Jan H Jensen

List of Publications by Year
in descending order

127	35,346	53939 47	23173 116
papers	citations	h-index	g-index

190	190	190	32153
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	1.5	19,020
2	PROPKA3: Consistent Treatment of Internal and Surface Residues in Empirical pK_a Predictions. Journal of Chemical Theory and Computation, 2011, 7, 525-537.	2.3	3,121
3	Very fast empirical prediction and rationalization of protein pKa values. Proteins: Structure, Function and Bioinformatics, 2005, 61, 704-721.	1.5	1,771
4	PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. Nucleic Acids Research, 2007, 35, W522-W525.	6.5	1,659
5	Improved Treatment of Ligands and Coupling Effects in Empirical Calculation and Rationalization of pK_a Values. Journal of Chemical Theory and Computation, 2011, 7, 2284-2295.	2.3	1,436
6	Very fast prediction and rationalization of pK_a values for proteinâ€“ligand complexes. Proteins: Structure, Function and Bioinformatics, 2008, 73, 765-783.	1.5	938
7	An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986.	1.2	578
8	The Effective Fragment Potential Method:Â A QM-Based MM Approach to Modeling Environmental Effects in Chemistry. Journal of Physical Chemistry A, 2001, 105, 293-307.	1.1	570
9	On the Number of Water Molecules Necessary To Stabilize the Glycine Zwitterion. Journal of the American Chemical Society, 1995, 117, 8159-8170.	6.6	419
10	Graphical analysis of pH-dependent properties of proteins predicted using PROPKA. BMC Structural Biology, 2011, 11, 6.	2.3	328
11	Conformational potential energy surface of glycine: a theoretical study. Journal of the American Chemical Society, 1991, 113, 7917-7924.	6.6	238
12	Chapter 10 The Effective Fragment Potential: A General Method for Predicting Intermolecular Interactions. Annual Reports in Computational Chemistry, 2007, 3, 177-193.	0.9	193
13	Understanding the Hydrogen Bond Using Quantum Chemistry. Accounts of Chemical Research, 1996, 29, 536-543.	7.6	188
14	FTIR Spectroscopy Combined with Isotope Labeling and Quantum Chemical Calculations to Investigate Adsorbed Bicarbonate Formation Following Reaction of Carbon Dioxide with Surface Hydroxyl Groups on Fe2O3and Al2O3. Journal of Physical Chemistry B, 2006, 110, 12005-12016.	1.2	170
15	The polarizable continuum model (PCM) interfaced with the fragment molecular orbital method (FMO). Journal of Computational Chemistry, 2006, 27, 976-985.	1.5	161
16	A graph-based genetic algorithm and generative model/Monte Carlo tree search for the exploration of chemical space. Chemical Science, 2019, 10, 3567-3572.	3.7	161
17	Evaluation of charge penetration between distributed multipolar expansions. Journal of Chemical Physics, 2000, 112, 7300-7306.	1.2	149
18	Improving the efficiency and convergence of geometry optimization with the polarizable continuum model: New energy gradients and molecular surface tessellation. Journal of Computational Chemistry, 2004, 25, 1449-1462.	1.5	144

