Jan H Jensen

List of Publications by Year
in descending order

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127 papers	35,346 citations	47006 47 h-index	20358 116 g-index
190 all docs	190 docs citations	190 times ranked	28894 citing authors

#	Article	IF	Citations
1	RegioML: predicting the regioselectivity of electrophilic aromatic substitution reactions using machine learning. , 2022, 1, 108-114.		6
2	A Neural Network Approach for Property Determination of Molecular Solar Cell Candidates. Journal of Physical Chemistry A, 2022, 126, 1681-1688.	2.5	4
3	Substituent Control of ϊf-Interference Effects in the Transmission of Saturated Molecules. ACS Physical Chemistry Au, 2022, 2, 282-288.	4.0	3
4	RegioSQM20: improved prediction of the regioselectivity of electrophilic aromatic substitutions. Journal of Cheminformatics, 2021, 13, 10.	6.1	10
5	Fast and automated identification of reactions with low barriers: the decomposition of 3-hydroperoxypropanal. SciPost Chemistry, 2021, 1, .	4.0	7
6	Virtual screening of norbornadiene-based molecular solar thermal energy storage systems using a genetic algorithm. Journal of Chemical Physics, 2021, 155, 184105.	3.0	7
7	A graph-based genetic algorithm and generative model/Monte Carlo tree search for the exploration of chemical space. Chemical Science, 2019, 10, 3567-3572.	7.4	161
8	Random versus Systematic Errors in Reaction Enthalpies Computed Using Semiempirical and Minimal Basis Set Methods. ACS Omega, 2018, 3, 4372-4377.	3.5	12
9	Fast and accurate prediction of the regioselectivity of electrophilic aromatic substitution reactions. Chemical Science, 2018, 9, 660-665.	7.4	59
10	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.	4.6	20
11	Improving solvation energy predictions using the SMD solvation method and semiempirical electronic structure methods. Journal of Chemical Physics, 2018, 149, 104102.	3.0	39
12	Empirical corrections and pair interaction energies in the fragment molecular orbital method. Chemical Physics Letters, 2018, 706, 328-333.	2.6	14
13	Protein structure refinement using a quantum mechanics-based chemical shielding predictor. Chemical Science, 2017, 8, 2061-2072.	7.4	10
14	Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods. Journal of Chemical Physics, 2017, 147, 161704.	3.0	9
15	Prediction of pK_a Values for Druglike Molecules Using Semiempirical Quantum Chemical Methods. Journal of Physical Chemistry A, 2017, 121, 699-707.	2.5	41
16	Towards a barrier height benchmark set for biologically relevant systems. PeerJ, 2016, 4, e1994.	2.0	22
17	Prediction of pKa values using the PM6 semiempirical method. PeerJ, 2016, 4, e2335.	2.0	29
18	Predicting accurate absolute binding energies in aqueous solution: thermodynamic considerations for electronic structure methods. Physical Chemistry Chemical Physics, 2015, 17, 12441-12451.	2.8	108

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19	Effect of mutations on the thermostability of Aspergillus aculeatus Î²-1,4-galactanase. Computational and Structural Biotechnology Journal, 2015, 13, 256-264.	4.1	14
20	ProCS15: a DFT-based chemical shift predictor for backbone and CÎ²atoms in proteins. PeerJ, 2015, 3, e1344.	2.0	13
21	Bayesian inference of protein structure from chemical shift data. PeerJ, 2015, 3, e861.	2.0	11
22	A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+. PeerJ, 2014, 2, e449.	2.0	46
23	Indium arsenide nanowire field-effect transistors for pH and biological sensing. Applied Physics Letters, 2014, 104, .	3.3	22
24	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.	5.4	58
25	Hybrid RHF/MP2 Geometry Optimizations with the Effective Fragment Molecular Orbital Method. PLoS ONE, 2014, 9, e88800.	2.5	11
26	In Silico Prediction of Mutant HIV-1 Proteases Cleaving a Target Sequence. PLoS ONE, 2014, 9, e95833.	2.5	12
27	FragBuilder: an efficient Python library to setup quantum chemistry calculations on peptides models. PeerJ, 2014, 2, e277.	2.0	6
28	The Molecule Calculator: A Web Application for Fast Quantum Mechanics-Based Estimation of Molecular Properties. Journal of Chemical Education, 2013, 90, 1093-1095.	2.3	36
29	Effects of buffer composition and dilution on nanowire field-effect biosensors. Nanotechnology, 2013, 24, 035501.	2.6	41
30	PHAISTOS: A framework for Markov chain Monte Carlo simulation and inference of protein structure. Journal of Computational Chemistry, 2013, 34, 1697-1705.	3.3	35
31	Fully Integrated Effective Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2013, 9, 2235-2249.	5.3	56
32	In silicoscreening of 393 mutants facilitates enzyme engineering of amidase activity in CalB. PeerJ, 2013, 1, e145.	2.0	7
33	Mapping Enzymatic Catalysis Using the Effective Fragment Molecular Orbital Method: Towards all ab initio Biochemistry. PLoS ONE, 2013, 8, e60602.	2.5	33
34	Interface of the Polarizable Continuum Model of Solvation with Semi-Empirical Methods in the GAMESS Program. PLoS ONE, 2013, 8, e67725.	2.5	13
35	Protein Structure Validation and Refinement Using Amide Proton Chemical Shifts Derived from Quantum Mechanics. PLoS ONE, 2013, 8, e84123.	2.5	21
36	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.	2.0	7

