Richard A Friesner

List of Publications by Year
in descending order

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156 papers	40,401 citations	13099 68 h-index	6996 154 g-index
158 all docs	158 docs citations	158 times ranked	32991 citing authors

#	Article	IF	Citations
1	Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. Journal of Chemical Theory and Computation, 2022, 18, 2845-2862.	5.3	18
2	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 3447-3459.	5.3	7
3	In silico prediction of annihilators for tripletâ€“triplet annihilation upconversion via auxiliary-field quantum Monte Carlo. Chemical Science, 2021, 12, 1068-1079.	7.4	7
4	Reliable and Accurate Solution to the Induced Fit Docking Problem for Proteinâ€“Ligand Binding. Journal of Chemical Theory and Computation, 2021, 17, 2630-2639.	5.3	60
5	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. Journal of Chemical Theory and Computation, 2021, 17, 4291-4300.	5.3	582
6	Highly efficient implementation of the analytical gradients of pseudospectral time-dependent density functional theory. Journal of Chemical Physics, 2021, 155, 024115.	3.0	2
7	Pseudospectral implementations of <scp>longâ€range</scp> corrected density functional theory. Journal of Computational Chemistry, 2021, 42, 2089-2102.	3.3	10
8	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. Cell Host and Microbe, 2020, 28, 867-879.e5.	11.0	316
9	Multiple Stable Isopreneâ€“Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. Journal of the American Chemical Society, 2020, 142, 10806-10813.	13.7	9
10	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. Journal of Chemical Theory and Computation, 2020, 16, 2109-2123.	5.3	2
11	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 3041-3054.	5.3	21
12	Singletâ€“Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 4924-4932.	5.3	37
13	On Achieving High Accuracy in Quantum Chemical Calculations of 3d Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. Journal of Chemical Theory and Computation, 2019, 15, 2346-2358.	5.3	62
14	Relative Binding Affinity Prediction of Charge-Changing Sequence Mutations with FEP in Proteinâ€“Protein Interfaces. Journal of Molecular Biology, 2019, 431, 1481-1493.	4.2	68
15	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1863-1874.	5.3	698
16	Modeling the value of predictive affinity scoring in preclinical drug discovery. Current Opinion in Structural Biology, 2018, 52, 103-110.	5.7	14
17	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 4109-4121.	5.3	35
18	Localized orbital corrections for density functional calculations on transition metal containing systems. Coordination Chemistry Reviews, 2017, 344, 205-213.	18.8	8

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19	Free Energy Perturbation Calculations of the Thermodynamics of Protein Side-Chain Mutations. Journal of Molecular Biology, 2017, 429, 923-929.	4.2	34
20	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2017, 13, 2667-2680.	5.3	33
21	Free Energy Perturbation Calculation of Relative Binding Free Energy between Broadly Neutralizing Antibodies and the gp120 Glycoprotein of HIV-1. Journal of Molecular Biology, 2017, 429, 930-947.	4.2	82
22	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. Journal of Chemical Theory and Computation, 2017, 13, 5780-5797.	5.3	125
23	Advancing Drug Discovery through Enhanced Free Energy Calculations. Accounts of Chemical Research, 2017, 50, 1625-1632.	15.6	211
24	Accelerating drug discovery through tight integration of expert molecular design and predictive scoring. Current Opinion in Structural Biology, 2017, 43, 38-44.	5.7	62
25	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. Journal of Chemical Theory and Computation, 2017, 13, 42-54.	5.3	103
