Frank Weinhold

List of Publications by Citations

251 papers	49,885 citations	67 h-index	223 g-index
277 ext. papers	53,336 ext. citations	6.4 avg, IF	7.72 L-index

#	Paper	IF	Citations
251	Intermolecular interactions from a natural bond orbital, donor-acceptor viewpoint. *Chemical Reviews*, **1988**, 88, 899-926	68.1	14317
250	Natural population analysis. *Journal of Chemical Physics*, **1985**, 83, 735-746	3.9	7663
249	Natural hybrid orbitals. *Journal of the American Chemical Society*, **1980**, 102, 7211-7218	16.4	4019
248	Natural bond orbital analysis of near-Hartree–Fock water dimer. *Journal of Chemical Physics*, **1983**, 78, 4066-4073	3.9	2460
247	Natural localized molecular orbitals. *Journal of Chemical Physics*, **1985**, 83, 1736-1740	3.9	1785
246	Analysis of the geometry of the hydroxymethyl radical by the "different hybrids for different spins" natural bond orbital procedure. *Computational and Theoretical Chemistry*, **1988**, 169, 41-62		1727
245	Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective **2003**,		1289
244	NBO 6.0: natural bond orbital analysis program. *Journal of Computational Chemistry*, **2013**, 34, 1429-37	3.5	916
243	Natural bond orbital methods. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 1-42	7.9	887
242	Electronic basis of improper hydrogen bonding: a subtle balance of hyperconjugation and rehybridization. *Journal of the American Chemical Society*, **2003**, 125, 5973-87	16.4	644
241	NATURAL BOND ORBITALS AND EXTENSIONS OF LOCALIZED BONDING CONCEPTS. *Chemistry Education Research and Practice*, **2001**, 2, 91-104	2.1	582
240	Natural resonance theory: I. General formalism. *Journal of Computational Chemistry*, **1998**, 19, 593-609	3.5	549
239	Metric geometry of equilibrium thermodynamics. *Journal of Chemical Physics*, **1975**, 63, 2479-2483	3.9	451
238	Natural resonance theory: II. Natural bond order and valency. *Journal of Computational Chemistry*, **1998**, 19, 610-627	3.5	432
237	Natural bond orbital analysis of molecular interactions: Theoretical studies of binary complexes of HF, H2O, NH3, N2, O2, F2, CO, and CO2 with HF, H2O, and NH3. *Journal of Chemical Physics*, **1986**, 84, 5687-5705	3.9	429
236	Natural resonance theory: III. Chemical applications. *Journal of Computational Chemistry*, **1998**, 19, 628-646	3.5	416
235	**2012**,		394

234	What is NBO analysis and how is it useful?. *International Reviews in Physical Chemistry*, **2016**, 35, 399-440	7	375
233	Natural bond orbital analysis: a critical overview of relationships to alternative bonding perspectives. *Journal of Computational Chemistry*, **2012**, 33, 2363-79	3.5	372
232	Resonance properties of complex-rotated hamiltonians. *Molecular Physics*, **1978**, 36, 1613-1630	1.7	340
231	The Natural Bond Orbital Lewis Structure Concept for Molecules, Radicals, and Radical Ions **1988**, 227-236		333
230	Quantum-mechanical studies on the origin of barriers to internal rotation about single bonds. *Journal of the American Chemical Society*, **1979**, 101, 1700-1709	16.4	281
229	Collagen stability: insights from NMR spectroscopic and hybrid density functional computational investigations of the effect of electronegative substituents on prolyl ring conformations. *Journal of the American Chemical Society*, **2002**, 124, 2497-505	16.4	276
228	Natural bond orbital analysis of steric interactions. *Journal of Chemical Physics*, **1997**, 107, 5406-5421	3.9	228
227	Natural chemical shielding analysis of nuclear magnetic resonance shielding tensors from gauge-including atomic orbital calculations. *Journal of Chemical Physics*, **1997**, 107, 1173-1184	3.9	216
226	Structure and spectroscopy of (HCN)n clusters: Cooperative and electronic delocalization effects in C□H???N hydrogen bonding. *Journal of Chemical Physics*, **1995**, 103, 333-347	3.9	210
225	Nature of H-bonding in clusters, liquids, and enzymes: an ab initio, natural bond orbital perspective. *Computational and Theoretical Chemistry*, **1997**, 398-399, 181-197		199
224	What is a hydrogen bond? Mutually consistent theoretical and experimental criteria for characterizing H-bonding interactions. *Molecular Physics*, **2012**, 110, 565-579	1.7	169
223	Natural Bond Orbital Analysis of Internal Rotation Barriers and Related Phenomena. *Israel Journal of Chemistry*, **1991**, 31, 277-285	3.4	160
222	Natural steric analysis of internal rotation barriers. *International Journal of Quantum Chemistry*, **1999**, 72, 269-280	2.1	159
221	Metric geometry of equilibrium thermodynamics. II. Scaling, homogeneity, and generalized Gibbs□Duhem relations. *Journal of Chemical Physics*, **1975**, 63, 2484-2487	3.9	152
220	Anti-electrostatic hydrogen bonds. *Angewandte Chemie - International Edition*, **2014**, 53, 11214-7	16.4	146
219	Natural steric analysis: Ab initio van der Waals radii of atoms and ions. *Journal of Chemical Physics*, **1997**, 107, 5422-5432	3.9	146
218	Rebuttal to the Bickelhaupt□Baerends Case for Steric Repulsion Causing the Staggered Conformation of Ethane. *Angewandte Chemie - International Edition*, **2003**, 42, 4188-4194	16.4	145
217	On the role of d orbitals in sulfur hexafluoride. *Journal of the American Chemical Society*, **1986**, 108, 3586-3593	15.4	144

