Jiali Gao

List of Publications by Year in descending order

192 papers	14,805 citations	14614 66 h-index	19690 117 g-index
198 all docs	198 docs citations	198 times ranked	9632 citing authors

#	Article	IF	Citations
1	How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations. Science, 2004, 303, 186-195.	6.0	1,048
2	QUANTUMMECHANICALMETHODS FORENZYMEKINETICS. Annual Review of Physical Chemistry, 2002, 53, 467-505.	4.8	730
3	Hybrid Quantum and Molecular Mechanical Simulations:â€‰ An Alternative Avenue to Solvent Effects in Organic Chemistry. Accounts of Chemical Research, 1996, 29, 298-305.	7.6	510
4	A Generalized Hybrid Orbital (GHO) Method for the Treatment of Boundary Atoms in Combined QM/MM Calculations. Journal of Physical Chemistry A, 1998, 102, 4714-4721.	1.1	481
5	Mechanisms and Free Energies of Enzymatic Reactions. Chemical Reviews, 2006, 106, 3188-3209.	23.0	355
6	Energy decomposition analysis of intermolecular interactions using a block-localized wave function approach. Journal of Chemical Physics, 2000, 112, 5530-5538.	1.2	346
7	Multidimensional Tunneling, Recrossing, and the Transmission Coefficient for Enzymatic Reactions. Chemical Reviews, 2006, 106, 3140-3169.	23.0	328
8	Monte Carlo simulations of the hydration of ammonium and carboxylate ions. The Journal of Physical Chemistry, 1986, 90, 2174-2182.	2.9	299
9	Enhanced receptor binding of SARS-CoV-2 through networks of hydrogen-bonding and hydrophobic interactions. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 13967-13974.	3.3	291
10	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	7.6	262
11	The Methionine-aromatic Motif Plays a Unique Role in Stabilizing Protein Structure. Journal of Biological Chemistry, 2012, 287, 34979-34991.	1.6	261
12	An Efficient Linear-Scaling Ewald Method for Long-Range Electrostatic Interactions in Combined QM/MM Calculations. Journal of Chemical Theory and Computation, 2005, 1, 2-13.	2.3	258
13	The Incorporation of Quantum Effects in Enzyme Kinetics Modeling. Accounts of Chemical Research, 2002, 35, 341-349.	7.6	240
14	Design of a Next Generation Force Field:â€‰ The X-POL Potential. Journal of Chemical Theory and Computation, 2007, 3, 1890-1900.	2.3	209
15	Toward a Molecular Orbital Derived Empirical Potential for Liquid Simulations. Journal of Physical Chemistry B, 1997, 101, 657-663.	1.2	207
16	Energy decomposition analysis based on a block-localized wavefunction and multistate density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 6760.	1.3	203
17	Reaction-Path Energetics and Kinetics of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase. Biochemistry, 2003, 42, 13558-13575.	1.2	202
18	Absolute free energy of solvation from Monte Carlo simulations using combined quantum and molecular mechanical potentials. The Journal of Physical Chemistry, 1992, 96, 537-540.	2.9	193

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19	Methods and Applications of Combined Quantum Mechanical and Molecular Mechanical Potentials. Reviews in Computational Chemistry, 2007, , 119-185.	1.5	189
20	Canonical Variational Theory for Enzyme Kinetics with the Protein Mean Force and Multidimensional Quantum Mechanical Tunneling Dynamics. Theory and Application to Liver Alcohol Dehydrogenase. Journal of Physical Chemistry B, 2001, 105, 11326-11340.	1.2	184
21	Quantum Dynamics of Hydride Transfer in Enzyme Catalysis. Journal of the American Chemical Society, 2000, 122, 8197-8203.	6.6	179
22	Theoretical Analysis of the Rotational Barrier of Ethane. Accounts of Chemical Research, 2007, 40, 113-119.	7.6	172
23	A molecular mechanics force field for NAD+ NADH, and the pyrophosphate groups of nucleotides. Journal of Computational Chemistry, 1997, 18, 221-239.	1.5	168
24	A Polarizable Intermolecular Potential Function for Simulation of Liquid Alcohols. The Journal of Physical Chemistry, 1995, 99, 16460-16467.	2.9	166
25	Optimization of the Lennard-Jones parameters for a combinedab initio quantum mechanical and molecular mechanical potential using the 3-21G basis set. Journal of Computational Chemistry, 1996, 17, 386-395.	1.5	148