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37	Predicting pK_afor proteins using COSMO-RS. PeerJ, 2013, 1, e198.	2.0	14
38	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.	0.8	0
39	BioFET-SIM Web Interface: Implementation and Two Applications. PLoS ONE, 2012, 7, e45379.	2.5	10
40	The Effective Fragment Molecular Orbital Method for Fragments Connected by Covalent Bonds. PLoS ONE, 2012, 7, e41117.	2.5	28
41	FragIt: A Tool to Prepare Input Files for Fragment Based Quantum Chemical Calculations. PLoS ONE, 2012, 7, e44480.	2.5	39
42	A Computational Methodology to Screen Activities of Enzyme Variants. PLoS ONE, 2012, 7, e49849.	2.5	15
43	Definitive Benchmark Study of Ring Current Effects on Amide Proton Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 2078-2084.	5.3	16
44	PROPKA3: Consistent Treatment of Internal and Surface Residues in Empirical pK_a Predictions. Journal of Chemical Theory and Computation, 2011, 7, 525-537.	5.3	3,121
45	Predicting and rationalizing the effect of surface charge distribution and orientation on nano-wire based FET bio-sensors. Nanoscale, 2011, 3, 3635.	5.6	35
46	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.	5.3	1,436
47	Quantifying signal changes in nano-wire based biosensors. Nanoscale, 2011, 3, 706-717.	5.6	37
48	Graphical analysis of pH-dependent properties of proteins predicted using PROPKA. BMC Structural Biology, 2011, 11, 6.	2.3	328
49	Energy gradients in combined fragment molecular orbital and polarizable continuum model (FMO/PCM) calculation. Journal of Computational Chemistry, 2010, 31, 778-790.	3.3	37
50	Exchange repulsion between effective fragment potentials and ab initio molecules. Theoretical Chemistry Accounts, 2010, 125, 481-491.	1.4	26
51	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.	2.5	80
52	Analytic gradient for the adaptive frozen orbital bond detachment in the fragment molecular orbital method. Chemical Physics Letters, 2009, 477, 169-175.	2.6	53
53	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
54	Proteinâ€“protein binding is often associated with changes in protonation state. Proteins: Structure, Function and Bioinformatics, 2008, 71, 81-91.	2.6	38

