Richard A Friesner

List of Publications by Year in Descending Order

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	Reliable and Accurate Solution to the Induced Fit Docking Problem for Protein-Ligand Binding. *Journal of Chemical Theory and Computation*, **2021**, 17, 2630-2639	6.4	13
151	OPLS4: Improving Force Field Accuracy on Challenging Regimes of Chemical Space. *Journal of Chemical Theory and Computation*, **2021**, 17, 4291-4300	6.4	92
150	Highly efficient implementation of the analytical gradients of pseudospectral time-dependent density functional theory. *Journal of Chemical Physics*, **2021**, 155, 024115	3.9	
149	Pseudospectral implementations of long-range corrected density functional theory. *Journal of Computational Chemistry*, **2021**, 42, 2089-2102	3.5	0
148	Multiple Stable Isoprene-Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. *Journal of the American Chemical Society*, **2020**, 142, 10806-10813	16.4	7
147	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	6.4	1
146	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	23.4	168
145	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2020**, 16, 3041-3054	6.4	10
144	prediction of annihilators for triplet-triplet annihilation upconversion auxiliary-field quantum Monte Carlo. *Chemical Science*, **2020**, 12, 1068-1079	9.4	1
143	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. *Journal of Chemical Theory and Computation*, **2019**, 15, 2346-2358	6.4	42
142	Singlet-Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2019**, 15, 4924-4932	6.4	22
141	Relative Binding Affinity Prediction of Charge-Changing Sequence Mutations with FEP in Protein-Protein Interfaces. *Journal of Molecular Biology*, **2019**, 431, 1481-1493	6.5	29
140	OPLS3e: Extending Force Field Coverage for Drug-Like Small Molecules. *Journal of Chemical Theory and Computation*, **2019**, 15, 1863-1874	6.4	337
139	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. *Journal of Chemical Theory and Computation*, **2018**, 14, 4109-4121	6.4	25
138	Modeling the value of predictive affinity scoring in preclinical drug discovery. *Current Opinion in Structural Biology*, **2018**, 52, 103-110	8.1	9
137	Localized orbital corrections for density functional calculations on transition metal containing systems. *Coordination Chemistry Reviews*, **2017**, 344, 205-213	23.2	3
136	Free Energy Perturbation Calculations of the Thermodynamics of Protein Side-Chain Mutations. *Journal of Molecular Biology*, **2017**, 429, 923-929	6.5	20

135	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2017**, 13, 2667-2680	6.4	21
134	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	6.5	47
133	Automated Transition State Search and Its Application to Diverse Types of Organic Reactions. *Journal of Chemical Theory and Computation*, **2017**, 13, 5780-5797	6.4	85
132	Advancing Drug Discovery through Enhanced Free Energy Calculations. *Accounts of Chemical Research*, **2017**, 50, 1625-1632	24.3	126
131	Accelerating drug discovery through tight integration of expert molecular design and predictive scoring. *Current Opinion in Structural Biology*, **2017**, 43, 38-44	8.1	47
130	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. *Journal of Chemical Theory and Computation*, **2017**, 13, 42-54	6.4	68
129	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	3	60
128	Highly efficient implementation of pseudospectral time-dependent density-functional theory for the calculation of excitation energies of large molecules. *Journal of Computational Chemistry*, **2016**, 37, 1425-41	3.5	17
127	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
126	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, 1121-8	6.4	48
125	OPLS3: A Force Field Providing Broad Coverage of Drug-like Small Molecules and Proteins. *Journal of Chemical Theory and Computation*, **2016**, 12, 281-96	6.4	1555
124	Successful application of the DBLOC method to the hydroxylation of camphor by cytochrome p450. *Protein Science*, **2016**, 25, 277-85	6.3	7
123	WScore: A Flexible and Accurate Treatment of Explicit Water Molecules in Ligand-Receptor Docking. *Journal of Medicinal Chemistry*, **2016**, 59, 4364-84	8.3	53
122	Prediction of Protein-Ligand Binding Poses via a Combination of Induced Fit Docking and Metadynamics Simulations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2990-8	6.4	120
121	Accurate Binding Free Energy Predictions in Fragment Optimization. *Journal of Chemical Information and Modeling*, **2015**, 55, 2411-20	6.1	83
120	Conformational preferences underlying reduced activity of a thermophilic ribonuclease H. *Journal of Molecular Biology*, **2015**, 427, 853-866	6.5	3
119	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, 2695-703	16.4	633
118	Antibody structure determination using a combination of homology modeling, energy-based refinement, and loop prediction. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1646-55	4.2	110