26	Ab initio QM/MM simulations with a molecular orbital-valence bond (MOVB) method: application to an SN2 reaction in water. Journal of Computational Chemistry, 2000, 21, 1458-1469.	1.5	146
27	The Magnitude of Hyperconjugation in Ethane: A Perspective from Ab Initio Valence Bond Theory. Angewandte Chemie - International Edition, 2004, 43, 1986-1990.	7.2	139
28	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions:â€‰ H, O, and P Atoms. Journal of Chemical Theory and Computation, 2007, 3, 486-504.	2.3	138
29	The Reaction Mechanism of Paraoxon Hydrolysis by Phosphotriesterase from Combined QM/MM Simulations. Biochemistry, 2007, 46, 13352-13369.	1.2	137
30	Cationâˆ'Ï€ Interactions:â€‰ An Energy Decomposition Analysis and Its Implication in Î´-Opioid Receptorâˆ'Ligand Binding. Journal of the American Chemical Society, 2002, 124, 4832-4837.	6.6	131
31	Dynamically committed, uncommitted, and quenched states encoded in protein kinase A revealed by NMR spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6969-6974.	3.3	129
32	Ab initio study of structures and binding energies for anion-water complexes. Journal of the American Chemical Society, 1986, 108, 4784-4790.	6.6	128
33	A Combined Quantum Mechanical and Molecular Mechanical Study of the Reaction Mechanism and Î±-Amino Acidity in Alanine Racemase. Journal of the American Chemical Society, 2006, 128, 16345-16357.	6.6	125
34	An Ab Initio Molecular Orbitalâˆ'Valence Bond (MOVB) Method for Simulating Chemical Reactions in Solution. Journal of Physical Chemistry A, 2000, 104, 3012-3020.	1.1	123
35	A two-dimensional energy surface for a type II SN2 reaction in aqueous solution. Journal of the American Chemical Society, 1993, 115, 9667-9675.	6.6	122
36	Ensemble-averaged variational transition state theory with optimized multidimensional tunneling for enzyme kinetics and other condensed-phase reactions. International Journal of Quantum Chemistry, 2004, 100, 1136-1152.	1.0	122

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37	X-Pol Potential: An Electronic Structure-Based Force Field for Molecular Dynamics Simulation of a Solvated Protein in Water. Journal of Chemical Theory and Computation, 2009, 5, 459-467.	2.3	121
38	Induced dipole moment and atomic charges based on average electrostatic potentials in aqueous solution. Journal of Chemical Physics, 1993, 98, 2975-2982.	1.2	118
39	Potential of mean force for the isomerization of DMF in aqueous solution: a Monte Carlo QM/MM simulation study. Journal of the American Chemical Society, 1993, 115, 2930-2935.	6.6	115
40	A Simple Electrostatic Model for Trisilylamine:Â Theoretical Examinations of the nâ†'Ïƒ* Negative Hyperconjugation, pï€â†'dï€Bonding, and Stereoelectronic Interaction. Journal of the American Chemical Society, 1999, 121, 5737-5742.	6.6	111
41	Simulation of Liquid Amides Using a Polarizable Intermolecular Potential Functionâ€. The Journal of Physical Chemistry, 1996, 100, 2689-2697.	2.9	110
42	The generalized hybrid orbital method for combined quantum mechanical/molecular mechanical calculations: formulation and tests of the analytical derivatives. Theoretical Chemistry Accounts, 2000, 104, 336-343.	0.5	110
43	Block-Localized Density Functional Theory (BLDFT), Diabatic Coupling, and Their Use in Valence Bond Theory for Representing Reactive Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2009, 5, 2702-2716.	2.3	110
44	Energy components of aqueous solution: Insight from hybrid QM/MM simulations using a polarizable solvent model. Journal of Computational Chemistry, 1997, 18, 1061-1071.	1.5	108
45	A molecular-orbital derived polarization potential for liquid water. Journal of Chemical Physics, 1998, 109, 2346-2354.	1.2	107
46	Development of a Polarizable Intermolecular Potential Function (PIPF) for Liquid Amides and Alkanes. Journal of Chemical Theory and Computation, 2007, 3, 1878-1889.	2.3	107
