

Richard A Friesner

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

152 papers	30,663 citations	65 h-index	158 g-index
158 ext. papers	35,826 ext. citations	7.4 avg, IF	6.91 L-index

#	Paper	IF	Citations
152	Glide: a new approach for rapid, accurate docking and scoring. 1. Method and assessment of docking accuracy. <i>Journal of Medicinal Chemistry</i> , 2004 , 47, 1739-49	8.3	5601
151	Extra precision glide: docking and scoring incorporating a model of hydrophobic enclosure for protein-ligand complexes. <i>Journal of Medicinal Chemistry</i> , 2006 , 49, 6177-96	8.3	3757
150	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 281-96	6.4	1555
149	A hierarchical approach to all-atom protein loop prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 55, 351-67	4.2	1329
148	Novel procedure for modeling ligand/receptor induced fit effects. <i>Journal of Medicinal Chemistry</i> , 2006 , 49, 534-53	8.3	1320
147	Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. <i>Journal of the American Chemical Society</i> , 1994 , 116, 11875-11882	16.4	953
146	New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 11775-11788		852
145	PHASE: a new engine for pharmacophore perception, 3D QSAR model development, and 3D database screening: 1. Methodology and preliminary results. <i>Journal of Computer-Aided Molecular Design</i> , 2006 , 20, 647-71	4.2	764
144	On the role of the crystal environment in determining protein side-chain conformations. <i>Journal of Molecular Biology</i> , 2002 , 320, 597-608	6.5	691
143	Accurate and reliable prediction of relative ligand binding potency in prospective drug discovery by way of a modern free-energy calculation protocol and force field. <i>Journal of the American Chemical Society</i> , 2015 , 137, 2695-703	16.4	633
142	Motifs for molecular recognition exploiting hydrophobic enclosure in protein-ligand binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 808-13	11.5	536
141	Role of the active-site solvent in the thermodynamics of factor Xa ligand binding. <i>Journal of the American Chemical Society</i> , 2008 , 130, 2817-31	16.4	500
140	The VSGB 2.0 model: a next generation energy model for high resolution protein structure modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 2794-812	4.2	483
139	Ab initio quantum chemical and mixed quantum mechanics/molecular mechanics (QM/MM) methods for studying enzymatic catalysis. <i>Annual Review of Physical Chemistry</i> , 2005 , 56, 389-427	15.7	447
138	Mechanistic studies on the hydroxylation of methane by methane monooxygenase. <i>Chemical Reviews</i> , 2003 , 103, 2385-419	68.1	407
137	Replica exchange with solute scaling: a more efficient version of replica exchange with solute tempering (REST2). <i>Journal of Physical Chemistry B</i> , 2011 , 115, 9431-8	3.4	387
136	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1863-1874	6.4	337

