

Richard A Friesner

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	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, 1739-1749.	2.9	7,428
2	Extra Precision Glide: Docking and Scoring Incorporating a Model of Hydrophobic Enclosure for Protein-Ligand Complexes. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 6177-6196.	2.9	5,196
3	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 281-296.	2.3	2,349
4	A hierarchical approach to all-atom protein loop prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 351-367.	1.5	1,874
5	Novel Procedure for Modeling Ligand/Receptor Induced Fit Effects. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 534-553.	2.9	1,671
6	Jaguar: A high-performance quantum chemistry software program with strengths in life and materials sciences. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2110-2142.	1.0	1,426
7	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.	6.6	1,026
8	On the Role of the Crystal Environment in Determining Protein Side-chain Conformations. <i>Journal of Molecular Biology</i> , 2002, 320, 597-608.	2.0	1,002
9	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, 647-671.	1.3	963
10	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.	2.9	936
11	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, 2695-2703.	6.6	931
12	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, 2794-2812.	1.5	773
13	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1863-1874.	2.3	698
14	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, 808-813.	3.3	633
15	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, 9431-9438.	1.2	595
16	Role of the Active-Site Solvent in the Thermodynamics of Factor Xa Ligand Binding. <i>Journal of the American Chemical Society</i> , 2008, 130, 2817-2831.	6.6	594
17	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4291-4300.	2.3	582
18	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.	4.8	493

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19	Mechanistic Studies on the Hydroxylation of Methane by Methane Monooxygenase. <i>Chemical Reviews</i> , 2003, 103, 2385-2420.	23.0	479
20	Computing Redox Potentials in Solution: A Density Functional Theory as A Tool for Rational Design of Redox Agents. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7407-7412.	1.1	374
21	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.	6.6	339
22	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.	5.1	316
23	Electronic Structure and Luminescence of 1.1- and 1.4-nm Silicon Nanocrystals: A Oxide Shell versus Hydrogen Passivation. <i>Nano Letters</i> , 2003, 3, 163-167.	4.5	292
24	Ab initio quantum chemistry: Methodology and applications. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6648-6653.	3.3	279
25	Correlated ab Initio Electronic Structure Calculations for Large Molecules. <i>Journal of Physical Chemistry A</i> , 1999, 103, 1913-1928.	1.1	274
26	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.	1.5	268
27	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.	1.2	267
28	Solution of self-consistent field electronic structure equations by a pseudospectral method. <i>Chemical Physics Letters</i> , 1985, 116, 39-43.	1.2	258
29	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.	1.2	251
30	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, 2553-2558.	2.3	239
31	Aqua, Alcohol, and Acetonitrile Adducts of Tris(perfluorophenyl)borane: A Evaluation of Brønsted Acidity and Ligand Lability with Experimental and Computational Methods. <i>Journal of the American Chemical Society</i> , 2000, 122, 10581-10590.	6.6	235
32	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.	1.1	221
33	Solvation Free Energies of Peptides: A 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.	1.2	214
34	Advancing Drug Discovery through Enhanced Free Energy Calculations. <i>Accounts of Chemical Research</i> , 2017, 50, 1625-1632.	7.6	211
35	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, 1937-1942.	3.3	204
36	Solution of the Hartree-Fock equations by a pseudospectral method: Application to diatomic molecules. <i>Journal of Chemical Physics</i> , 1986, 85, 1462-1468.	1.2	193