47	Monte Carlo Quantum Mechanical-Configuration Interaction and Molecular Mechanics Simulation of Solvent Effects on the n .fwdarw. .pi.* Blue Shift of Acetone. Journal of the American Chemical Society, 1994, 116, 9324-9328.	6.6	106
48	The variational explicit polarization potential and analytical first derivative of energy: Towards a next generation force field. Journal of Chemical Physics, 2008, 128, 234108.	1.2	104
49	Hybrid ab Initio QM/MM Simulation of N-Methylacetamide in Aqueous Solution. Journal of Physical Chemistry A, 1997, 101, 3182-3188.	1.1	103
50	Combining Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) with Molecular Mechanics by the Generalized Hybrid Orbital (GHO) Method. Journal of Physical Chemistry A, 2004, 108, 5454-5463.	1.1	94
51	Balancing Kinetic and Thermodynamic Control:Â the Mechanism of Carbocation Cyclization by Squalene Cyclase. Journal of the American Chemical Society, 2003, 125, 12768-12781.	6.6	91
52	Polarization and Charge-Transfer Effects in Lewis Acidâ^'Base Complexes. Journal of Physical Chemistry A, 2001, 105, 6530-6536.	1.1	87
53	An Integrated Path Integral and Free-Energy Perturbationâ^'Umbrella Sampling Method for Computing Kinetic Isotope Effects of Chemical Reactions in Solution and in Enzymes. Journal of Chemical Theory and Computation, 2007, 3, 949-960.	2.3	86
54	Inclusion of quantum-mechanical vibrational energy in reactive potentials of mean force. Journal of Chemical Physics, 2001, 114, 9953-9958.	1.2	84

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55	Hydrophobic and Hydrogen-Bonding Effects on the Rate of Dielsâ^'Alder Reactions in Aqueous Solution. Journal of Organic Chemistry, 1996, 61, 5492-5497.	1.7	83
56	Molecular Dynamics Simulations of the Catalytic Pathway of a Cysteine Protease:â€‰ A Combined QM/MM Study of Human Cathepsin K. Journal of the American Chemical Society, 2007, 129, 13633-13645.	6.6	82
57	Explicit Polarization: A Quantum Mechanical Framework for Developing Next Generation Force Fields. Accounts of Chemical Research, 2014, 47, 2837-2845.	7.6	82
58	Combined QM/MM study of the opsin shift in bacteriorhodopsin. Journal of Computational Chemistry, 2002, 23, 96-105.	1.5	81
59	Combined QM/MM Simulation Study of the Claisen Rearrangement of Allyl Vinyl Ether in Aqueous Solution. Journal of the American Chemical Society, 1994, 116, 1563-1564.	6.6	80
60	Importance of Substrate and Cofactor Polarization in the Active Site of Dihydrofolate Reductase. Journal of Molecular Biology, 2003, 327, 549-560.	2.0	78
61	Combined QM/MM Study of the Mechanism and Kinetic Isotope Effect of the Nucleophilic Substitution Reaction in Haloalkane Dehalogenase. Journal of the American Chemical Society, 2003, 125, 1532-1540.	6.6	75
62	Free Energy Surface, Reaction Paths, and Kinetic Isotope Effect of Short-Chain Acyl-CoA Dehydrogenase. Journal of Physical Chemistry B, 2003, 107, 9567-9578.	1.2	75
63	An Automated Procedure for Simulating Chemical Reactions in Solution. Application to the Decarboxylation of 3-Carboxybenzisoxazole in Water. Journal of the American Chemical Society, 1995, 117, 8600-8607.	6.6	70
64	Solvent effects on the nÏ€* transition of pyrimidine in aqueous solution. Theoretical Chemistry Accounts, 1997, 96, 151-156.	0.5	69
65	Differential quantum tunneling contributions in nitroalkane oxidase catalyzed and the uncatalyzed proton transfer reaction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20734-20739.	3.3	69
66	Hybrid QM/MM Simulations Yield the Ground and Excited State pKaDifference:Â Phenol in Aqueous Solution. Journal of the American Chemical Society, 1996, 118, 4912-4913.	6.6	68
67	Aqueous basicity of the carboxylate lone pairs and the carbon-oxygen barrier in acetic acid: a combined quantum and statistical mechanical study. Journal of the American Chemical Society, 1992, 114, 1912-1914.	6.6	67
68	Beyond Kohnâ€“Sham Approximation: Hybrid Multistate Wave Function and Density Functional Theory. Journal of Physical Chemistry Letters, 2016, 7, 5143-5149.	2.1	66