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19	QM/MM Boundaries Across Covalent Bonds:Â A Frozen Localized Molecular Orbital-Based Approach for the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2000, 104, 6656-6665.	1.1	136
20	Determinants of the Relative Reduction Potentials of Type-1 Copper Sites in Proteins. Journal of the American Chemical Society, 2004, 126, 8010-8019.	6.6	134
21	Prediction and Rationalization of Protein pKa Values Using QM and QM/MM Methods. Journal of Physical Chemistry A, 2005, 109, 6634-6643.	1.1	131
22	FTIR spectroscopy combined with quantum chemical calculations to investigate adsorbed nitrate on aluminium oxide surfaces in the presence and absence of co-adsorbed water. Physical Chemistry Chemical Physics, 2007, 9, 4970.	1.3	119
23	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. Molecular Physics, 1996, 89, 1313-1325.	0.8	110
24	Partial Hessian vibrational analysis: the localization of the molecular vibrational energy and entropy. Theoretical Chemistry Accounts, 2002, 107, 211-219.	0.5	109
25	Predicting accurate absolute binding energies in aqueous solution: thermodynamic considerations for electronic structure methods. Physical Chemistry Chemical Physics, 2015, 17, 12441-12451.	1.3	108
26	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. II. Application to the effective fragment potential method. Journal of Chemical Physics, 1998, 108, 4772-4782.	1.2	105
27	Continuum solvation of large molecules described by QM/MM: a semi-iterative implementation of the PCM/EFP interface. Theoretical Chemistry Accounts, 2003, 109, 71-84.	0.5	91
28	Uncatalyzed peptide bond formation in the gas phase. The Journal of Physical Chemistry, 1992, 96, 8340-8351.	2.9	90
29	The Prediction of Protein pKa's Using QM/MM:Â The pKaof Lysine 55 in Turkey Ovomucoid Third Domain. Journal of Physical Chemistry B, 2002, 106, 3486-3494.	1.2	90
30	The determinants of carboxyl pKa values in turkey ovomucoid third domain. Proteins: Structure, Function and Bioinformatics, 2004, 55, 689-704.	1.5	84
31	Toward a General Theory of Hydrogen Bonding:Â The Short, Strong Hydrogen Bond [HOHÂ·Â·Â·OH]-. Journal of Physical Chemistry A, 2000, 104, 9266-9275.	1.1	81
32	Effective Fragment Molecular Orbital Method: A Merger of the Effective Fragment Potential and Fragment Molecular Orbital Methods^{â€}. Journal of Physical Chemistry A, 2010, 114, 8705-8712.	1.1	80
33	Covalent Bond Fragmentation Suitable To Describe Solids in the Fragment Molecular Orbital Method. Journal of Physical Chemistry A, 2008, 112, 11808-11816.	1.1	76
34	Charge transfer interaction in the effective fragment potential method. Journal of Chemical Physics, 2006, 124, 214108.	1.2	74
35	1,3-Transposition of Allylic Alcohols Catalyzed by Methyltrioxorhenium. Organometallics, 1998, 17, 1835-1840.	1.1	71
36	Nature of the silicon-nitrogen bond in silatranes. Organometallics, 1991, 10, 2657-2660.	1.1	70

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37	Cooperative Hydrogen Bonding Effects Are Key Determinants of Backbone Amide Proton Chemical Shifts in Proteins. Journal of the American Chemical Society, 2006, 128, 9863-9872.	6.6	69
38	Surface Reactions of Carbon Dioxide at the Adsorbed Waterâ^'Oxide Interface. Journal of Physical Chemistry C, 2007, 111, 14870-14880.	1.5	69
39	Regiocontrol by remote substituents. An enantioselective total synthesis of frenolicin B via a highly regioselective Diels-Alder reaction. Journal of the American Chemical Society, 1993, 115, 5859-5860.	6.6	68
40	Evaluation of the charge penetration energy between non-orthogonal molecular orbitals using the Spherical Gaussian Overlap approximation. Chemical Physics Letters, 1999, 315, 140-144.	1.2	61
41	Fast and accurate prediction of the regioselectivity of electrophilic aromatic substitution reactions. Chemical Science, 2018, 9, 660-665.	3.7	59
42	Rationalization of the pK_a Values of Alcohols and Thiols Using Atomic Charge Descriptors and Its Application to the Prediction of Amino Acid pK_aâ€™s. Journal of Chemical Information and Modeling, 2014, 54, 2200-2213.	2.5	58
43	Boundary Conditions for the Swainâ^'Schaad Relationship as a Criterion for Hydrogen Tunneling. Journal of the American Chemical Society, 2002, 124, 3858-3864.	6.6	56
44	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	2.3	56
45	Pathways for H2 elimination from ethylene: A theoretical study. Journal of Chemical Physics, 1994, 100, 1981-1987.	1.2	53
46	Analytic gradient for the adaptive frozen orbital bond detachment in the fragment molecular orbital method. Chemical Physics Letters, 2009, 477, 169-175.	1.2	53
47	Direct Total Syntheses of Frenolicin B and Kalafungin via Highly Regioselective Diels-Alder Reactions. Journal of Organic Chemistry, 1995, 60, 1154-1159.	1.7	51
48	Effective Fragment Method for Modeling Intermolecular Hydrogen-Bonding Effects on Quantum Mechanical Calculations. ACS Symposium Series, 1994, , 139-151.	0.5	47
49	Short strong hydrogen bonds in proteins: a case study of rhamnogalacturonan acetylesterase. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 851-863.	2.5	46
50	A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. PeerJ, 2014, 2, e449.	0.9	46
51	Accurate Intraprotein Electrostatics Derived from First Principles:Â An Effective Fragment Potential Method Study of the Proton Affinities of Lysine 55 and Tyrosine 20 in Turkey Ovomucoid Third Domain. Journal of Physical Chemistry A, 2001, 105, 3829-3837.	1.1	45
52	Intermolecular exchange-induction and charge transfer: Derivation of approximate formulas using nonorthogonal localized molecular orbitals. Journal of Chemical Physics, 2001, 114, 8775-8783.	1.2	41
53	Effects of buffer composition and dilution on nanowire field-effect biosensors. Nanotechnology, 2013, 24, 035501.	1.3	41
54	Prediction of pK_a Values for Druglike Molecules Using Semiempirical Quantum Chemical Methods. Journal of Physical Chemistry A, 2017, 121, 699-707.	1.1	41