216	Dynamic polarizabilities of two-electron atoms, with rigorous upper and lower bounds. *Journal of Chemical Physics*, **1976**, 65, 4913-4926	3.9	131
215	Moment-theory investigations of photoabsorption and dispersion profiles in atoms and ions. *Physical Review A*, **1976**, 14, 1042-1056	2.6	128
214	Quantum cluster equilibrium theory of liquids: General theory and computer implementation. *Journal of Chemical Physics*, **1998**, 109, 367-372	3.9	124
213	Experimental and theoretical determination of the temperature dependence of deuteron and oxygen quadrupole coupling constants of liquid water. *Journal of Chemical Physics*, **1995**, 103, 6941-6950	3.9	114
212	The Nature of the Silicon□Oxygen Bond. *Organometallics*, **2011**, 30, 5815-5824	3.8	110
211	Origin of Methyl Internal Rotation Barriers. *Accounts of Chemical Research*, **1999**, 32, 983-993	24.3	107
210	Understanding barriers to internal rotation in substituted toluenes and their cations. *Journal of Chemical Physics*, **1995**, 102, 6787-6805	3.9	101
209	Spectroscopic Evidence for Clusters of Like-Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding. *ChemPhysChem*, **2016**, 17, 458-62	3.2	100
208	Quantum Cluster Equilibrium Theory of Liquids: Temperature Dependence of Hydrogen Bonding in Liquid N-Methylacetamide Studied by IR Spectra. *Journal of Physical Chemistry B*, **1998**, 102, 9312-9318	3.4	99
207	Investigation of the differences in stability of the OC???HF and CO???HF complexes. *Journal of Chemical Physics*, **1985**, 82, 2679-2687	3.9	99
206	Natural J-coupling analysis: interpretation of scalar J-couplings in terms of natural bond orbitals. *Journal of the American Chemical Society*, **2001**, 123, 12026-36	16.4	93
205	Metric geometry of equilibrium thermodynamics. V. Aspects of heterogeneous equilibrium. *Journal of Chemical Physics*, **1976**, 65, 559-564	3.9	93
204	Origin of trans-bent geometries in maximally bonded transition metal and main group molecules. *Journal of the American Chemical Society*, **2006**, 128, 7335-45	16.4	90
203	Quantum cluster equilibrium theory of liquids: Illustrative application to water. *Journal of Chemical Physics*, **1998**, 109, 373-384	3.9	90
202	Theoretical study of hydrogen bonding in liquid and gaseous N-methylformamide. *Journal of Chemical Physics*, **1997**, 107, 499-507	3.9	89
201	Reduced Density Matrices of Atoms and Molecules. II. On the N-Representability Problem. *Journal of Chemical Physics*, **1967**, 47, 2298-2311	3.9	89
200	NMR Investigations of Clostridium pasteurianum Rubredoxin. Origin of Hyperfine 1H, 2H, 13C, and 15N NMR Chemical Shifts in Iron□Sulfur Proteins As Determined by Comparison of Experimental Data with Hybrid Density Functional Calculations□ *Journal of the American Chemical Society*, **1998**, 120, 4806-4814	16.4	86
199	NBO 7.0: New vistas in localized and delocalized chemical bonding theory. *Journal of Computational Chemistry*, **2019**, 40, 2234-2241	3.5	85