69	Synthetic Efficiency in Enzyme Mechanisms Involving Carbocations:â€‰ Aristolochene Synthase. Journal of the American Chemical Society, 2007, 129, 13008-13013.	6.6	61
70	Solvent Effects on the Bond Length Alternation and Absorption Energy of Conjugated Compounds. Journal of the American Chemical Society, 1997, 119, 2962-2963.	6.6	60
71	Importance of Electronic Delocalization on the Câ^'N Bond Rotation in HCX(NH2) (X = O, NH, CH2, S, and) Tj ETQq1 1 0.784314 rgBT	1.1	59
72	On the Construction of Diabatic and Adiabatic Potential Energy Surfaces Based on Ab Initio Valence Bond Theory. Journal of Physical Chemistry A, 2008, 112, 12925-12935.	1.1	59

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73	Multistate Density Functional Theory for Effective Diabatic Electronic Coupling. Journal of Physical Chemistry Letters, 2016, 7, 2286-2293.	2.1	59
74	Catalysis by enzyme conformational change as illustrated by orotidine 5â€²-monophosphate decarboxylase. Current Opinion in Structural Biology, 2003, 13, 184-192.	2.6	58
75	Path Integral Simulations of Proton Transfer Reactions in Aqueous Solution Using Combined QM/MM Potentials. Journal of Chemical Theory and Computation, 2006, 2, 236-245.	2.3	57
76	Implementation of the bisection sampling method in path integral simulations. Journal of Molecular Graphics and Modelling, 2005, 24, 121-127.	1.3	54
77	NMR mapping of protein conformational landscapes using coordinated behavior of chemical shifts upon ligand binding. Physical Chemistry Chemical Physics, 2014, 16, 6508-6518.	1.3	54
78	Solvatochromic Shifts of the n â†’ Ï€* Transition of Acetone from Steam Vapor to Ambient Aqueous Solution:â€‰ A Combined Configuration Interaction QM/MM Simulation Study Incorporating Solvent Polarization. Journal of Chemical Theory and Computation, 2007, 3, 1484-1493.	2.3	53
79	Oxidation increases the strength of the methionine-aromatic interaction. Nature Chemical Biology, 2016, 12, 860-866.	3.9	53
80	Importance of bimolecular interactions in developing empirical potential functions for liquid ammonia. The Journal of Physical Chemistry, 1993, 97, 9241-9247.	2.9	50
81	Solvent Polarization and Kinetic Isotope Effects in Nitroethane Deprotonation and Implications to the Nitroalkane Oxidase Reaction. Journal of the American Chemical Society, 2005, 127, 16374-16375.	6.6	50
82	Transition Structure and Substituent Effects on Aqueous Acceleration of the Claisen Rearrangement. Journal of the American Chemical Society, 1995, 117, 11337-11340.	6.6	49
83	Explicit Polarization (X-Pol) Potential Using ab Initio Molecular Orbital Theory and Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 11656-11664.	1.1	49
84	Diabatic-At-Construction Method for Diabatic and Adiabatic Ground and Excited States Based on Multistate Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 1176-1187.	2.3	49
85	A hybrid semiempirical quantum mechanical and lattice-sum method for electrostatic interactions in fluid simulations. Journal of Chemical Physics, 1997, 107, 1212-1217.	1.2	48
86	Theoretical Evidence for a Concerted Mechanism of the Oxirane Cleavage and A-Ring Formation in Oxidosqualene Cyclization. Journal of the American Chemical Society, 1998, 120, 4045-4046.	6.6	48
87	Chemical Control in the Battle against Fidelity in Promiscuous Natural Product Biosynthesis: The Case of Trichodiene Synthase. ACS Catalysis, 2017, 7, 812-818.	5.5	48
88	Combined QM/MM and path integral simulations of kinetic isotope effects in the proton transfer reaction between nitroethane and acetate ion in water. Journal of Computational Chemistry, 2008, 29, 514-522.	1.5	45
89	Perspective on Diabatic Models of Chemical Reactivity as Illustrated by the Gas-Phase SN2 Reaction of Acetate Ion with 1,2-Dichloroethane. Journal of Chemical Theory and Computation, 2009, 5, 1-22.	2.3	45
90	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. Israel Journal of Chemistry, 2014, 54, 1250-1263.	1.0	45