117	Covalent O-H bonds as electron traps in proton-rich rutile TiO2 nanoparticles. *Nano Letters*, **2014**, 14, 1785-9	11.5	25
116	Leveraging Data Fusion Strategies in Multireceptor Lead Optimization MM/GBSA End-Point Methods. *Journal of Chemical Theory and Computation*, **2014**, 10, 3207-20	6.4	16
115	Accurate pKa prediction in first-row hexaaqua transition metal complexes using the B3LYP-DBLOC method. *Journal of Physical Chemistry B*, **2014**, 118, 8008-16	3.4	19
114	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	3.9	1
113	Role of Desolvation in Thermodynamics and Kinetics of Ligand Binding to a Kinase. *Journal of Chemical Theory and Computation*, **2014**, 10, 5696-5705	6.4	44
112	Conformational Dynamics of the Partially Disordered Yeast Transcription Factor GCN4. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	29
111	Computational methods for high resolution prediction and refinement of protein structures. *Current Opinion in Structural Biology*, **2013**, 23, 177-84	8.1	17
110	Prediction of Long Loops with Embedded Secondary Structure using the Protein Local Optimization Program. *Journal of Chemical Theory and Computation*, **2013**, 9, 1846-4864	6.4	7
109	Accurate Force Field Development for Modeling Conjugated Polymers. *Journal of Chemical Theory and Computation*, **2012**, 8, 4556-69	6.4	85
108	Improving the Prediction of Absolute Solvation Free Energies Using the Next Generation OPLS Force Field. *Journal of Chemical Theory and Computation*, **2012**, 8, 2553-8	6.4	159
107	On achieving high accuracy and reliability in the calculation of relative protein-ligand binding affinities. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 1937-42	11.5	151
106	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, 7724-38	3.6	30
105	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, 442-59	6.4	58
104	Realistic cluster modeling of electron transport and trapping in solvated TiO2 nanoparticles. *Journal of the American Chemical Society*, **2012**, 134, 12028-42	16.4	48
103	Correcting Systematic Errors in DFT Spin-Splitting Energetics for Transition Metal Complexes. *Journal of Chemical Theory and Computation*, **2011**, 7, 19-32	6.4	73
102	Replica exchange with solute scaling: a more efficient version of replica exchange with solute tempering (REST2). *Journal of Physical Chemistry B*, **2011**, 115, 9431-8	3.4	387
101	The VSGB 2.0 model: a next generation energy model for high resolution protein structure modeling. *Proteins: Structure, Function and Bioinformatics*, **2011**, 79, 2794-812	4.2	483
100	Continuous Localized Orbital Corrections to Density Functional Theory: B3LYP-CLOC. *Journal of Chemical Theory and Computation*, **2010**, 6, 3647-3663	6.4	8

99	Computational Modeling of the Electronic Structure of Oligothiophenes with Various Side Chains. *Journal of Physical Chemistry C*, **2009**, 113, 2553-2561	3.8	10
98	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	3.8	30
97	QM/MM Simulation on P450 BM3 Enzyme Catalysis Mechanism. *Journal of Chemical Theory and Computation*, **2009**, 5, 1421-1431	6.4	28
96	Localized orbital corrections for the calculation of barrier heights in density functional theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 2996-3009	6.4	19
95	Role of the active-site solvent in the thermodynamics of factor Xa ligand binding. *Journal of the American Chemical Society*, **2008**, 130, 2817-31	16.4	500
94	Density functional localized orbital corrections for transition metals. *Journal of Chemical Physics*, **2008**, 129, 164108	3.9	37
93	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	3.9	18
92	Structural and mechanistic studies of AlkB. *FASEB Journal*, **2008**, 22, 526.3	0.9	
91	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. *Journal of Chemical Theory and Computation*, **2007**, 3, 2108-19	6.4	89
90	Multiscale Optimization of a Truncated Newton Minimization Algorithm and Application to Proteins and Protein-Ligand Complexes. *Journal of Chemical Theory and Computation*, **2007**, 3, 640-8	6.4	27
89	The Redfield Equation in Condensed-Phase Quantum Dynamics. *Advances in Chemical Physics*, **2007**, 77-134		124
88	Motifs for molecular recognition exploiting hydrophobic enclosure in protein-ligand binding. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 808-13	11.5	536
87	The effect of heme environment on the hydrogen abstraction reaction of camphor in P450cam catalysis: a QM/MM study. *Journal of the American Chemical Society*, **2006**, 128, 3924-5	16.4	98
86	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	3.9	52
85	Novel procedure for modeling ligand/receptor induced fit effects. *Journal of Medicinal Chemistry*, **2006**, 49, 534-53	8.3	1320
84	Localized orbital corrections for the calculation of ionization potentials and electron affinities in density functional theory. *Journal of Physical Chemistry B*, **2006**, 110, 18787-802	3.4	29
83	Extra precision glide: docking and scoring incorporating a model of hydrophobic enclosure for protein-ligand complexes. *Journal of Medicinal Chemistry*, **2006**, 49, 6177-96	8.3	3757
82	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, 647-71	4.2	764

