32	Bonding in Sulfurâ€“Oxygen Compoundsâ€”HSO/SOH and SOO/OSO: An Example of Recoupled Pair Ï€ Bonding. Journal of Chemical Theory and Computation, 2013, 9, 4444-4452.	5.3	24
33	Bonding in FSSF₃: Breakdown in Bond Length-Strength Correlations and Implications for SF₂ Dimerization. Journal of Physical Chemistry Letters, 2013, 4, 3139-3143.	4.6	24
34	Hypervalency and recoupled pair bonding in the p-block elements. Computational and Theoretical Chemistry, 2011, 963, 7-12.	2.5	23
35	Fundamental aspects of recoupled pair bonds. I. Recoupled pair bonds in carbon and sulfur monofluoride. Journal of Chemical Physics, 2015, 142, 034113.	3.0	19
36	Orbital Hybridization in Modern Valence Bond Wave Functions: Methane, Ethylene, and Acetylene. Journal of Physical Chemistry A, 2020, 124, 204-214.	2.5	18

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37	Generalized Valence Bond Description of the Ground States (X¹Î£_g⁺) of Homonuclear Pnictogen Diatomic Molecules: N₂, P₂, and As₂. Journal of Chemical Theory and Computation, 2015, 11, 2496-2507.	5.3	17
38	The nature of the SO bond of chlorinated sulfurâ€“oxygen compounds. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	15
39	Fundamental aspects of recoupled pair bonds. II. Recoupled pair bond dyads in carbon and sulfur difluoride. Journal of Chemical Physics, 2015, 142, 034114.	3.0	15
40	Generalized Valence Bond Description of Chalcogenâ€“Nitrogen Compounds. II. NO, F(NO), and H(NO). Journal of Physical Chemistry A, 2015, 119, 1456-1463.	2.5	13
41	Generalized Valence Bond Description of Chalcogenâ€“Nitrogen Compounds. I. NS, F(NS), and H(NS). Journal of Physical Chemistry A, 2015, 119, 1446-1455.	2.5	13
42	Variations in the Nature of Triple Bonds: The N₂, HCN, and HC₂H Series. Journal of Physical Chemistry A, 2016, 120, 4526-4533.	2.5	13
43	SiH2, a critical study. Molecular Physics, 2004, 102, 2597-2606.	1.7	12
44	Why edge inversion? Theoretical characterization of the bonding in the transition states for inversion in F n NH(3â^'n) and FnPH(3â^'n) (nÂ=Â0â€“3). Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	12
45	Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another. Journal of Chemical Education, 2021, 98, 3617-3620.	2.3	12
46	Spin-Coupled Generalized Valence Bond Description of Group 14 Species: The Carbon, Silicon and Germanium Hydrides, XH_n (n = 1â€“4). Journal of Physical Chemistry A, 2019, 123, 2401-2419.	2.5	11
47	High Level ab Initio Calculations for ClF_n⁺ (n = 1â€“6) Ions: Refining the Recoupled Pair Bonding Model. Journal of Physical Chemistry A, 2013, 117, 4251-4266.	2.5	10
48	Insights into the Electronic Structure of Disulfur Tetrafluoride Isomers from Generalized Valence Bond Theory. Journal of Physical Chemistry A, 2014, 118, 10117-10126.	2.5	10
49	The electronic structure of the two lowest states of CuC. Journal of Chemical Physics, 2008, 129, 174306.	3.0	9
50	Effects of Ligand Electronegativity on Recoupled Pair Bonds with Application to Sulfurane Precursors. Journal of Physical Chemistry A, 2014, 118, 5709-5719.	2.5	9
51	Insights into the Electronic Structure of Ozone and Sulfur Dioxide from Generalized Valence Bond Theory: Addition of Hydrogen Atoms. Journal of Physical Chemistry A, 2016, 120, 2720-2726.	2.5	9
52	Bonding in PF2Cl, PF3Cl, and PF4Cl: insight into isomerism and apicophilicity from ab initio calculations and the recoupled pair bonding model. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	8
53	Generalized Valence Bond Description of Chalcogenâ€“Nitrogen Compounds. III. Why the NOâ€“OH and NSâ€“OH Bonds Are So Different. Journal of Physical Chemistry A, 2016, 120, 6846-6850.	2.5	7
54	Resolving a puzzling anomaly in the spinâ€coupled generalized valence bond description of benzene. Journal of Computational Chemistry, 2020, 41, 1421-1426.	3.3	6

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55	Fundamental Aspects of Recoupled Pair Bonds. III. The Frustrated Recoupled Pair Bond in Oxygen Monofluoride. Journal of Physical Chemistry A, 2016, 120, 9607-9611.	2.5	5
56	The nature of the chemical bond and the role of non-dynamical and dynamical correlation in Be2. Journal of Chemical Physics, 2020, 152, 214111.	3.0	5
57	High level ab initio calculations on ClF n â^' (n = 1â€“6): Recoupled pair bonding involving a closed-shell central ion. Computational and Theoretical Chemistry, 2017, 1116, 73-85.	2.5	4
58	A cautionary tale: Problems in the valence-CASSCF description of the ground state (X1Î£+) of BF. Journal of Chemical Physics, 2020, 153, 114113.	3.0	4
59	Quantum chemical calculations using the floating point systems, Inc. Model 164 attached processor. International Journal of Quantum Chemistry, 1983, 24, 613-622.	2.0	2
60	Reply to â€œComment on â€˜Insights into the Electronic Structure of Ozone and Sulfur Dioxide from Generalized Valence Bond Theory: Bonding in O3 and SO2â€™â€•. Journal of Physical Chemistry A, 2016, 120, 171-172.	2.5	2
61	New Insights into the Remarkable Difference between CH₅^{â€“} and SiH₅^{â€“}. Journal of Physical Chemistry A, 2021, 125, 7414-7424.	2.5	2
62	Dynamical electron correlation and the chemical bond. I. Covalent bonds in AH and AF (A = B-F). Journal of Chemical Physics, 0, , .	3.0	2
63	Nature of the Bonding in the Bifluoride Anion, FHF^{â€“}. Journal of Physical Chemistry Letters, 2021, 12, 7293-7298.	4.6	1