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91	The opsin shift and mechanism of spectral tuning in rhodopsin. Journal of Computational Chemistry, 2011, 32, 854-865.	1.5	44
92	Dysfunctional conformational dynamics of protein kinase A induced by a lethal mutant of phospholamban hinder phosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3716-3721.	3.3	43
93	Cushingâ€™s syndrome driver mutation disrupts protein kinase A allosteric network, altering both regulation and substrate specificity. Science Advances, 2019, 5, eaaw9298.	4.7	43
94	The polarization contribution to the free energy of hydration. Journal of Chemical Physics, 1995, 102, 6145-6152.	1.2	41
95	The hydration and solvent polarization effects of nucleotide bases. Biophysical Chemistry, 1994, 51, 253-261.	1.5	40
96	Internal Proton Transfer in the External Pyridoxal 5â€²-Phosphate Schiff Base in Dopa Decarboxylase. Biochemistry, 2010, 49, 84-94.	1.2	37
97	Spin-Multiplet Components and Energy Splittings by Multistate Density Functional Theory. Journal of Physical Chemistry Letters, 2017, 8, 4838-4845.	2.1	37
98	Quantum mechanical force field for water with explicit electronic polarization. Journal of Chemical Physics, 2013, 139, 054503.	1.2	36
99	Generalized hybrid orbital for the treatment of boundary atoms in combined quantum mechanical and molecular mechanical calculations using the semiempirical parameterized model 3 method. Theoretical Chemistry Accounts, 2004, 111, 280-286.	0.5	35
100	Solvent and Protein Effects on the Vibrational Frequency Shift and Energy Relaxation of the Azide Ligand in Carbonic Anhydrase. Journal of Physical Chemistry B, 2004, 108, 13501-13512.	1.2	34
101	Catalytic hydrogen atom transfer from hydrosilanes to vinylarenes for hydrosilylation and polymerization. Nature Catalysis, 2019, 2, 164-173.	16.1	33
102	Multilevel X-Pol: A Fragment-Based Method with Mixed Quantum Mechanical Representations of Different Fragments. Journal of Physical Chemistry B, 2012, 116, 6781-6788.	1.2	32
103	AM1/d-CB1: A Semiempirical Model for QM/MM Simulations of Chemical Glycobiology Systems. Journal of Chemical Theory and Computation, 2014, 10, 4694-4707.	2.3	32
104	Incorporation of a QM/MM Buffer Zone in the Variational Double Self-Consistent Field Method. Journal of Physical Chemistry B, 2008, 112, 14124-14131.	1.2	31
105	Perturbation Approach to Combined QM/MM Simulation of Soluteâ^'Solvent Interactions in Solution. Journal of Physical Chemistry B, 2003, 107, 1664-1671.	1.2	30
106	Communication: Variational many-body expansion: Accounting for exchange repulsion, charge delocalization, and dispersion in the fragment-based explicit polarization method. Journal of Chemical Physics, 2012, 136, 071101.	1.2	30
107	The Third Dimension of a More Oâ€™Ferrallâ€“Jencks Diagram for Hydrogen Atom Transfer in the Isoelectronic Hydrogen Exchange Reactions of (PhX)₂H^{â€¢} with X = O, NH, and CH₂. Journal of Chemical Theory and Computation, 2012, 8, 4347-4358.	2.3	30
108	Kinetic Isotope Effects of <scp>L</scp>-Dopa Decarboxylase. Journal of the American Chemical Society, 2011, 133, 4398-4403.	6.6	29

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109	Dynamical and allosteric regulation of photoprotection in light harvesting complex II. Science China Chemistry, 2020, 63, 1121-1133.	4.2	29
110	Polarization Effects on the Tautomeric Equilibria of 2- and 4-Hydroxypyridine in Aqueous and Organic Solution. The Journal of Physical Chemistry, 1994, 98, 13772-13779.	2.9	27
111	On the Interfragment Exchange in the X-Pol Method. Journal of Chemical Theory and Computation, 2010, 6, 2469-2476.	2.3	27
112	Polarized Molecular Orbital Model Chemistry. 2. The PMO Method. Journal of Chemical Theory and Computation, 2011, 7, 857-867.	2.3	27
113	Dipole preserving and polarization consistent charges. Journal of Computational Chemistry, 2011, 32, 2127-2139.	1.5	27
114	Hydrogen fluoride phase behavior and molecular structure: A QM/MM potential model approach. Journal of Chemical Physics, 2003, 119, 7365-7371.	1.2	26