81	Efficient Simulation Method for Polarizable Protein Force Fields: Application to the Simulation of BPTI in Liquid Water. *Journal of Chemical Theory and Computation*, **2005**, 1, 169-80	6.4	65
80	Substrate hydroxylation in methane monooxygenase: quantitative modeling via mixed quantum mechanics/molecular mechanics techniques. *Journal of the American Chemical Society*, **2005**, 127, 1025-37	16.4	56
79	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	15.7	447
78	Modeling Polarization in Proteins and Protein-ligand Complexes: Methods and Preliminary Results. *Advances in Protein Chemistry*, **2005**, 72, 79-104		60
77	Ab initio quantum chemistry: methodology and applications. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6648-53	11.5	217
76	Glide: a new approach for rapid, accurate docking and scoring. 1. Method and assessment of docking accuracy. *Journal of Medicinal Chemistry*, **2004**, 47, 1739-49	8.3	5601
75	A hierarchical approach to all-atom protein loop prediction. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 351-67	4.2	1329
74	Dioxygen activation in methane monooxygenase: a theoretical study. *Journal of the American Chemical Society*, **2004**, 126, 2978-90	16.4	114
73	Combined quantum and molecular mechanics (QM/MM). *Drug Discovery Today: Technologies*, **2004**, 1, 253-60	7.1	16
72	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	2.8	209
71	Cytochrome P450CAM enzymatic catalysis cycle: a quantum mechanics/molecular mechanics study. *Journal of the American Chemical Society*, **2004**, 126, 8501-8	16.4	126
70	Electronic Structure and Luminescence of 1.1- and 1.4-nm Silicon Nanocrystals: Oxide Shell versus Hydrogen Passivation. *Nano Letters*, **2003**, 3, 163-167	11.5	264
69	Mechanistic studies on the hydroxylation of methane by methane monooxygenase. *Chemical Reviews*, **2003**, 103, 2385-419	68.1	407
68	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	11.5	138
67	Ab Initio Protein Structure Prediction Using a Size-dependent Tertiary Folding Potential. *Advances in Chemical Physics*, **2002**, 223-263		1
66	Reactions of methane monooxygenase intermediate Q with derivatized methanes. *Journal of the American Chemical Society*, **2002**, 124, 8770-1	16.4	67
65	Hydroxylation of methane by non-heme diiron enzymes: molecular orbital analysis of C-H bond activation by reactive intermediate Q. *Journal of the American Chemical Society*, **2002**, 124, 14608-15	16.4	61
64	Computational Modeling for Scanning Tunneling Microscopy of Physisorbed Molecules via Ab Initio Quantum Chemistry. *Journal of Physical Chemistry A*, **2002**, 106, 1802-1814	2.8	9