26	A Critical Review of Validation, Blind Testing, and Real- World Use of Alchemical Protein-Ligand Binding Free Energy Calculations. Current Topics in Medicinal Chemistry, 2017, 17, 2577-2585.	2.1	88
27	Efficient simulation of large materials clusters using the jaguar quantum chemistry program: Parallelization and wavefunction initialization. International Journal of Quantum Chemistry, 2016, 116, 357-368.	2.0	5
28	Successful application of the <scp>DBLOC</scp> method to the hydroxylation of camphor by cytochrome p450. Protein Science, 2016, 25, 277-285.	7.6	8
29	WScore: A Flexible and Accurate Treatment of Explicit Water Molecules in Ligandâ€“Receptor Docking. Journal of Medicinal Chemistry, 2016, 59, 4364-4384.	6.4	75
30	Prediction of Proteinâ€“Ligand Binding Poses via a Combination of Induced Fit Docking and Metadynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 2990-2998.	5.3	184
31	Highly efficient implementation of pseudospectral timeâ€dependent densityâ€functional theory for the calculation of excitation energies of large molecules. Journal of Computational Chemistry, 2016, 37, 1425-1441.	3.3	29
32	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
33	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. Journal of Chemical Theory and Computation, 2016, 12, 1121-1128.	5.3	62
34	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. Journal of Chemical Theory and Computation, 2016, 12, 281-296.	5.3	2,349
35	Conformational Preferences Underlying Reduced Activity of a Thermophilic Ribonuclease H. Journal of Molecular Biology, 2015, 427, 853-866.	4.2	4
36	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. Journal of the American Chemical Society, 2015, 137, 2695-2703.	13.7	931

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37	Accurate Binding Free Energy Predictions in Fragment Optimization. Journal of Chemical Information and Modeling, 2015, 55, 2411-2420.	5.4	119
38	A first-principles polarized Raman method for determining whether a uniform region of a sample is crystalline or isotropic. Journal of Chemical Physics, 2014, 141, 224702.	3.0	1
39	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. Journal of Chemical Theory and Computation, 2014, 10, 5696-5705.	5.3	61
40	Antibody structure determination using a combination of homology modeling, energyâ€based refinement, and loop prediction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1646-1655.	2.6	167
41	Covalent Oâ€“H Bonds as Electron Traps in Proton-Rich Rutile TiO₂ Nanoparticles. Nano Letters, 2014, 14, 1785-1789.	9.1	27
42	Leveraging Data Fusion Strategies in Multireceptor Lead Optimization MM/GBSA End-Point Methods. Journal of Chemical Theory and Computation, 2014, 10, 3207-3220.	5.3	26
43	Accurate pK_a Prediction in First-Row Hexaaqua Transition Metal Complexes Using the B3LYP-DBLOC Method. Journal of Physical Chemistry B, 2014, 118, 8008-8016.	2.6	20
44	Conformational Dynamics of the Partially Disordered Yeast Transcription Factor GCN4. Journal of Chemical Theory and Computation, 2013, 9, 5190-5200.	5.3	36
45	Jaguar: A highâ€performance quantum chemistry software program with strengths in life and materials sciences. International Journal of Quantum Chemistry, 2013, 113, 2110-2142.	2.0	1,426
46	Computational methods for high resolution prediction and refinement of protein structures. Current Opinion in Structural Biology, 2013, 23, 177-184.	5.7	18
47	Prediction of Long Loops with Embedded Secondary Structure Using the Protein Local Optimization Program. Journal of Chemical Theory and Computation, 2013, 9, 1846-1864.	5.3	9
48	Accurate Force Field Development for Modeling Conjugated Polymers. Journal of Chemical Theory and Computation, 2012, 8, 4556-4569.	5.3	109