115	Generalized X-Pol Theory and Charge Delocalization States. Journal of Chemical Theory and Computation, 2010, 6, 2402-2410.	2.3	26
116	Insight into the phosphodiesterase mechanism from combined QM/MM free energy simulations. FEBS Journal, 2011, 278, 2579-2595.	2.2	25
117	Fragment-based quantum mechanical methods for periodic systems with Ewald summation and mean image charge convention for long-range electrostatic interactions. Physical Chemistry Chemical Physics, 2012, 14, 7821.	1.3	23
118	Conformational Landscape of the PRKACA-DNAJB1 Chimeric Kinase, the Driver for Fibrolamellar Hepatocellular Carcinoma. Scientific Reports, 2018, 8, 720.	1.6	23
119	Computation of Intermolecular Interactions with a Combined Quantum Mechanical and Classical Approach. ACS Symposium Series, 1994, , 8-21.	0.5	22
120	An Effective Hamiltonian Molecular Orbital-Valence Bond (MOVB) Approach for Chemical Reactions as Applied to the Nucleophilic Substitution Reaction of Hydrosulfide Ion and Chloromethane. Journal of Chemical Theory and Computation, 2009, 5, 174-185.	2.3	22
121	The Stories Tryptophans Tell: Exploring Protein Dynamics of Heptosyltransferase I from Escherichia coli. Biochemistry, 2017, 56, 886-895.	1.2	20
122	A leap in quantum efficiency through light harvesting in photoreceptor UVR8. Nature Communications, 2020, 11, 4316.	5.8	20
123	Multistate density functional theory applied with 3 unpaired electrons in 3 orbitals: The singdoublet and tripdoublet states of the ethylene cation. Chemical Physics Letters, 2019, 736, 136803.	1.2	19
124	Dynamic-then-Static Approach for Core Excitations of Open-Shell Molecules. Journal of Physical Chemistry Letters, 2021, 12, 7409-7417.	2.1	19
125	A theoretical investigation of the enol content of acetic acid and the acetate ion in aqueous solution. Computational and Theoretical Chemistry, 1996, 370, 203-208.	1.5	18
126	A Coupled Polarization-Matrix Inversion and Iteration Approach for Accelerating the Dipole Convergence in a Polarizable Potential Function. Journal of Physical Chemistry A, 2009, 113, 2109-2116.	1.1	18

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127	Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 2009, 131, 2687-2698.	6.6	18
128	A Non-Orthogonal Block-Localized Effective Hamiltonian Approach for Chemical and Enzymatic Reactions. Journal of Chemical Theory and Computation, 2010, 6, 2242-2251.	2.3	18
129	Block-Localized Excitation for Excimer Complex and Diabatic Coupling. Journal of Chemical Theory and Computation, 2021, 17, 240-254.	2.3	18
130	Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants. Journal of Chemical Theory and Computation, 2021, 17, 277-289.	2.3	18
131	Comment on â€œSubstrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivityâ€. ACS Catalysis, 2018, 8, 1371-1375.	5.5	17
132	XSOL, a Combined Integral Equation (XRISM) and Quantum Mechanical Solvation Model:Â Free Energies of Hydration and Applications to Solvent Effects on Organic Equilibria. Journal of Physical Chemistry A, 1998, 102, 10366-10373.	1.1	16
133	Hydrogen-bonding interactions in the active site of a low molecular weight protein-tyrosine phosphatase. Journal of Computational Chemistry, 2000, 21, 1192-1203.	1.5	16
134	Incorporation of charge transfer into the explicit polarization fragment method by grand canonical density functional theory. Journal of Chemical Physics, 2011, 135, 084107.	1.2	16
135	Origin of Free Energy Barriers of Decarboxylation and the Reverse Process of CO₂ Capture in Dimethylformamide and in Water. Journal of the American Chemical Society, 2021, 143, 137-141.	6.6	16
136	Multi-state recognition pathway of the intrinsically disordered protein kinase inhibitor by protein kinase A. ELife, 2020, 9, .	2.8	16
137	Simulating Solvent Effects on Reactivity and Interactions in Ambient and Supercritical Water. ACS Symposium Series, 1994, , 212-228.	0.5	15
138	Optimization of the explicit polarization (X-Pol) potential using a hybrid density functional. Theoretical Chemistry Accounts, 2012, 131, 1161.	0.5	15