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55	Very fast prediction and rationalization of pK_a values for proteinâ€“ligand complexes. Proteins: Structure, Function and Bioinformatics, 2008, 73, 765-783.	2.6	938
56	Covalent Bond Fragmentation Suitable To Describe Solids in the Fragment Molecular Orbital Method. Journal of Physical Chemistry A, 2008, 112, 11808-11816.	2.5	76
57	Application driven software for chemistry. , 2008, , .		2
58	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.	2.6	0
59	Role of the virtual orbitals and HOMO-LUMO gap in mean-field approximations to the conductance of molecular junctions. Physical Review B, 2008, 77, .	3.2	20
60	Calculating pH and Salt Dependence of Protein-Protein Binding. Current Pharmaceutical Biotechnology, 2008, 9, 96-102.	1.6	35
61	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 1. Journal of Chemical Theory and Computation, 2007, 3, 1620-1628.	5.3	17
62	Sugar Folding:â€‰ A Novel Structural Prediction Tool for Oligosaccharides and Polysaccharides 2. Journal of Chemical Theory and Computation, 2007, 3, 1629-1643.	5.3	30
63	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.	2.8	119
64	Chapter 10 The Effective Fragment Potential: A General Method for Predicting Intermolecular Interactions. Annual Reports in Computational Chemistry, 2007, 3, 177-193.	1.7	193
65	PDB2PQR: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. Nucleic Acids Research, 2007, 35, W522-W525.	14.5	1,659
66	Prediction and Rationalization of the pH Dependence of the Activity and Stability of Family 11 Xylanases. Biochemistry, 2007, 46, 13581-13592.	2.5	24
67	Surface Reactions of Carbon Dioxide at the Adsorbed Waterâ^'Oxide Interface. Journal of Physical Chemistry C, 2007, 111, 14870-14880.	3.1	69
68	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.	2.6	170
69	Charge transfer interaction in the effective fragment potential method. Journal of Chemical Physics, 2006, 124, 214108.	3.0	74
70	Exploring the Role of the Active Site Cysteine in Human Muscle Creatine Kinaseâ€. Biochemistry, 2006, 45, 11464-11472.	2.5	21
71	Hydride Transfer versus Hydrogen Radical Transfer in Thymidylate Synthase. Journal of the American Chemical Society, 2006, 128, 5636-5637.	13.7	35
72	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.	13.7	69

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73	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.	2.6	21
74	Molecular quantum mechanics to biodynamics: Essential connections. Computational and Theoretical Chemistry, 2006, 764, 1-8.	1.5	9
75	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.	2.8	16
76	The polarizable continuum model (PCM) interfaced with the fragment molecular orbital method (FMO). Journal of Computational Chemistry, 2006, 27, 976-985.	3.3	161
77	Regiochemical Control by Remote Substituents - A Selective Synthesis of Angularly Fused Ring Systems. European Journal of Organic Chemistry, 2005, 2005, 3040-3044.	2.4	3
78	Regiochemical Control by Remote Substituents â€" A Selective Synthesis of Angularly Fused Ring Systems.. ChemInform, 2005, 36, no.	0.0	0
79	Very fast empirical prediction and rationalization of protein pKa values. Proteins: Structure, Function and Bioinformatics, 2005, 61, 704-721.	2.6	1,771
80	Prediction and Rationalization of Protein pKa Values Using QM and QM/MM Methods. Journal of Physical Chemistry A, 2005, 109, 6634-6643.	2.5	131
81	Determinants of cysteine pKa values in creatine kinase and Î±1-antitrypsin. Proteins: Structure, Function and Bioinformatics, 2004, 57, 799-803.	2.6	40
82	The determinants of carboxyl pKa values in turkey ovomucoid third domain. Proteins: Structure, Function and Bioinformatics, 2004, 55, 689-704.	2.6	84
83	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.	3.3	144
84	Determinants of the Relative Reduction Potentials of Type-1 Copper Sites in Proteins. Journal of the American Chemical Society, 2004, 126, 8010-8019.	13.7	134
85	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.	1.4	32
86	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.	1.4	91
87	Intraprotein electrostatics derived from first principles: Divide-and-conquer approaches for QM/MM calculations. Journal of Computational Chemistry, 2003, 24, 1971-1979.	3.3	11
88	A Predictive Model of Strong Hydrogen Bonding in Proteins:Â The NÎ´1â^'Hâ^'OÎ´1Hydrogen Bond in Low-pH Î±-Chymotrypsin and Î±-Lytic Protease. Journal of Physical Chemistry B, 2003, 107, 6226-6233.	2.6	37
89	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.	13.7	29
90	Boundary Conditions for the Swainâ^'Schaad Relationship as a Criterion for Hydrogen Tunneling. Journal of the American Chemical Society, 2002, 124, 3858-3864.	13.7	56