49	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. Journal of Chemical Theory and Computation, 2012, 8, 2553-2558.	5.3	239
50	On achieving high accuracy and reliability in the calculation of relative proteinâ€“ligand binding affinities. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 1937-1942.	7.1	204
51	A B3LYP-DBLOC empirical correction scheme for ligand removal enthalpies of transition metal complexes: parameterization against experimental and CCSD(T)-F12 heats of formation. Physical Chemistry Chemical Physics, 2012, 14, 7724.	2.8	31
52	Development of Accurate DFT Methods for Computing Redox Potentials of Transition Metal Complexes: Results for Model Complexes and Application to Cytochrome P450. Journal of Chemical Theory and Computation, 2012, 8, 442-459.	5.3	67
53	Realistic Cluster Modeling of Electron Transport and Trapping in Solvated TiO2Nanoparticles. Journal of the American Chemical Society, 2012, 134, 12028-12042.	13.7	55
54	Correcting Systematic Errors in DFT Spin-Splitting Energetics for Transition Metal Complexes. Journal of Chemical Theory and Computation, 2011, 7, 19-32.	5.3	83

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55	Replica Exchange with Solute Scaling: A More Efficient Version of Replica Exchange with Solute Tempering (REST2). Journal of Physical Chemistry B, 2011, 115, 9431-9438.	2.6	595
56	The VSGB 2.0 model: A next generation energy model for high resolution protein structure modeling. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2794-2812.	2.6	773
57	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. Journal of Chemical Theory and Computation, 2010, 6, 3647-3663.	5.3	9
58	Computational Modeling of the Electronic Structure of Oligothiophenes with Various Side Chains. Journal of Physical Chemistry C, 2009, 113, 2553-2561.	3.1	11
59	Quantum Chemical Investigation of Cluster Models for TiO₂ Nanoparticles with Water-Derived Ligand Passivation: Studies of Excess Electron States and Implications for Charge Transport in the Gratzel Cell. Journal of Physical Chemistry C, 2009, 113, 19806-19811.	3.1	32
60	QM/MM Simulation on P450 BM3 Enzyme Catalysis Mechanism. Journal of Chemical Theory and Computation, 2009, 5, 1421-1431.	5.3	33
61	Localized Orbital Corrections for the Barrier Heights in Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 2996-3009.	5.3	21
62	Role of the Active-Site Solvent in the Thermodynamics of Factor Xa Ligand Binding. Journal of the American Chemical Society, 2008, 130, 2817-2831.	13.7	594
63	Density functional localized orbital corrections for transition metals. Journal of Chemical Physics, 2008, 129, 164108.	3.0	42
64	Localized orbital corrections applied to thermochemical errors in density functional theory: The role of basis set and application to molecular reactions. Journal of Chemical Physics, 2008, 129, 214105.	3.0	19
65	Structural and mechanistic studies of AlkB. FASEB Journal, 2008, 22, 526.3.	0.5	0
66	Motifs for molecular recognition exploiting hydrophobic enclosure in proteinâ€“ligand binding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 808-813.	7.1	633
67	Improved Methods for Side Chain and Loop Predictions via the Protein Local Optimization Program:â€‰Variable Dielectric Model for Implicitly Improving the Treatment of Polarization Effects. Journal of Chemical Theory and Computation, 2007, 3, 2108-2119.	5.3	104
68	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Proteinâ^'Ligand Complexes. Journal of Chemical Theory and Computation, 2007, 3, 640-648.	5.3	29
69	The Redfield Equation in Condensed-Phase Quantum Dynamics. Advances in Chemical Physics, 2007, , 77-134.	0.3	135