63	Force Field Validation Using Protein Side Chain Prediction. *Journal of Physical Chemistry B*, **2002**, 106, 11673-11680	3.4	155
62	Computing Redox Potentials in Solution: Density Functional Theory as A Tool for Rational Design of Redox Agents. *Journal of Physical Chemistry A*, **2002**, 106, 7407-7412	2.8	319
61	On the role of the crystal environment in determining protein side-chain conformations. *Journal of Molecular Biology*, **2002**, 320, 597-608	6.5	691
60	Protein structure prediction using a combination of sequence-based alignment, constrained energy minimization, and structural alignment. *Proteins: Structure, Function and Bioinformatics*, **2001**, Suppl 5, 133-9	4.2	15
59	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	3.5	108
58	Photodissociation of acetaldehyde: The CH4+CO channel. *Journal of Chemical Physics*, **2001**, 114, 6128-6133	3.9	49
57	Combined fluctuating charge and polarizable dipole models: Application to a five-site water potential function. *Journal of Chemical Physics*, **2001**, 115, 2237-2251	3.9	256
56	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	3.4	8
55	Large-scale ab initio quantum chemical calculations on biological systems. *Accounts of Chemical Research*, **2001**, 34, 351-8	24.3	92
54	Application and development of multiconfigurational localized perturbation theory. *Journal of Chemical Physics*, **2001**, 115, 11052-11067	3.9	19
53	Activation of the C-H bond of methane by intermediate Q of methane monooxygenase: a theoretical study. *Journal of the American Chemical Society*, **2001**, 123, 3836-7	16.4	96
52	An experimental and computational analysis of the formation of the terminal nitrido complex (eta3-Cp*)2Mo(N)(N3) by elimination of N2 from Cp*2Mo(N3)2: the barrier to elimination is strongly influenced by the exo versus endo configuration of the azide ligand. *Journal of the American Chemical Society*, **2001**, 123, 10111-2	16.4	19
51	Reduced dynamics in spin-boson models: A method for both slow and fast bath. *Journal of Chemical Physics*, **2000**, 112, 2095-2105	3.9	41
50	Aqua, Alcohol, and Acetonitrile Adducts of Tris(perfluorophenyl)borane: Evaluation of Br□sted Acidity and Ligand Lability with Experimental and Computational Methods. *Journal of the American Chemical Society*, **2000**, 122, 10581-10590	16.4	197
49	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. *Dalton Transactions RSC*, **2000**, 4491-4496		63
48	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. *Journal of the American Chemical Society*, **2000**, 122, 12651-12658	16.4	34
47	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	16.4	157
46	Efficient memory equation algorithm for reduced dynamics in spin-boson models. *Journal of Chemical Physics*, **1999**, 110, 138-146	3.9	47

45	Mixed ab initio QM/MM modeling using frozen orbitals and tests with alanine dipeptide and tetrapeptide. *Journal of Computational Chemistry*, **1999**, 20, 1468-1494	3.5	232
44	Protein tertiary structure prediction using a branch and bound algorithm. *Proteins: Structure, Function and Bioinformatics*, **1999**, 35, 41-57	4.2	44
43	Prediction of loop geometries using a generalized born model of solvation effects **1999**, 35, 173-183		81
42	Spin–spin model for two-level system/bath problems: A numerical study. *Journal of Chemical Physics*, **1999**, 111, 9918-9923	3.9	19
41	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. *Journal of Chemical Physics*, **1999**, 110, 741-754	3.9	225
40	Calculation of atomization energies by a multiconfigurational localized perturbation theory—Application for closed shell cases. *Journal of Chemical Physics*, **1999**, 110, 1921-1930	3.9	14
39	Mechanistic and Theoretical Analysis of the Oxidative Addition of H2 to Six-Coordinate Molybdenum and Tungsten Complexes M(PMe3)4X2 (M = Mo, W; X = F, Cl, Br, I): An Inverse Equilibrium Isotope Effect and an Unprecedented Halide Dependence. *Journal of the American Chemical Society*, **1999**, 121, 11402-11417	16.4	56
38	1,3-Dipolar Addition of Phenylazide to the Carbon−Carbon Double Bond: An ab Initio Study. *Journal of Physical Chemistry A*, **1999**, 103, 1276-1282	2.8	20
37	Correlated ab Initio Electronic Structure Calculations for Large Molecules. *Journal of Physical Chemistry A*, **1999**, 103, 1913-1928	2.8	258
36	Prediction of loop geometries using a generalized born model of solvation effects **1999**, 35, 173		3
35	Parallel pseudospectral electronic structure: I. Hartree–Fock calculations. *Journal of Computational Chemistry*, **1998**, 19, 1017-1029	3.5	15
34	Parallel pseudospectral electronic structure: II. Localized Møller–Plesset calculations. *Journal of Computational Chemistry*, **1998**, 19, 1030-1038	3.5	13
33	Tertiary structure prediction of mixed α/β proteins via energy minimization. *Proteins: Structure, Function and Bioinformatics*, **1998**, 33, 240-252	4.2	16
32	Constructing ab initio force fields for molecular dynamics simulations. *Journal of Chemical Physics*, **1998**, 108, 4739-4755	3.9	126
31	A three-dimensional reduction of the Ornstein–Zernicke equation for molecular liquids. *Journal of Chemical Physics*, **1997**, 107, 6400-6414	3.9	75
30	Pseudospectral localized generalized Mo/ller–Plesset methods with a generalized valence bond reference wave function: Theory and calculation of conformational energies. *Journal of Chemical Physics*, **1997**, 106, 5073-5084	3.9	68
29	Solvation Free Energies of Peptides: Comparison of Approximate Continuum Solvation Models with Accurate Solution of the Poisson–Boltzmann Equation. *Journal of Physical Chemistry B*, **1997**, 101, 1190-1197	3.4	192
28	Hydrogen Bonding between Amino Acid Backbone and Side Chain Analogues: A High-Level ab Initio Study. *Journal of the American Chemical Society*, **1997**, 119, 12952-12961	16.4	61