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91	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.	2.6	90
92	Partial Hessian vibrational analysis: the localization of the molecular vibrational energy and entropy. Theoretical Chemistry Accounts, 2002, 107, 211-219.	1.4	109
93	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.	2.5	570
94	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.	2.5	45
95	Regiochemical Control by Remote Substituents. A Direct Synthesis of Tetrangulol. Synlett, 2001, 2001, 0521-0522.	1.8	13
96	Intermolecular exchange-induction and charge transfer: Derivation of approximate formulas using nonorthogonal localized molecular orbitals. Journal of Chemical Physics, 2001, 114, 8775-8783.	3.0	41
97	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.	2.0	7
98	Perspective on "The physical nature of the chemical bond". Theoretical Chemistry Accounts, 2000, 103, 248-251.	1.4	14
99	Evaluation of charge penetration between distributed multipolar expansions. Journal of Chemical Physics, 2000, 112, 7300-7306.	3.0	149
100	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.	2.5	81
101	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.	2.5	136
102	Perspective on â€œThe physical nature of the chemical bondâ€• , 2000, , 248-251.		1
103	Evaluation of the charge penetration energy between non-orthogonal molecular orbitals using the Spherical Gaussian Overlap approximation. Chemical Physics Letters, 1999, 315, 140-144.	2.6	61
104	1,3-Transposition of Allylic Alcohols Catalyzed by Methyltrioxorhenium. Organometallics, 1998, 17, 1835-1840.	2.3	71
105	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.	3.0	105
106	Modeling intermolecular exchange integrals between nonorthogonal molecular orbitals. Journal of Chemical Physics, 1996, 104, 7795-7796.	3.0	39
107	Understanding the Hydrogen Bond Using Quantum Chemistry. Accounts of Chemical Research, 1996, 29, 536-543.	15.6	188
108	An effective fragment method for modeling solvent effects in quantum mechanical calculations. Journal of Chemical Physics, 1996, 105, 1968-1986.	3.0	578

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109	An approximate formula for the intermolecular Pauli repulsion between closed shell molecules. Molecular Physics, 1996, 89, 1313-1325.	1.7	110
110	Applications of Parallel GAMESS. ACS Symposium Series, 1995, , 29-46.	0.5	2
111	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
112	Direct Total Syntheses of Frenolicin B and Kalafungin via Highly Regioselective Diels-Alder Reactions. Journal of Organic Chemistry, 1995, 60, 1154-1159.	3.2	51
113	On the Number of Water Molecules Necessary To Stabilize the Glycine Zwitterion. Journal of the American Chemical Society, 1995, 117, 8159-8170.	13.7	419
114	Pathways for H2 elimination from ethylene: A theoretical study. Journal of Chemical Physics, 1994, 100, 1981-1987.	3.0	53
115	Effective Fragment Method for Modeling Intermolecular Hydrogen-Bonding Effects on Quantum Mechanical Calculations. ACS Symposium Series, 1994, , 139-151.	0.5	47
116	Regiocontrol by Remote Substituents. A Direct Total Synthesis of Racemic Hongconin. Journal of Organic Chemistry, 1994, 59, 2219-2222.	3.2	31
117	General atomic and molecular electronic structure system. Journal of Computational Chemistry, 1993, 14, 1347-1363.	3.3	19,020
118	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.	13.7	68
119	Uncatalyzed peptide bond formation in the gas phase. The Journal of Physical Chemistry, 1992, 96, 8340-8351.	2.9	90
120	Nature of the silicon-nitrogen bond in silatranes. Organometallics, 1991, 10, 2657-2660.	2.3	70
121	Conformational potential energy surface of glycine: a theoretical study. Journal of the American Chemical Society, 1991, 113, 7917-7924.	13.7	238
122	Splicing I: Using mixed basis sets inab initio calculations. Journal of Computational Chemistry, 1991, 12, 421-426.	3.3	12
123	High throughput virtual screening of 230 billion molecular solar heat battery candidates. PeerJ Physical Chemistry, 0, 3, e16.	0.0	15
124	Using a genetic algorithm to find molecules with good docking scores. PeerJ Physical Chemistry, 0, 3, e18.	0.0	13
125	Chemical space exploration: how genetic algorithms find the needle in the haystack. PeerJ Physical Chemistry, 0, 2, e11.	0.0	25
126	Fast and automatic estimation of transition state structures using tight binding quantum chemical calculations. PeerJ Physical Chemistry, 0, 2, e15.	0.0	15

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127	Fast and automated identification of reactions with low barriers using meta-MD simulations. PeerJ Physical Chemistry, 0, 4, e22.	0.0	5