70	The Effect of Heme Environment on the Hydrogen Abstraction Reaction of Camphor in P450camCatalysis:Â A QM/MM Study. Journal of the American Chemical Society, 2006, 128, 3924-3925.	13.7	105
71	A localized orbital analysis of the thermochemical errors in hybrid density functional theory: Achieving chemical accuracy via a simple empirical correction scheme. Journal of Chemical Physics, 2006, 125, 124107.	3.0	56
72	Novel Procedure for Modeling Ligand/Receptor Induced Fit Effects. Journal of Medicinal Chemistry, 2006, 49, 534-553.	6.4	1,671

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73	Localized Orbital Corrections for the Calculation of Ionization Potentials and Electron Affinities in Density Functional Theory. Journal of Physical Chemistry B, 2006, 110, 18787-18802.	2.6	30
74	Extra Precision Glide:Â Docking and Scoring Incorporating a Model of Hydrophobic Enclosure for Proteinâ˜Ligand Complexes. Journal of Medicinal Chemistry, 2006, 49, 6177-6196.	6.4	5,196
75	PHASE: a new engine for pharmacophore perception, 3D QSAR model development, and 3D database screening: 1. Methodology and preliminary results. Journal of Computer-Aided Molecular Design, 2006, 20, 647-671.	2.9	963
76	Modeling Polarization in Proteins and Proteinâ€“ligand Complexes: Methods and Preliminary Results. Advances in Protein Chemistry, 2005, 72, 79-104.	4.4	68
77	Ab initio quantum chemistry: Methodology and applications. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6648-6653.	7.1	279
78	Efficient Simulation Method for Polarizable Protein Force Fields:â€‰ Application to the Simulation of BPTI in Liquid Water. Journal of Chemical Theory and Computation, 2005, 1, 169-180.	5.3	68
79	Substrate Hydroxylation in Methane Monooxygenase:Â Quantitative Modeling via Mixed Quantum Mechanics/Molecular Mechanics Techniques. Journal of the American Chemical Society, 2005, 127, 1025-1037.	13.7	63
80	AB INITIO QUANTUM CHEMICAL AND MIXED QUANTUM MECHANICS/MOLECULAR MECHANICS (QM/MM) METHODS FOR STUDYING ENZYMATIC CATALYSIS. Annual Review of Physical Chemistry, 2005, 56, 389-427.	10.8	493
81	Glide:Â A New Approach for Rapid, Accurate Docking and Scoring. 1. Method and Assessment of Docking Accuracy. Journal of Medicinal Chemistry, 2004, 47, 1739-1749.	6.4	7,428
82	A hierarchical approach to all-atom protein loop prediction. Proteins: Structure, Function and Bioinformatics, 2004, 55, 351-367.	2.6	1,874
83	Dioxygen Activation in Methane Monooxygenase:Â A Theoretical Study. Journal of the American Chemical Society, 2004, 126, 2978-2990.	13.7	118
84	Combined quantum and molecular mechanics (QM/MM). Drug Discovery Today: Technologies, 2004, 1, 253-260.	4.0	20
85	Development of an Accurate and Robust Polarizable Molecular Mechanics Force Field from ab Initio Quantum Chemistry. Journal of Physical Chemistry A, 2004, 108, 621-627.	2.5	221
86	Cytochrome P450CAM Enzymatic Catalysis Cycle:Â A Quantum Mechanics/Molecular Mechanics Study. Journal of the American Chemical Society, 2004, 126, 8501-8508.	13.7	130
87	Electronic Structure and Luminescence of 1.1- and 1.4-nm Silicon Nanocrystals:Â Oxide Shell versus Hydrogen Passivation. Nano Letters, 2003, 3, 163-167.	9.1	292
88	Mechanistic Studies on the Hydroxylation of Methane by Methane Monooxygenase. Chemical Reviews, 2003, 103, 2385-2420.	47.7	479
89	Peripheral heme substituents control the hydrogen-atom abstraction chemistry in cytochromes P450. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 6998-7002.	7.1	143
90	Reactions of Methane Monooxygenase Intermediate Q with Derivatized Methanes. Journal of the American Chemical Society, 2002, 124, 8770-8771.	13.7	74