135	Accurate ab Initio Quantum Chemical Determination of the Relative Energetics of Peptide Conformations and Assessment of Empirical Force Fields. <i>Journal of the American Chemical Society</i> , 1997 , 119, 5908-5920	16.4	323
134	Computing Redox Potentials in Solution: Density Functional Theory as A Tool for Rational Design of Redox Agents. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 7407-7412	2.8	319
133	Electronic Structure and Luminescence of 1.1- and 1.4-nm Silicon Nanocrystals: Oxide Shell versus Hydrogen Passivation. <i>Nano Letters</i> , 2003 , 3, 163-167	11.5	264
132	Correlated ab Initio Electronic Structure Calculations for Large Molecules. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 1913-1928	2.8	258
131	Combined fluctuating charge and polarizable dipole models: Application to a five-site water potential function. <i>Journal of Chemical Physics</i> , 2001 , 115, 2237-2251	3.9	256
130	Mixed ab initio QM/MM modeling using frozen orbitals and tests with alanine dipeptide and tetrapeptide. <i>Journal of Computational Chemistry</i> , 1999 , 20, 1468-1494	3.5	232
129	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. <i>Journal of Chemical Physics</i> , 1999 , 110, 741-754	3.9	225
128	Solution of self-consistent field electronic structure equations by a pseudospectral method. <i>Chemical Physics Letters</i> , 1985 , 116, 39-43	2.5	224
127	Ab initio quantum chemistry: methodology and applications. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 6648-53	11.5	217
126	Development of an Accurate and Robust Polarizable Molecular Mechanics Force Field from ab Initio Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 621-627	2.8	209
125	Aqua, Alcohol, and Acetonitrile Adducts of Tris(perfluorophenyl)borane: Evaluation of Brønsted Acidity and Ligand Lability with Experimental and Computational Methods. <i>Journal of the American Chemical Society</i> , 2000 , 122, 10581-10590	16.4	197
124	Solvation Free Energies of Peptides: Comparison of Approximate Continuum Solvation Models with Accurate Solution of the Poisson-Boltzmann Equation. <i>Journal of Physical Chemistry B</i> , 1997 , 101, 1190-1197	3.4	192
123	Solution of the Hartree-Fock equations by a pseudospectral method: Application to diatomic molecules. <i>Journal of Chemical Physics</i> , 1986 , 85, 1462-1468	3.9	172
122	Cryo-EM Structures of SARS-CoV-2 Spike without and with ACE2 Reveal a pH-Dependent Switch to Mediate Endosomal Positioning of Receptor-Binding Domains. <i>Cell Host and Microbe</i> , 2020 , 28, 867-879.e5	23.4	168
121	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2553-8	6.4	159
120	Pseudospectral localized Møller-Plesset methods: Theory and calculation of conformational energies. <i>Journal of Chemical Physics</i> , 1995 , 103, 1481-1490	3.9	159
119	Large Scale ab Initio Quantum Chemical Calculation of the Intermediates in the Soluble Methane Monooxygenase Catalytic Cycle. <i>Journal of the American Chemical Society</i> , 2000 , 122, 2828-2839	16.4	157
118	Force Field Validation Using Protein Side Chain Prediction. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 11673-11680	3.4	155

117	Numerical solution of the Poisson-Boltzmann equation using tetrahedral finite-element meshes. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1591-1608	3.5	154
116	On achieving high accuracy and reliability in the calculation of relative protein-ligand binding affinities. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 1937-42	11.5	151
115	Peripheral heme substituents control the hydrogen-atom abstraction chemistry in cytochromes P450. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003 , 100, 6998-7002	11.5	138
114	Advancing Drug Discovery through Enhanced Free Energy Calculations. <i>Accounts of Chemical Research</i> , 2017 , 50, 1625-1632	24.3	126
113	Cytochrome P450CAM enzymatic catalysis cycle: a quantum mechanics/molecular mechanics study. <i>Journal of the American Chemical Society</i> , 2004 , 126, 8501-8	16.4	126
112	Constructing ab initio force fields for molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1998 , 108, 4739-4755	3.9	126
111	The Redfield Equation in Condensed-Phase Quantum Dynamics. <i>Advances in Chemical Physics</i> , 2007 , 77-134		124
110	Solution of the Hartree-Fock equations for polyatomic molecules by a pseudospectral method. <i>Journal of Chemical Physics</i> , 1987 , 86, 3522-3531	3.9	123
109	Prediction of Protein-Ligand Binding Poses via a Combination of Induced Fit Docking and Metadynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2990-8	6.4	120
108	Dioxygen activation in methane monooxygenase: a theoretical study. <i>Journal of the American Chemical Society</i> , 2004 , 126, 2978-90	16.4	114
107	Antibody structure determination using a combination of homology modeling, energy-based refinement, and loop prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 1646-55	4.2	110
106	Solvent models for protein-ligand binding: Comparison of implicit solvent poisson and surface generalized born models with explicit solvent simulations. <i>Journal of Computational Chemistry</i> , 2001 , 22, 591-607	3.5	108
105	The effect of heme environment on the hydrogen abstraction reaction of camphor in P450cam catalysis: a QM/MM study. <i>Journal of the American Chemical Society</i> , 2006 , 128, 3924-5	16.4	98
104	Activation of the C-H bond of methane by intermediate Q of methane monooxygenase: a theoretical study. <i>Journal of the American Chemical Society</i> , 2001 , 123, 3836-7	16.4	96
103	Large-scale ab initio quantum chemical calculations on biological systems. <i>Accounts of Chemical Research</i> , 2001 , 34, 351-8	24.3	92
102	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 4291-4300	6.4	92
101	A method for exponential propagation of large systems of stiff nonlinear differential equations. <i>Journal of Scientific Computing</i> , 1989 , 4, 327-354	2.3	91
100	Improved Methods for Side Chain and Loop Predictions via the Protein Local Optimization Program: Variable Dielectric Model for Implicitly Improving the Treatment of Polarization Effects. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 2108-19	6.4	89