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55	Determinants of cysteine pKa values in creatine kinase and Î±1-antitrypsin. Proteins: Structure, Function and Bioinformatics, 2004, 57, 799-803.	1.5	40
56	Modeling intermolecular exchange integrals between nonorthogonal molecular orbitals. Journal of Chemical Physics, 1996, 104, 7795-7796.	1.2	39
57	FragIt: A Tool to Prepare Input Files for Fragment Based Quantum Chemical Calculations. PLoS ONE, 2012, 7, e44480.	1.1	39
58	Improving solvation energy predictions using the SMD solvation method and semiempirical electronic structure methods. Journal of Chemical Physics, 2018, 149, 104102.	1.2	39
59	Proteinâ€“protein binding is often associated with changes in protonation state. Proteins: Structure, Function and Bioinformatics, 2008, 71, 81-91.	1.5	38
60	A Predictive Model of Strong Hydrogen Bonding in Proteins:Â The NÎ´1âˆ’Hâˆ’OÎ´1Hydrogen Bond in Low-pH Î±-Chymotrypsin and Î±-Lytic Protease. Journal of Physical Chemistry B, 2003, 107, 6226-6233.	1.2	37
61	Energy gradients in combined fragment molecular orbital and polarizable continuum model (FMO/PCM) calculation. Journal of Computational Chemistry, 2010, 31, 778-790.	1.5	37
62	Quantifying signal changes in nano-wire based biosensors. Nanoscale, 2011, 3, 706-717.	2.8	37
63	The Molecule Calculator: A Web Application for Fast Quantum Mechanics-Based Estimation of Molecular Properties. Journal of Chemical Education, 2013, 90, 1093-1095.	1.1	36
64	Hydride Transfer versus Hydrogen Radical Transfer in Thymidylate Synthase. Journal of the American Chemical Society, 2006, 128, 5636-5637.	6.6	35
65	Calculating pH and Salt Dependence of Protein-Protein Binding. Current Pharmaceutical Biotechnology, 2008, 9, 96-102.	0.9	35
66	Predicting and rationalizing the effect of surface charge distribution and orientation on nano-wire based FET bio-sensors. Nanoscale, 2011, 3, 3635.	2.8	35
67	PHAISTOS: A framework for Markov chain Monte Carlo simulation and inference of protein structure. Journal of Computational Chemistry, 2013, 34, 1697-1705.	1.5	35
68	Mapping Enzymatic Catalysis Using the Effective Fragment Molecular Orbital Method: Towards all ab initio Biochemistry. PLoS ONE, 2013, 8, e60602.	1.1	33
69	NMR chemical shifts in the low-pH form of a-chymotrypsin. A QM/MM and ONIOM-NMR study. Theoretical Chemistry Accounts, 2003, 109, 100-107.	0.5	32
70	Regiocontrol by Remote Substituents. A Direct Total Synthesis of Racemic Hongconin. Journal of Organic Chemistry, 1994, 59, 2219-2222.	1.7	31
71	Ab Initio Localized Charge Distributions: Theory and a Detailed Analysis of the Water Dimer-Hydrogen Bond. The Journal of Physical Chemistry, 1995, 99, 8091-8107.	2.9	30
72	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 2. Journal of Chemical Theory and Computation, 2007, 3, 1629-1643.	2.3	30