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37	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, 2990-2998.	2.3	184
38	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.	6.6	176
39	Pseudospectral localized Møller-Plesset methods: Theory and calculation of conformational energies. <i>Journal of Chemical Physics</i> , 1995, 103, 1481-1490.	1.2	168
40	Antibody structure determination using a combination of homology modeling, energy-based refinement, and loop prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1646-1655.	1.5	167
41	Numerical solution of the Poisson-Boltzmann equation using tetrahedral finite-element meshes. <i>Journal of Computational Chemistry</i> , 1997, 18, 1591-1608.	1.5	166
42	Force Field Validation Using Protein Side Chain Prediction. <i>Journal of Physical Chemistry B</i> , 2002, 106, 11673-11680.	1.2	165
43	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.	3.3	143
44	Solution of the Hartree-Fock equations for polyatomic molecules by a pseudospectral method. <i>Journal of Chemical Physics</i> , 1987, 86, 3522-3531.	1.2	142
45	The Redfield Equation in Condensed-Phase Quantum Dynamics. <i>Advances in Chemical Physics</i> , 2007, , 77-134.	0.3	135
46	Constructing ab initio force fields for molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 1998, 108, 4739-4755.	1.2	133
47	Cytochrome P450 _{cam} Enzymatic Catalysis Cycle: A Quantum Mechanics/Molecular Mechanics Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 8501-8508.	6.6	130
48	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.	2.3	125
49	Accurate Binding Free Energy Predictions in Fragment Optimization. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2411-2420.	2.5	119
50	Dioxygen Activation in Methane Monooxygenase: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 2978-2990.	6.6	118
51	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.	1.5	113
52	Accurate Force Field Development for Modeling Conjugated Polymers. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4556-4569.	2.3	109
53	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, 3836-3837.	6.6	108
54	The Effect of Heme Environment on the Hydrogen Abstraction Reaction of Camphor in P450 _{cam} Catalysis: A QM/MM Study. <i>Journal of the American Chemical Society</i> , 2006, 128, 3924-3925.	6.6	105

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55	Improved Methods for Side Chain and Loop Predictions via the Protein Local Optimization Program: a Variable Dielectric Model for Implicitly Improving the Treatment of Polarization Effects. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2108-2119.	2.3	104
56	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 42-54.	2.3	103
57	Large-Scale ab Initio Quantum Chemical Calculations on Biological Systems. <i>Accounts of Chemical Research</i> , 2001, 34, 351-358.	7.6	101
58	A method for exponential propagation of large systems of stiff nonlinear differential equations. <i>Journal of Scientific Computing</i> , 1989, 4, 327-354.	1.1	100
59	Pseudospectral Hartree-Fock theory: Applications and algorithmic improvements. <i>Journal of Chemical Physics</i> , 1990, 93, 3397-3407.	1.2	93
60	Prediction of loop geometries using a generalized born model of solvation effects. , 1999, 35, 173-183.		92
61	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.	1.0	88
62	An automatic three-dimensional finite element mesh generation system for the Poisson-Boltzmann equation. <i>Journal of Computational Chemistry</i> , 1997, 18, 1570-1590.	1.5	86
63	Correcting Systematic Errors in DFT Spin-Splitting Energetics for Transition Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 19-32.	2.3	83
64	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.	2.0	82
65	Pseudospectral localized generalized Møller-Plesset 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.	1.2	76
66	Pseudospectral generalized valence bond calculations: Application to methylene, ethylene, and silylene. <i>Journal of Chemical Physics</i> , 1990, 92, 7488-7497.	1.2	75
67	A three-dimensional reduction of the Ornstein-Zernicke equation for molecular liquids. <i>Journal of Chemical Physics</i> , 1997, 107, 6400-6414.	1.2	75
68	Hydroxylation of Methane by Non-Heme Diiron Enzymes: A Molecular Orbital Analysis of C-H Bond Activation by Reactive Intermediate Q. <i>Journal of the American Chemical Society</i> , 2002, 124, 14608-14615.	6.6	75
69	WScore: A Flexible and Accurate Treatment of Explicit Water Molecules in Ligand-Receptor Docking. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 4364-4384.	2.9	75
70	Reactions of Methane Monooxygenase Intermediate Q with Derivatized Methanes. <i>Journal of the American Chemical Society</i> , 2002, 124, 8770-8771.	6.6	74
71	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.	2.9	73
72	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, , 4494-4496.	2.3	69