99	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5780-5797	6.4	85
98	Accurate Force Field Development for Modeling Conjugated Polymers. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4556-69	6.4	85
97	Accurate Binding Free Energy Predictions in Fragment Optimization. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2411-20	6.1	83
96	Pseudospectral HartreeFock theory: Applications and algorithmic improvements. <i>Journal of Chemical Physics</i> , 1990 , 93, 3397-3407	3.9	82
95	Prediction of loop geometries using a generalized born model of solvation effects 1999 , 35, 173-183		81
94	A three-dimensional reduction of the OrnsteinZernicke equation for molecular liquids. <i>Journal of Chemical Physics</i> , 1997 , 107, 6400-6414	3.9	75
93	An automatic three-dimensional finite element mesh generation system for the PoissonBoltzmann equation. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1570-1590	3.5	75
92	Correcting Systematic Errors in DFT Spin-Splitting Energetics for Transition Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 19-32	6.4	73
91	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 42-54	6.4	68
90	Pseudospectral localized generalized Mo/llerPlesset methods with a generalized valence bond reference wave function: Theory and calculation of conformational energies. <i>Journal of Chemical Physics</i> , 1997 , 106, 5073-5084	3.9	68
89	Reactions of methane monooxygenase intermediate Q with derivatized methanes. <i>Journal of the American Chemical Society</i> , 2002 , 124, 8770-1	16.4	67
88	Efficient Simulation Method for Polarizable Protein Force Fields: Application to the Simulation of BPTI in Liquid Water. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 169-80	6.4	65
87	An automatic grid generation scheme for pseudospectral self-consistent field calculations on polyatomic molecules. <i>The Journal of Physical Chemistry</i> , 1988 , 92, 3091-3096		65
86	A zinc thiolate species which mimics aspects of the chemistry of the Ada repair protein and matrix metalloproteinases: the synthesis, structure and reactivity of the tris(2-mercapto-1-phenylimidazolyl)hydroborato complex [TmPh]ZnSPh. <i>Dalton Transactions RSC</i> , 2000 , 4434-4436		63
85	Pseudospectral generalized valence-bond calculations: Application to methylene, ethylene, and silylene. <i>Journal of Chemical Physics</i> , 1990 , 92, 7488-7497	3.9	63
84	Hydrogen Bonding between Amino Acid Backbone and Side Chain Analogues: A High-Level ab Initio Study. <i>Journal of the American Chemical Society</i> , 1997 , 119, 12952-12961	16.4	61
83	Hydroxylation of methane by non-heme diiron enzymes: molecular orbital analysis of C-H bond activation by reactive intermediate Q. <i>Journal of the American Chemical Society</i> , 2002 , 124, 14608-15	16.4	61
82	Modeling Polarization in Proteins and Protein-ligand Complexes: Methods and Preliminary Results. <i>Advances in Protein Chemistry</i> , 2005 , 72, 79-104		60