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91	Hydroxylation of Methane by Non-Heme Diiron Enzymes:Â Molecular Orbital Analysis of Câ”H Bond Activation by Reactive Intermediate Q. Journal of the American Chemical Society, 2002, 124, 14608-14615.	13.7	75
92	Computational Modeling for Scanning Tunneling Microscopy of Physisorbed Molecules via Ab Initio Quantum Chemistry. Journal of Physical Chemistry A, 2002, 106, 1802-1814.	2.5	10
93	Force Field Validation Using Protein Side Chain Prediction. Journal of Physical Chemistry B, 2002, 106, 11673-11680.	2.6	165
94	Computing Redox Potentials in Solution:Â Density Functional Theory as A Tool for Rational Design of Redox Agents. Journal of Physical Chemistry A, 2002, 106, 7407-7412.	2.5	374
95	On the Role of the Crystal Environment in Determining Protein Side-chain Conformations. Journal of Molecular Biology, 2002, 320, 597-608.	4.2	1,002
96	Ab Initio Protein Structure Prediction Using a Size-dependent Tertiary Folding Potential. Advances in Chemical Physics, 2002, , 223-263.	0.3	4
97	Theoretical studies of diiron(II) complexes that model features of the dioxygen-activating centers in non-heme diiron enzymes. Israel Journal of Chemistry, 2001, 41, 173-186.	2.3	9
98	Large-Scale ab Initio Quantum Chemical Calculations on Biological Systems. Accounts of Chemical Research, 2001, 34, 351-358.	15.6	101
99	Application and development of multiconfigurational localized perturbation theory. Journal of Chemical Physics, 2001, 115, 11052-11067.	3.0	19
100	Activation of the Câ”H Bond of Methane by Intermediate Q of Methane Monooxygenase:Â A Theoretical Study. Journal of the American Chemical Society, 2001, 123, 3836-3837.	13.7	108
101	An Experimental and Computational Analysis of the Formation of the Terminal Nitrido Complex (Î·3-Cp*)2Mo(N)(N3) by Elimination of N2from Cp*2Mo(N3)2:Â The Barrier to Elimination Is Strongly Influenced by theexoversusendoConfiguration of the Azide Ligand. Journal of the American Chemical Society, 2001, 123, 10111-10112.	13.7	21
102	Protein structure prediction using a combination of sequence-based alignment, constrained energy minimization, and structural alignment. Proteins: Structure, Function and Bioinformatics, 2001, 45, 133-139.	2.6	17
103	Solvent models for protein-ligand binding: Comparison of implicit solvent poisson and surface generalized born models with explicit solvent simulations. Journal of Computational Chemistry, 2001, 22, 591-607.	3.3	113
104	Photodissociation of acetaldehyde: The CH4+CO channel. Journal of Chemical Physics, 2001, 114, 6128-6133.	3.0	52
105	Combined fluctuating charge and polarizable dipole models: Application to a five-site water potential function. Journal of Chemical Physics, 2001, 115, 2237-2251.	3.0	267
106	Reduced dynamics in spin-boson models: A method for both slow and fast bath. Journal of Chemical Physics, 2000, 112, 2095-2105.	3.0	43
107	Aqua, Alcohol, and Acetonitrile Adducts of Tris(perfluorophenyl)borane:Â Evaluation of BrÃ¸nsted Acidity and Ligand Lability with Experimental and Computational Methods. Journal of the American Chemical Society, 2000, 122, 10581-10590.	13.7	235
108	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]ZnSPhâ€Šâ€. Dalton Transactions RSC, 2000, , 4494-4496.	2.3	69

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109	Factors Influencing the Thermodynamics of Zinc Alkoxide Formation by Alcoholysis of the Terminal Hydroxide Complex, [TpBut,Me]ZnOH:Â An Experimental and Theoretical Study Relevant to the Mechanism of Action of Liver Alcohol Dehydrogenase. Journal of the American Chemical Society, 2000, 122, 12651-12658.	13.7	43
110	Large Scale ab Initio Quantum Chemical Calculation of the Intermediates in the Soluble Methane Monooxygenase Catalytic Cycle. Journal of the American Chemical Society, 2000, 122, 2828-2839.	13.7	176