139	Investigating the role of a backbone to substrate hydrogen bond in OMP decarboxylase using a site-specific amide to ester substitution. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15066-15071.	3.3	15
140	Beyond QM/MM: Fragment Quantum Mechanical Methods. Accounts of Chemical Research, 2014, 47, 2711-2711.	7.6	14
141	Activation mechanism of Drosophila cryptochrome through an allosteric switch. Science Advances, 2021, 7, .	4.7	14
142	Solvent effect on the potential surface of the proton transfer in [H3N?H?NH3]+. International Journal of Quantum Chemistry, 1993, 48, 491-499.	1.0	13
143	The Geometry of Water in Liquid Water from Hybrid Ab Initio-Monte Carlo and Density Functional-Molecular Dynamics Simulations. ACS Symposium Series, 1998, , 35-49.	0.5	13
144	Diabatic States at Construction (DAC) through Generalized Singular Value Decomposition. Journal of Physical Chemistry Letters, 2018, 9, 6038-6046.	2.1	13

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145	Fragment Exchange Potential for Realizing Pauli Deformation of Interfragment Interactions. Journal of Physical Chemistry Letters, 2020, 11, 4008-4016.	2.1	13
146	Origin of the solvent effects on the barrier to amide isomerization from the combined QM/MM Monte Carlo simulations. Journal of Chemical Sciences, 1994, 106, 507-519.	0.7	13
147	Molecular Dynamics Simulations of Biotin Carboxylase. Journal of Physical Chemistry B, 2008, 112, 3149-3156.	1.2	12
148	Minimal-active-space multistate density functional theory for excitation energy involving local and charge transfer states. Npj Computational Materials, 2021, 7, .	3.5	12
149	The charger transfer electronic coupling in diabatic perspective: A multi-state density functional theory study. Chemical Physics Letters, 2018, 691, 91-97.	1.2	11
150	Using multipole point charge distributions to provide the electrostatic potential in the variational explicit polarization (X-Pol) potential. Theoretical Chemistry Accounts, 2011, 129, 3-13.	0.5	10
151	Quantum mechanical force field for hydrogen fluoride with explicit electronic polarization. Journal of Chemical Physics, 2014, 140, 204501.	1.2	10
152	Enhanced vibrational solvatochromism and spectral diffusion by electron rich substituents on small molecule silanes. Journal of Chemical Physics, 2017, 147, 124302.	1.2	10
153	Perturbation Approach for Computing Infrared Spectra of the Local Mode of Probe Molecules. Journal of Chemical Theory and Computation, 2017, 13, 191-201.	2.3	10
154	Active-Site Heterogeneity of Lactate Dehydrogenase. ACS Catalysis, 2019, 9, 4236-4246.	5.5	10
155	Conserved Conformational Hierarchy across Functionally Divergent Glycosyltransferases of the GT-B Structural Superfamily as Determined from Microsecond Molecular Dynamics. International Journal of Molecular Sciences, 2021, 22, 4619.	1.8	10
156	Sunitinib inhibits RNase L by destabilizing its active dimer conformation. Biochemical Journal, 2020, 477, 3387-3399.	1.7	10
157	CARNOT: a Fragment-Based Direct Molecular Dynamics and Virtualâ€“Reality Simulation Package for Reactive Systems. Journal of Chemical Theory and Computation, 2022, 18, 1297-1313.	2.3	10
158	Probing Protein-Protein Interactions Using Asymmetric Labeling and Carbonyl-Carbon Selective Heteronuclear NMR Spectroscopy. Molecules, 2018, 23, 1937.	1.7	9
159	Dynamics and mechanism of dimer dissociation of photoreceptor UVR8. Nature Communications, 2022, 13, 93.	5.8	9
160	Potential energy functions for an intramolecular proton transfer reaction in the ground and excited state. Theoretical Chemistry Accounts, 2007, 118, 211-218.	0.5	8
161	Computation of kinetic isotope effects for enzymatic reactions. Science China Chemistry, 2011, 54, 1841-1850.	4.2	8
162	Intrinsically disordered HAX-1 regulates Ca2+ cycling by interacting with lipid membranes and the phospholamban cytoplasmic region. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183034.	1.4	8

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