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73	A Planar Tetracoordinate Carbon and Unusual Bonding in an Organodimetallic Propynylidene Complex Arising from Double Câ^'H Activation of an Allene Ligand. Journal of the American Chemical Society, 2003, 125, 1688-1689.	6.6	29
74	Prediction of pKa values using the PM6 semiempirical method. PeerJ, 2016, 4, e2335.	0.9	29
75	The Effective Fragment Molecular Orbital Method for Fragments Connected by Covalent Bonds. PLoS ONE, 2012, 7, e41117.	1.1	28
76	Exchange repulsion between effective fragment potentials and ab initio molecules. Theoretical Chemistry Accounts, 2010, 125, 481-491.	0.5	26
77	Chemical space exploration: how genetic algorithms find the needle in the haystack. PeerJ Physical Chemistry, 0, 2, e11.	0.0	25
78	Prediction and Rationalization of the pH Dependence of the Activity and Stability of Family 11 Xylanases. Biochemistry, 2007, 46, 13581-13592.	1.2	24
79	Indium arsenide nanowire field-effect transistors for pH and biological sensing. Applied Physics Letters, 2014, 104, .	1.5	22
80	Towards a barrier height benchmark set for biologically relevant systems. PeerJ, 2016, 4, e1994.	0.9	22
81	Exploring the Role of the Active Site Cysteine in Human Muscle Creatine Kinaseâ€. Biochemistry, 2006, 45, 11464-11472.	1.2	21
82	Hydrogen bonding is the prime determinant of carboxyl pKa values at the N-termini of Î±-helices. Proteins: Structure, Function and Bioinformatics, 2006, 63, 621-635.	1.5	21
83	Protein Structure Validation and Refinement Using Amide Proton Chemical Shifts Derived from Quantum Mechanics. PLoS ONE, 2013, 8, e84123.	1.1	21
84	Role of the virtual orbitals and HOMO-LUMO gap in mean-field approximations to the conductance of molecular junctions. Physical Review B, 2008, 77, .	1.1	20
85	The Bicyclo[2.2.2]octane Motif: A Class of Saturated Group 14 Quantum Interference Based Single-Molecule Insulators. Journal of Physical Chemistry Letters, 2018, 9, 6941-6947.	2.1	20
86	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 1. Journal of Chemical Theory and Computation, 2007, 3, 1620-1628.	2.3	17
87	Chemically accurate protein structures: Validation of protein NMR structures by comparison of measured and predicted pK a values. Journal of Biomolecular NMR, 2006, 35, 39-51.	1.6	16
88	Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 2078-2084.	2.3	16
89	A Computational Methodology to Screen Activities of Enzyme Variants. PLoS ONE, 2012, 7, e49849.	1.1	15
90	High throughput virtual screening of 230 billion molecular solar heat battery candidates. PeerJ Physical Chemistry, 0, 3, e16.	0.0	15

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91	Fast and automatic estimation of transition state structures using tight binding quantum chemical calculations. PeerJ Physical Chemistry, 0, 2, e15.	0.0	15
92	Perspective on "The physical nature of the chemical bond". Theoretical Chemistry Accounts, 2000, 103, 248-251.	0.5	14
93	Effect of mutations on the thermostability of Aspergillus aculeatus Î²-1,4-galactanase. Computational and Structural Biotechnology Journal, 2015, 13, 256-264.	1.9	14
94	Empirical corrections and pair interaction energies in the fragment molecular orbital method. Chemical Physics Letters, 2018, 706, 328-333.	1.2	14
95	Predicting pK_afor proteins using COSMO-RS. PeerJ, 2013, 1, e198.	0.9	14
96	Regiochemical Control by Remote Substituents. A Direct Synthesis of Tetrangulol. Synlett, 2001, 2001, 0521-0522.	1.0	13
97	Interface of the Polarizable Continuum Model of Solvation with Semi-Empirical Methods in the GAMESS Program. PLoS ONE, 2013, 8, e67725.	1.1	13
98	Using a genetic algorithm to find molecules with good docking scores. PeerJ Physical Chemistry, 0, 3, e18.	0.0	13
99	ProCS15: a DFT-based chemical shift predictor for backbone and CÎ²atoms in proteins. PeerJ, 2015, 3, e1344.	0.9	13
100	Splicing I: Using mixed basis sets inab initio calculations. Journal of Computational Chemistry, 1991, 12, 421-426.	1.5	12
101	Random versus Systematic Errors in Reaction Enthalpies Computed Using Semiempirical and Minimal Basis Set Methods. ACS Omega, 2018, 3, 4372-4377.	1.6	12
102	In Silico Prediction of Mutant HIV-1 Proteases Cleaving a Target Sequence. PLoS ONE, 2014, 9, e95833.	1.1	12
103	Intraprotein electrostatics derived from first principles: Divide-and-conquer approaches for QM/MM calculations. Journal of Computational Chemistry, 2003, 24, 1971-1979.	1.5	11
104	Hybrid RHF/MP2 Geometry Optimizations with the Effective Fragment Molecular Orbital Method. PLoS ONE, 2014, 9, e88800.	1.1	11
105	Bayesian inference of protein structure from chemical shift data. PeerJ, 2015, 3, e861.	0.9	11
106	BioFET-SIM Web Interface: Implementation and Two Applications. PLoS ONE, 2012, 7, e45379.	1.1	10
107	Protein structure refinement using a quantum mechanics-based chemical shielding predictor. Chemical Science, 2017, 8, 2061-2072.	3.7	10
108	RegioSQM20: improved prediction of the regioselectivity of electrophilic aromatic substitutions. Journal of Cheminformatics, 2021, 13, 10.	2.8	10