81	A Critical Review of Validation, Blind Testing, and Real- World Use of Alchemical Protein-Ligand Binding Free Energy Calculations. <i>Current Topics in Medicinal Chemistry</i> , 2017 , 17, 2577-2585	3	60
80	Development of Accurate DFT Methods for Computing Redox Potentials of Transition Metal Complexes: Results for Model Complexes and Application to Cytochrome P450. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 442-59	6.4	58
79	Substrate hydroxylation in methane monooxygenase: quantitative modeling via mixed quantum mechanics/molecular mechanics techniques. <i>Journal of the American Chemical Society</i> , 2005 , 127, 1025-37	16.4	56
78	Mechanistic and Theoretical Analysis of the Oxidative Addition of H ₂ to Six-Coordinate Molybdenum and Tungsten Complexes M(PMe ₃) ₄ X ₂ (M = Mo, W; X = F, Cl, Br, I): An Inverse Equilibrium Isotope Effect and an Unprecedented Halide Dependence. <i>Journal of the American Chemical Society</i> , 1999 , 121, 11402-11417	16.4	56
77	WScore: A Flexible and Accurate Treatment of Explicit Water Molecules in Ligand-Receptor Docking. <i>Journal of Medicinal Chemistry</i> , 2016 , 59, 4364-84	8.3	53
76	A localized orbital analysis of the thermochemical errors in hybrid density functional theory: achieving chemical accuracy via a simple empirical correction scheme. <i>Journal of Chemical Physics</i> , 2006 , 125, 124107	3.9	52
75	Photodissociation of acetaldehyde: The CH ₄ +CO channel. <i>Journal of Chemical Physics</i> , 2001 , 114, 6128-6133	3.3	49
74	Evaluation of the Performance of the B3LYP, PBE0, and M06 DFT Functionals, and DBLOC-Corrected Versions, in the Calculation of Redox Potentials and Spin Splittings for Transition Metal Containing Systems. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1121-8	6.4	48
73	Realistic cluster modeling of electron transport and trapping in solvated TiO ₂ nanoparticles. <i>Journal of the American Chemical Society</i> , 2012 , 134, 12028-42	16.4	48
72	Free Energy Perturbation Calculation of Relative Binding Free Energy between Broadly Neutralizing Antibodies and the gp120 Glycoprotein of HIV-1. <i>Journal of Molecular Biology</i> , 2017 , 429, 930-947	6.5	47
71	Accelerating drug discovery through tight integration of expert molecular design and predictive scoring. <i>Current Opinion in Structural Biology</i> , 2017 , 43, 38-44	8.1	47
70	Efficient memory equation algorithm for reduced dynamics in spin-boson models. <i>Journal of Chemical Physics</i> , 1999 , 110, 138-146	3.9	47
69	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5696-5705	6.4	44
68	Protein tertiary structure prediction using a branch and bound algorithm. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 35, 41-57	4.2	44
67	On Achieving High Accuracy in Quantum Chemical Calculations of 3 d Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2346-2358	6.4	42
66	Quantum mechanical geometry optimization in solution using a finite element continuum electrostatics method. <i>Journal of Chemical Physics</i> , 1996 , 105, 5472-5484	3.9	42
65	Reduced dynamics in spin-boson models: A method for both slow and fast bath. <i>Journal of Chemical Physics</i> , 2000 , 112, 2095-2105	3.9	41
64	Pseudospectral Hartree-Fock calculations on glycine. <i>Journal of Chemical Physics</i> , 1990 , 92, 1163-1173	3.9	38