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73	Modeling Polarization in Proteins and Protein-Ligand Complexes: Methods and Preliminary Results. <i>Advances in Protein Chemistry</i> , 2005, 72, 79-104.	4.4	68
74	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, 169-180.	2.3	68
75	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.	2.0	68
76	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, 442-459.	2.3	67
77	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.	6.6	63
78	Substrate Hydroxylation in Methane Monooxygenase: Quantitative Modeling via Mixed Quantum Mechanics/Molecular Mechanics Techniques. <i>Journal of the American Chemical Society</i> , 2005, 127, 1025-1037.	6.6	63
79	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.	6.6	62
80	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, 1121-1128.	2.3	62
81	Accelerating drug discovery through tight integration of expert molecular design and predictive scoring. <i>Current Opinion in Structural Biology</i> , 2017, 43, 38-44.	2.6	62
82	On Achieving High Accuracy in Quantum Chemical Calculations of 3 <i>d</i> 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.	2.3	62
83	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.	2.3	61
84	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.	2.3	60
85	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.	1.2	56
86	Realistic Cluster Modeling of Electron Transport and Trapping in Solvated TiO ₂ Nanoparticles. <i>Journal of the American Chemical Society</i> , 2012, 134, 12028-12042.	6.6	55
87	Efficient memory equation algorithm for reduced dynamics in spin-boson models. <i>Journal of Chemical Physics</i> , 1999, 110, 138-146.	1.2	52
88	Photodissociation of acetaldehyde: The CH ₄ +CO channel. <i>Journal of Chemical Physics</i> , 2001, 114, 6128-6133.	1.2	52
89	Protein tertiary structure prediction using a branch and bound algorithm. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 35, 41-57.	1.5	48
90	Quantum mechanical geometry optimization in solution using a finite element continuum electrostatics method. <i>Journal of Chemical Physics</i> , 1996, 105, 5472-5484.	1.2	44

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91	Pseudospectral Hartree-Fock calculations on glycine. <i>Journal of Chemical Physics</i> , 1990, 92, 1163-1173.	1.2	43
92	Reduced dynamics in spin-boson models: A method for both slow and fast bath. <i>Journal of Chemical Physics</i> , 2000, 112, 2095-2105.	1.2	43
93	Factors Influencing the Thermodynamics of Zinc Alkoxide Formation by Alcoholysis of the Terminal Hydroxide Complex, [TpBut,Me]ZnOH: A 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.	6.6	43
94	Density functional localized orbital corrections for transition metals. <i>Journal of Chemical Physics</i> , 2008, 129, 164108.	1.2	42
95	ENERGY TRANSFER BETWEEN THE PRIMARY DONOR BACTERIOCHLOROPHYLL AND CAROTENOIDS IN <i>Rhodospseudomonas sphaeroides</i> . <i>Photochemistry and Photobiology</i> , 1983, 38, 451-455.	1.3	39
96	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.	2.3	37
97	Conformational Dynamics of the Partially Disordered Yeast Transcription Factor GCN4. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5190-5200.	2.3	36
98	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4109-4121.	2.3	35
99	Free Energy Perturbation Calculations of the Thermodynamics of Protein Side-Chain Mutations. <i>Journal of Molecular Biology</i> , 2017, 429, 923-929.	2.0	34
100	QM/MM Simulation on P450 BM3 Enzyme Catalysis Mechanism. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1421-1431.	2.3	33
101	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.	2.3	33
102	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.	1.5	32
103	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.	1.3	31
104	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, 18787-18802.	1.2	30
105	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, 640-648.	2.3	29
106	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, 1425-1441.	1.5	29
107	Natural expansion of vibrational wave functions: RRGm with residue algebra. <i>Journal of Chemical Physics</i> , 1986, 85, 331-336.	1.2	28
108	Covalent O-H Bonds as Electron Traps in Proton-Rich Rutile TiO ₂ Nanoparticles. <i>Nano Letters</i> , 2014, 14, 1785-1789.	4.5	27