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109	Molecular quantum mechanics to biodynamics: Essential connections. Computational and Theoretical Chemistry, 2006, 764, 1-8.	1.5	9
110	Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods. Journal of Chemical Physics, 2017, 147, 161704.	1.2	9
111	Toward a general theory of hydrogen bonding: A study of hydrogen bonds involving H2O and HF. International Journal of Quantum Chemistry, 2000, 76, 341-358.	1.0	7
112	In silicoscreening of 393 mutants facilitates enzyme engineering of amidase activity in CalB. PeerJ, 2013, 1, e145.	0.9	7
113	Fast and automated identification of reactions with low barriers: the decomposition of 3-hydroperoxypropanal. SciPost Chemistry, 2021, 1, .	2.0	7
114	A computational method for the systematic screening of reaction barriers in enzymes: searching forBacillus circulansxylanase mutants with greater activity towards a synthetic substrate. PeerJ, 2013, 1, e111.	0.9	7
115	Virtual screening of norbornadiene-based molecular solar thermal energy storage systems using a genetic algorithm. Journal of Chemical Physics, 2021, 155, 184105.	1.2	7
116	FragBuilder: an efficient Python library to setup quantum chemistry calculations on peptides models. PeerJ, 2014, 2, e277.	0.9	6
117	RegioML: predicting the regioselectivity of electrophilic aromatic substitution reactions using machine learning. , 2022, 1, 108-114.		6
118	Fast and automated identification of reactions with low barriers using meta-MD simulations. PeerJ Physical Chemistry, 0, 4, e22.	0.0	5
119	A Neural Network Approach for Property Determination of Molecular Solar Cell Candidates. Journal of Physical Chemistry A, 2022, 126, 1681-1688.	1.1	4
120	Regiochemical Control by Remote Substituents - A Selective Synthesis of Angularly Fused Ring Systems. European Journal of Organic Chemistry, 2005, 2005, 3040-3044.	1.2	3
121	Substituent Control of Ïƒ-Interference Effects in the Transmission of Saturated Molecules. ACS Physical Chemistry Au, 2022, 2, 282-288.	1.9	3
122	Applications of Parallel GAMESS. ACS Symposium Series, 1995, , 29-46.	0.5	2
123	Application driven software for chemistry. , 2008, , .		2
124	Perspective on â€œThe physical nature of the chemical bondâ€• , 2000, , 248-251.		1
125	Regiochemical Control by Remote Substituents â€" A Selective Synthesis of Angularly Fused Ring Systems.. ChemInform, 2005, 36, no.	0.1	0
126	Rationalization of the Difference in Lifetime of Two Covalent Sialosylâ^'Enzyme Intermediates of Trypanosoma rangeli Sialidase. Journal of Physical Chemistry B, 2008, 112, 14093-14095.	1.2	0

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127	BioFET-SIM: A Tool for the Analysis and Prediction of Signal Changes in Nanowire-Based Field Effect Transistor Biosensors. Lecture Notes in Nanoscale Science and Technology, 2013, , 55-86.	0.4	0