63	ENERGY TRANSFER BETWEEN THE PRIMARY DONOR BACTERIOCHLOROPHYLL AND CAROTENOIDS IN <i>Rhodopseudomonas sphaeroides</i> . <i>Photochemistry and Photobiology</i> , 1983 , 38, 451-455 ^{3.6}	38
62	Density functional localized orbital corrections for transition metals. <i>Journal of Chemical Physics</i> , 2008 , 129, 164108	3.9 37
61	Factors Influencing the Thermodynamics of Zinc Alkoxide Formation by Alcoholysis of the Terminal Hydroxide Complex, [TpBut,Me]ZnOH: An Experimental and Theoretical Study Relevant to the Mechanism of Action of Liver Alcohol Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2000 , 122, 12651-12658	16.4 34
60	A B3LYP-DBLOC empirical correction scheme for ligand removal enthalpies of transition metal complexes: parameterization against experimental and CCSD(T)-F12 heats of formation. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 7724-38	3.6 30
59	Quantum Chemical Investigation of Cluster Models for TiO ₂ Nanoparticles with Water-Derived Ligand Passivation: Studies of Excess Electron States and Implications for Charge Transport in the Gratzel Cell. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 19806-19811	3.8 30
58	Conformational Dynamics of the Partially Disordered Yeast Transcription Factor GCN4. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9,	6.4 29
57	Localized orbital corrections for the calculation of ionization potentials and electron affinities in density functional theory. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 18787-802	3.4 29
56	Relative Binding Affinity Prediction of Charge-Changing Sequence Mutations with FEP in Protein-Protein Interfaces. <i>Journal of Molecular Biology</i> , 2019 , 431, 1481-1493	6.5 29
55	QM/MM Simulation on P450 BM3 Enzyme Catalysis Mechanism. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1421-1431	6.4 28
54	Natural expansion of vibrational wave functions: RRGm with residue algebra. <i>Journal of Chemical Physics</i> , 1986 , 85, 331-336	3.9 28
53	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Protein-Ligand Complexes. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 640-8	6.4 27
52	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4109-4121	6.4 25
51	Covalent O-H bonds as electron traps in proton-rich rutile TiO ₂ nanoparticles. <i>Nano Letters</i> , 2014 , 14, 1785-9	11.5 25
50	Calculation of temperature-dependent multimode resonance Raman line shapes for harmonic potential surfaces). <i>Journal of Chemical Physics</i> , 1985 , 82, 2918-2926	3.9 23
49	Singlet-Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4924-4932	6.4 22
48	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 2667-2680 ^{6.4}	21
47	Pseudospectral Hartree-Fock gradient calculations. <i>Journal of Chemical Physics</i> , 1991 , 94, 8152-8157	3.9 21
46	Calculation of optical line shapes for generalized multilevel vibronic systems. <i>Journal of Chemical Physics</i> , 1984 , 81, 5899-5905	3.9 21

45	Free Energy Perturbation Calculations of the Thermodynamics of Protein Side-Chain Mutations. <i>Journal of Molecular Biology</i> , 2017 , 429, 923-929	6.5	20
44	1,3-Dipolar Addition of Phenylazide to the Carbon-Carbon Double Bond: An ab Initio Study. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 1276-1282	2.8	20
43	Accurate pKa prediction in first-row hexaaqua transition metal complexes using the B3LYP-DBLOC method. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 8008-16	3.4	19
42	Localized orbital corrections for the calculation of barrier heights in density functional theory. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2996-3009	6.4	19
41	Application and development of multiconfigurational localized perturbation theory. <i>Journal of Chemical Physics</i> , 2001 , 115, 11052-11067	3.9	19
40	An experimental and computational analysis of the formation of the terminal nitrido complex (eta ³ -Cp*) ₂ Mo(N)(N ₃) by elimination of N ₂ from Cp* ₂ Mo(N ₃) ₂ : the barrier to elimination is strongly influenced by the exo versus endo configuration of the azide ligand. <i>Journal of the American Chemical Society</i> , 2001 , 123, 10111-2	16.4	19
39	Spin-spin model for two-level system/bath problems: A numerical study. <i>Journal of Chemical Physics</i> , 1999 , 111, 9918-9923	3.9	19
38	Localized orbital corrections applied to thermochemical errors in density functional theory: The role of basis set and application to molecular reactions. <i>Journal of Chemical Physics</i> , 2008 , 129, 214105	3.9	18
37	Highly efficient implementation of pseudospectral time-dependent density-functional theory for the calculation of excitation energies of large molecules. <i>Journal of Computational Chemistry</i> , 2016 , 37, 1425-41	3.5	17
36	Computational methods for high resolution prediction and refinement of protein structures. <i>Current Opinion in Structural Biology</i> , 2013 , 23, 177-84	8.1	17
35	Leveraging Data Fusion Strategies in Multireceptor Lead Optimization MM/GBSA End-Point Methods. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3207-20	6.4	16
34	Tertiary structure prediction of mixed α/β proteins via energy minimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 1998 , 33, 240-252	4.2	16
33	Combined quantum and molecular mechanics (QM/MM). <i>Drug Discovery Today: Technologies</i> , 2004 , 1, 253-60	7.1	16
32	Classical and Quantum Models of Activationless Reaction Dynamics. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1991 , 95, 253-258		16
31	Parallel pseudospectral electronic structure: I. Hartree-Fock calculations. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1017-1029	3.5	15
30	Protein structure prediction using a combination of sequence-based alignment, constrained energy minimization, and structural alignment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001 , Suppl 5, 133-9	4.2	15
29	Calculation of atomization energies by a multiconfigurational localized perturbation theory: Application for closed shell cases. <i>Journal of Chemical Physics</i> , 1999 , 110, 1921-1930	3.9	14
28	Parallel pseudospectral electronic structure: II. Localized Møller-Plesset calculations. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1030-1038	3.5	13