27	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	16.4	323
26	An automatic three-dimensional finite element mesh generation system for the PoissonBoltzmann equation. *Journal of Computational Chemistry*, **1997**, 18, 1570-1590	3.5	75
25	Numerical solution of the PoissonBoltzmann equation using tetrahedral finite-element meshes. *Journal of Computational Chemistry*, **1997**, 18, 1591-1608	3.5	154
24	Extension of the PS-GVB electronic structure code to transition metal complexes. *Journal of Computational Chemistry*, **1997**, 18, 1863-1874	3.5	5
23	New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. *The Journal of Physical Chemistry*, **1996**, 100, 11775-11788		852
22	Parallel implementation of a protein structure refinement algorithm. *Journal of Computational Chemistry*, **1996**, 17, 1217-1228	3.5	5
21	Quantum mechanical geometry optimization in solution using a finite element continuum electrostatics method. *Journal of Chemical Physics*, **1996**, 105, 5472-5484	3.9	42
20	Pseudospectral localized Mo/llerPlesset methods: Theory and calculation of conformational energies. *Journal of Chemical Physics*, **1995**, 103, 1481-1490	3.9	159
19	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	16.4	953
18	A hierarchical algorithm for polymer simulations. *Journal of Chemical Physics*, **1992**, 97, 9355-9365	3.9	8
17	Classical and Quantum Models of Activationless Reaction Dynamics. *Zeitschrift Fur Elektrotechnik Und Elektrochemie*, **1991**, 95, 253-258		16
16	Pseudospectral HartreeFock gradient calculations. *Journal of Chemical Physics*, **1991**, 94, 8152-8157	3.9	21
15	Pseudospectral HartreeFock calculations on glycine. *Journal of Chemical Physics*, **1990**, 92, 1163-1173	3.9	38
14	Pseudospectral HartreeFock theory: Applications and algorithmic improvements. *Journal of Chemical Physics*, **1990**, 93, 3397-3407	3.9	82
13	Pseudospectral generalized valence-bond calculations: Application to methylene, ethylene, and silylene. *Journal of Chemical Physics*, **1990**, 92, 7488-7497	3.9	63
12	A method for exponential propagation of large systems of stiff nonlinear differential equations. *Journal of Scientific Computing*, **1989**, 4, 327-354	2.3	91
11	An automatic grid generation scheme for pseudospectral self-consistent field calculations on polyatomic molecules. *The Journal of Physical Chemistry*, **1988**, 92, 3091-3096		65
10	A Thermal Expansion Model for the Special Pair of the Bacterial Reaction Center. *Israel Journal of Chemistry*, **1988**, 28, 67-72	3.4	7

9	Solution of the Hartree–Fock equations for polyatomic molecules by a pseudospectral method. *Journal of Chemical Physics*, **1987**, 86, 3522-3531	3.9	123
8	Natural expansion of vibrational wave functions: RRGM with residue algebra. *Journal of Chemical Physics*, **1986**, 85, 331-336	3.9	28
7	Solution of the Hartree–Fock equations by a pseudospectral method: Application to diatomic molecules. *Journal of Chemical Physics*, **1986**, 85, 1462-1468	3.9	172
6	An accurate and efficient decoupling approximation for temperature-dependent multimode resonance Raman spectra. *Journal of Chemical Physics*, **1986**, 85, 2353-2364	3.9	3
5	Solution of self-consistent field electronic structure equations by a pseudospectral method. *Chemical Physics Letters*, **1985**, 116, 39-43	2.5	224
4	Calculation of temperature-dependent multimode resonance Raman line shapes for harmonic potential surfacesa). *Journal of Chemical Physics*, **1985**, 82, 2918-2926	3.9	23
3	Calculation of optical line shapes for generalized multilevel vibronic systems. *Journal of Chemical Physics*, **1984**, 81, 5899-5905	3.9	21
2	ENERGY TRANSFER BETWEEN THE PRIMARY DONOR BACTERIOCHLOROPHYLL AND CAROTENOIDS IN Rhodopseudomonas sphaeroides. *Photochemistry and Photobiology*, **1983**, 38, 451-455	3.6	38
1	Green's functions and optical line shapes of a general two-level system in the strong electronic coupling limit. *Journal of Chemical Physics*, **1982**, 76, 2129-2135	3.9	5