111	Efficient memory equation algorithm for reduced dynamics in spin-boson models. Journal of Chemical Physics, 1999, 110, 138-146.	3.0	52
112	Mixedab initio QM/MM modeling using frozen orbitals and tests with alanine dipeptide and tetrapeptide. Journal of Computational Chemistry, 1999, 20, 1468-1494.	3.3	268
113	Protein tertiary structure prediction using a branch and bound algorithm. Proteins: Structure, Function and Bioinformatics, 1999, 35, 41-57.	2.6	48
114	Prediction of loop geometries using a generalized born model of solvation effects. , 1999, 35, 173-183.		92
115	Spinâ€“spin model for two-level system/bath problems: A numerical study. Journal of Chemical Physics, 1999, 111, 9918-9923.	3.0	19
116	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. Journal of Chemical Physics, 1999, 110, 741-754.	3.0	251
117	Calculation of atomization energies by a multiconfigurational localized perturbation theoryâ€”Application for closed shell cases. Journal of Chemical Physics, 1999, 110, 1921-1930.	3.0	14
118	Mechanistic and Theoretical Analysis of the Oxidative Addition of H2to Six-Coordinate Molybdenum and Tungsten Complexes M(PMe3)4X2(M = Mo, W; X = F, Cl, Br, I):Â An Inverse Equilibrium Isotope Effect and an Unprecedented Halide Dependence. Journal of the American Chemical Society, 1999, 121, 11402-11417.	13.7	62
119	1,3-Dipolar Addition of Phenylazide to the Carbonâ^'Carbon Double Bond:Â An ab Initio Study. Journal of Physical Chemistry A, 1999, 103, 1276-1282.	2.5	23
120	Correlated ab Initio Electronic Structure Calculations for Large Molecules. Journal of Physical Chemistry A, 1999, 103, 1913-1928.	2.5	274
121	Prediction of loop geometries using a generalized born model of solvation effects. Proteins: Structure, Function and Bioinformatics, 1999, 35, 173-183.	2.6	3
122	Parallel pseudospectral electronic structure: I. Hartree-Fock calculations. Journal of Computational Chemistry, 1998, 19, 1017-1029.	3.3	18
123	Parallel pseudospectral electronic structure: II. Localized Mï¿½ller-Plesset calculations. Journal of Computational Chemistry, 1998, 19, 1030-1038.	3.3	17
124	Tertiary structure prediction of mixed Î±/Î² proteins via energy minimization. Proteins: Structure, Function and Bioinformatics, 1998, 33, 240-252.	2.6	19
125	Constructing ab initio force fields for molecular dynamics simulations. Journal of Chemical Physics, 1998, 108, 4739-4755.	3.0	133
126	A three-dimensional reduction of the Ornsteinâ€“Zernicke equation for molecular liquids. Journal of Chemical Physics, 1997, 107, 6400-6414.	3.0	75

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127	Pseudospectral localized generalized Mo/llerâ€“Plesset methods with a generalized valence bond reference wave function: Theory and calculation of conformational energies. Journal of Chemical Physics, 1997, 106, 5073-5084.	3.0	76
128	Solvation Free Energies of Peptides:â€‰ Comparison of Approximate Continuum Solvation Models with Accurate Solution of the Poissonâ^'Boltzmann Equation. Journal of Physical Chemistry B, 1997, 101, 1190-1197.	2.6	214
129	Hydrogen Bonding between Amino Acid Backbone and Side Chain Analogues:â€‰ A High-Level ab Initio Study. Journal of the American Chemical Society, 1997, 119, 12952-12961.	13.7	63
130	Accurate ab Initio Quantum Chemical Determination of the Relative Energetics of Peptide Conformations and Assessment of Empirical Force Fields. Journal of the American Chemical Society, 1997, 119, 5908-5920.	13.7	339
131	An automatic three-dimensional finite element mesh generation system for the Poisson-Boltzmann equation. Journal of Computational Chemistry, 1997, 18, 1570-1590.	3.3	86
132	Numerical solution of the Poisson-Boltzmann equation using tetrahedral finite-element meshes. Journal of Computational Chemistry, 1997, 18, 1591-1608.	3.3	166