198	The role of delocalization in benzene. *Journal of the American Chemical Society*, **1993**, 115, 10952-10957	16.4	85
197	What is a hydrogen bond? Resonance covalency in the supramolecular domain. *Chemistry Education Research and Practice*, **2014**, 15, 276-285	2.1	82
196	Reduced Density Matrices of Atoms and Molecules. I. The 2 Matrix of Double-Occupancy, Configuration-Interaction Wavefunctions for Singlet States. *Journal of Chemical Physics*, **1967**, 46, 2752-2758	3.9	81
195	Experimental and theoretical studies of hydrogen bonding in neat, liquid formamide. *Journal of Chemical Physics*, **1995**, 102, 5118-5125	3.9	80
194	Metric geometry of equilibrium thermodynamics. III. Elementary formal structure of a vector-algebraic representation of equilibrium thermodynamics. *Journal of Chemical Physics*, **1975**, 63, 2488-2495	3.9	78
193	Observation of an Eclipsed C-CH3 Bond in a Tricyclic Orthoamide; Experimental and Theoretical Evidence for C?H O Hydrogen Bonds. *Angewandte Chemie International Edition in English*, **1987**, 26, 1175-1177		76
192	Hyperconjugative interactions in permethylated siloxanes and ethers: the nature of the SiO bond. *Journal of the American Chemical Society*, **2013**, 135, 5762-7	16.4	75
191	Upper and Lower Bounds to Quantum-Mechanical Properties. *Advances in Quantum Chemistry*, **1972**, 299-331	1.4	74
190	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
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184	Quantum cluster equilibrium theory of liquids: molecular clusters and thermodynamics of liquid ethanol. *Molecular Physics*, **1999**, 97, 465-477	1.7	66
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182	Some remarks on nonorthogonal orbitals in quantum chemistry. *Computational and Theoretical Chemistry*, **1988**, 165, 189-202		65
181	Metric geometry of equilibrium thermodynamics. IV. Vector-algebraic evaluation of thermodynamic derivatives. *Journal of Chemical Physics*, **1975**, 63, 2496-2501	3.9	65

180	Dipole oscillator strengths, with rigorous limits of error, for He and Li+. *Physical Review A*, **1974**, 9, 118-128	2.8	65
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177	Complex-coordinate studies of helium autoionizing resonances. *International Journal of Quantum Chemistry*, **1978**, 14, 727-736	2.1	58
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175	Transferability of natural bond orbitals. *Journal of the American Chemical Society*, **1988**, 110, 368-372	16.4	57
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170	Common Textbook and Teaching Misrepresentations of Lewis Structures. *Journal of Chemical Education*, **1995**, 72, 583	2.4	52
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167	Resonance Character of Hydrogen-bonding Interactions in Water and Other H-bonded Species. *Advances in Protein Chemistry*, **2005**, 72, 121-55		50
166	A theoretical model of bonding in hyperlithiated carbon compounds. *Journal of the American Chemical Society*, **1985**, 107, 1919-1921	16.4	50
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164	Joint treatment of ab initio and experimental data in molecular force field calculations with Tikhonov□ method of regularization. *Journal of Chemical Physics*, **1994**, 100, 1414-1424	3.9	46
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156	Some remarks on the C□H bond dipole moment. *Journal of Chemical Physics*, **1986**, 84, 2428-2430	3.9	41
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137	Threshold photoionization spectra of benzyl radical: Cation vibrational states and ab initio calculations. *Journal of Chemical Physics*, **1996**, 104, 8886-8895	3.9	29
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120	Quantum cluster equilibrium theory of liquids part II: Temperature dependent chemical shifts, quadrupole coupling constants and vibrational frequencies in liquid ammonia. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1998**, 102, 205-212		24
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