27	Reliable and Accurate Solution to the Induced Fit Docking Problem for Protein-Ligand Binding. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 2630-2639	6.4	13
26	Computational Modeling of the Electronic Structure of Oligothiophenes with Various Side Chains. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 2553-2561	3.8	10
25	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3041-3054	6.4	10
24	Computational Modeling for Scanning Tunneling Microscopy of Physisorbed Molecules via Ab Initio Quantum Chemistry. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 1802-1814	2.8	9
23	Modeling the value of predictive affinity scoring in preclinical drug discovery. <i>Current Opinion in Structural Biology</i> , 2018 , 52, 103-110	8.1	9
22	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3647-3663	6.4	8
21	Theoretical studies of diiron(II) complexes that model features of the dioxygen-activating centers in non-heme diiron enzymes. <i>Israel Journal of Chemistry</i> , 2001 , 41, 173-186	3.4	8
20	A hierarchical algorithm for polymer simulations. <i>Journal of Chemical Physics</i> , 1992 , 97, 9355-9365	3.9	8
19	Multiple Stable Isoprene-Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. <i>Journal of the American Chemical Society</i> , 2020 , 142, 10806-10813	16.4	7
18	Prediction of Long Loops with Embedded Secondary Structure using the Protein Local Optimization Program. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1846-4864	6.4	7
17	A Thermal Expansion Model for the Special Pair of the Bacterial Reaction Center. <i>Israel Journal of Chemistry</i> , 1988 , 28, 67-72	3.4	7
16	Successful application of the DBLOC method to the hydroxylation of camphor by cytochrome p450. <i>Protein Science</i> , 2016 , 25, 277-85	6.3	7
15	Extension of the PS-GVB electronic structure code to transition metal complexes. <i>Journal of Computational Chemistry</i> , 1997 , 18, 1863-1874	3.5	5
14	Parallel implementation of a protein structure refinement algorithm. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1217-1228	3.5	5
13	Green's functions and optical line shapes of a general two-level system in the strong electronic coupling limit. <i>Journal of Chemical Physics</i> , 1982 , 76, 2129-2135	3.9	5
12	Localized orbital corrections for density functional calculations on transition metal containing systems. <i>Coordination Chemistry Reviews</i> , 2017 , 344, 205-213	23.2	3
11	Conformational preferences underlying reduced activity of a thermophilic ribonuclease H. <i>Journal of Molecular Biology</i> , 2015 , 427, 853-866	6.5	3
10	An accurate and efficient decoupling approximation for temperature-dependent multimode resonance Raman spectra. <i>Journal of Chemical Physics</i> , 1986 , 85, 2353-2364	3.9	3

9	Prediction of loop geometries using a generalized born model of solvation effects 1999 , 35, 173		3
8	Accurate Quantum Chemical Calculation of Ionization Potentials: Validation of the DFT-LOC Approach via a Large Data Set Obtained from Experiments and Benchmark Quantum Chemical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 2109-2123	6.4	1
7	A first-principles polarized Raman method for determining whether a uniform region of a sample is crystalline or isotropic. <i>Journal of Chemical Physics</i> , 2014 , 141, 224702	3.9	1
6	Ab Initio Protein Structure Prediction Using a Size-dependent Tertiary Folding Potential. <i>Advances in Chemical Physics</i> , 2002 , 223-263		1
5	prediction of annihilators for triplet-triplet annihilation upconversion auxiliary-field quantum Monte Carlo. <i>Chemical Science</i> , 2020 , 12, 1068-1079	9.4	1
4	Pseudospectral implementations of long-range corrected density functional theory. <i>Journal of Computational Chemistry</i> , 2021 , 42, 2089-2102	3.5	0
3	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. <i>Journal of Cheminformatics</i> , 2016 , 8, 18	8.6	
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