133	Extension of the PS-GVB electronic structure code to transition metal complexes. Journal of Computational Chemistry, 1997, 18, 1863-1874.	3.3	7
134	New Model for Calculation of Solvation Free Energies:Â Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. The Journal of Physical Chemistry, 1996, 100, 11775-11788.	2.9	936
135	Parallel implementation of a protein structure refinement algorithm. Journal of Computational Chemistry, 1996, 17, 1217-1228.	3.3	6
136	Quantum mechanical geometry optimization in solution using a finite element continuum electrostatics method. Journal of Chemical Physics, 1996, 105, 5472-5484.	3.0	44
137	Pseudospectral localized Mo/llerâ€“Plesset methods: Theory and calculation of conformational energies. Journal of Chemical Physics, 1995, 103, 1481-1490.	3.0	168
138	Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. Journal of the American Chemical Society, 1994, 116, 11875-11882.	13.7	1,026
139	A hierarchical algorithm for polymer simulations. Journal of Chemical Physics, 1992, 97, 9355-9365.	3.0	9
140	Classical and Quantum Models of Activationless Reaction Dynamics. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1991, 95, 253-258.	0.9	17
141	Pseudospectral Hartreeâ€“Fock gradient calculations. Journal of Chemical Physics, 1991, 94, 8152-8157.	3.0	26
142	Pseudospectral Hartreeâ€“Fock calculations on glycine. Journal of Chemical Physics, 1990, 92, 1163-1173.	3.0	43
143	Pseudospectral Hartreeâ€“Fock theory: Applications and algorithmic improvements. Journal of Chemical Physics, 1990, 93, 3397-3407.	3.0	93
144	Pseudospectral generalized valenceâ€bond calculations: Application to methylene, ethylene, and silylene. Journal of Chemical Physics, 1990, 92, 7488-7497.	3.0	75

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145	A method for exponential propagation of large systems of stiff nonlinear differential equations. Journal of Scientific Computing, 1989, 4, 327-354.	2.3	100
146	An automatic grid generation scheme for pseudospectral self-consistent field calculations on polyatomic molecules. The Journal of Physical Chemistry, 1988, 92, 3091-3096.	2.9	73
147	A Thermal Expansion Model for the Special Pair of the Bacterial Reaction Center. Israel Journal of Chemistry, 1988, 28, 67-72.	2.3	10
148	Solution of the Hartreeâ€“Fock equations for polyatomic molecules by a pseudospectral method. Journal of Chemical Physics, 1987, 86, 3522-3531.	3.0	142
149	Natural expansion of vibrational wave functions: RRGM with residue algebra. Journal of Chemical Physics, 1986, 85, 331-336.	3.0	28
150	Solution of the Hartreeâ€“Fock equations by a pseudospectral method: Application to diatomic molecules. Journal of Chemical Physics, 1986, 85, 1462-1468.	3.0	193
151	An accurate and efficient decoupling approximation for temperatureâ€dependent multimode resonance Raman spectra. Journal of Chemical Physics, 1986, 85, 2353-2364.	3.0	3
152	Solution of self-consistent field electronic structure equations by a pseudospectral method. Chemical Physics Letters, 1985, 116, 39-43.	2.6	258
153	Calculation of temperatureâ€dependent multimode resonance Raman line shapes for harmonic potential	3.0	23
154	Calculation of optical line shapes for generalized multilevel vibronic systems. Journal of Chemical Physics, 1984, 81, 5899-5905.	3.0	21
155	ENERGY TRANSFER BETWEEN THE PRIMARY DONOR BACTERIOCHLOROPHYLL AND CAROTENOIDS IN Rhodopseudomonas sphaeroides. Photochemistry and Photobiology, 1983, 38, 451-455.	2.5	39
156	Greenâ€™s functions and optical line shapes of a general twoâ€level system in the strong electronic coupling limit. Journal of Chemical Physics, 1982, 76, 2129-2135.	3.0	5