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109	Pseudospectral Hartree-Fock gradient calculations. <i>Journal of Chemical Physics</i> , 1991, 94, 8152-8157.	1.2	26
110	Leveraging Data Fusion Strategies in Multireceptor Lead Optimization MM/GBSA End-Point Methods. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3207-3220.	2.3	26
111	Calculation of temperature-dependent multimode resonance Raman line shapes for harmonic potential	1.2	23
112	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.	1.1	23
113	Calculation of optical line shapes for generalized multilevel vibronic systems. <i>Journal of Chemical Physics</i> , 1984, 81, 5899-5905.	1.2	21
114	An Experimental and Computational Analysis of the Formation of the Terminal Nitrido Complex ($\eta^3\text{-Cp}^*\text{2Mo(N)(N3)}$) by Elimination of N_2 from $\text{Cp}^*\text{2Mo(N3)}_2$: 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, 10111-10112.	6.6	21
115	Localized Orbital Corrections for the Barrier Heights in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2996-3009.	2.3	21
116	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.	2.3	21
117	Combined quantum and molecular mechanics (QM/MM). <i>Drug Discovery Today: Technologies</i> , 2004, 1, 253-260.	4.0	20
118	Accurate $\text{p} \rightarrow \text{K} \rightarrow \text{a}$ Prediction in First-Row Hexaaqua Transition Metal Complexes Using the B3LYP-DBLOC Method. <i>Journal of Physical Chemistry B</i> , 2014, 118, 8008-8016.	1.2	20
119	Tertiary structure prediction of mixed α/β proteins via energy minimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 1998, 33, 240-252.	1.5	19
120	Spin-spin model for two-level system/bath problems: A numerical study. <i>Journal of Chemical Physics</i> , 1999, 111, 9918-9923.	1.2	19
121	Application and development of multiconfigurational localized perturbation theory. <i>Journal of Chemical Physics</i> , 2001, 115, 11052-11067.	1.2	19
122	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.	1.2	19
123	Parallel pseudospectral electronic structure: I. Hartree-Fock calculations. <i>Journal of Computational Chemistry</i> , 1998, 19, 1017-1029.	1.5	18
124	Computational methods for high resolution prediction and refinement of protein structures. <i>Current Opinion in Structural Biology</i> , 2013, 23, 177-184.	2.6	18
125	Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2845-2862.	2.3	18
126	Classical and Quantum Models of Activationless Reaction Dynamics. <i>Zeitschrift Fur Elektrotechnik Und Elektrochemie</i> , 1991, 95, 253-258.	0.9	17

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127	Parallel pseudospectral electronic structure: II. Localized Møller-Plesset calculations. <i>Journal of Computational Chemistry</i> , 1998, 19, 1030-1038.	1.5	17
128	Protein structure prediction using a combination of sequence-based alignment, constrained energy minimization, and structural alignment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 45, 133-139.	1.5	17
129	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.	1.2	14
130	Modeling the value of predictive affinity scoring in preclinical drug discovery. <i>Current Opinion in Structural Biology</i> , 2018, 52, 103-110.	2.6	14
131	Computational Modeling of the Electronic Structure of Oligothiophenes with Various Side Chains. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2553-2561.	1.5	11
132	A Thermal Expansion Model for the Special Pair of the Bacterial Reaction Center. <i>Israel Journal of Chemistry</i> , 1988, 28, 67-72.	1.0	10
133	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.	1.1	10
134	Pseudospectral implementations of long-range corrected density functional theory. <i>Journal of Computational Chemistry</i> , 2021, 42, 2089-2102.	1.5	10
135	A hierarchical algorithm for polymer simulations. <i>Journal of Chemical Physics</i> , 1992, 97, 9355-9365.	1.2	9
136	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.	1.0	9
137	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3647-3663.	2.3	9
138	Prediction of Long Loops with Embedded Secondary Structure Using the Protein Local Optimization Program. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1846-1864.	2.3	9
139	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.	6.6	9
140	Successful application of the DBLOC method to the hydroxylation of camphor by cytochrome p450. <i>Protein Science</i> , 2016, 25, 277-285.	3.1	8
141	Localized orbital corrections for density functional calculations on transition metal containing systems. <i>Coordination Chemistry Reviews</i> , 2017, 344, 205-213.	9.5	8
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