Jiali Gao

List of Publications by Year in descending order

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192	14,805	14655	19749
papers	citations	66 h-index	117 g-index

198	198	198	9632
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structural Basis for the Friedelâ€“Crafts Alkylation in Cylindrocyclophane Biosynthesis. ACS Catalysis, 2022, 12, 2108-2117.	11.2	7
2	Quantum vibration perturbation approach with polyatomic probe in simulating infrared spectra. Physical Chemistry Chemical Physics, 2022, 24, 1174-1182.	2.8	2
3	Dynamics and mechanism of dimer dissociation of photoreceptor UVR8. Nature Communications, 2022, 13, 93.	12.8	9
4	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.	5.3	10
5	The Age of Direct Chemical Dynamics. Accounts of Chemical Research, 2022, 55, 471-472.	15.6	0
6	Origin of thiocyanate spectral shifts in water and organic solvents. Journal of Chemical Physics, 2022, 156, 104106.	3.0	6
7	Community Reaction Network Reduction for Constructing a Coarse-Grained Representation of Combustion Reaction Mechanisms. Journal of Chemical Information and Modeling, 2022, 62, 2352-2364.	5.4	6
8	Minimal Active Space for Diradicals Using Multistate Density Functional Theory. Molecules, 2022, 27, 3466.	3.8	1
9	Solvation Induction of Free Energy Barriers of Decarboxylation Reactions in Aqueous Solution from Dual-Level QM/MM Simulations. Jacs Au, 2021, 1, 233-244.	7.9	8
10	SARS-CoV-2 spike protein N501Y mutation causes differential species transmissibility and antibody sensitivity: a molecular dynamics and alchemical free energy study. Molecular Systems Design and Engineering, 2021, 6, 964-974.	3.4	8
11	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.	4.1	10
12	Activation mechanism of Drosophila cryptochrome through an allosteric switch. Science Advances, 2021, 7, .	10.3	14
13	Exact-two-component block-localized wave function: A simple scheme for the automatic computation of relativistic Î”SCF. Journal of Chemical Physics, 2021, 155, 014103.	3.0	5
14	Dynamic-then-Static Approach for Core Excitations of Open-Shell Molecules. Journal of Physical Chemistry Letters, 2021, 12, 7409-7417.	4.6	19
15	Variational Energy Decomposition Analysis of Charge-Transfer Interactions between Metals and Ligands in Carbonyl Complexes. Inorganic Chemistry, 2021, 60, 14060-14071.	4.0	5
16	Is Disrupted Nucleotide-Substrate Cooperativity a Common Trait for Cushing's Syndrome Driving Mutations of Protein Kinase A?. Journal of Molecular Biology, 2021, 433, 167123.	4.2	8
17	Minimal-active-space multistate density functional theory for excitation energy involving local and charge transfer states. Npj Computational Materials, 2021, 7, .	8.7	12
18	Block-Localized Excitation for Excimer Complex and Diabatic Coupling. Journal of Chemical Theory and Computation, 2021, 17, 240-254.	5.3	18

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19	Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants. Journal of Chemical Theory and Computation, 2021, 17, 277-289.	5.3	18
20	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.	13.7	16
21	Deuterium Isotope Effects on Acid-Base Equilibrium of Organic Compounds. Molecules, 2021, 26, 7687.	3.8	1
22	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.	2.6	8
23	Source code, input data, and sample output concerning the application of multistate density functional theory to the singdoublet and tripdoublet states of the ethylene cation. Data in Brief, 2020, 28, 104984.	1.0	1
24	Coupled electron and proton transfer in the piperidine drug metabolism pathway by the active species of cytochromes P450. Dalton Transactions, 2020, 49, 11099-11107.	3.3	4
25	Dynamics and mechanism of light harvesting in UV photoreceptor UVR8. Chemical Science, 2020, 11, 12553-12569.	7.4	3
26	A leap in quantum efficiency through light harvesting in photoreceptor UVR8. Nature Communications, 2020, 11, 4316.	12.8	20
27	Exploring the Reaction Mechanism of HIV Reverse Transcriptase with a Nucleotide Substrate. Journal of Physical Chemistry B, 2020, 124, 4270-4283.	2.6	7
28	A selfâ€consistent coulomb bath model using density fitting. Journal of Computational Chemistry, 2020, 41, 1698-1708.	3.3	6
29	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.	7.1	291
30	Dynamical and allosteric regulation of photoprotection in light harvesting complex II. Science China Chemistry, 2020, 63, 1121-1133.	8.2	29
31	Fragment Exchange Potential for Realizing Pauli Deformation of Interfragment Interactions. Journal of Physical Chemistry Letters, 2020, 11, 4008-4016.	4.6	13
32	Sunitinib inhibits RNase L by destabilizing its active dimer conformation. Biochemical Journal, 2020, 477, 3387-3399.	3.7	10
33	Multi-state recognition pathway of the intrinsically disordered protein kinase inhibitor by protein kinase A. ELife, 2020, 9, .	6.0	16
34	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.	2.6	19
35	Cushingâ€™s syndrome driver mutation disrupts protein kinase A allosteric network, altering both regulation and substrate specificity. Science Advances, 2019, 5, eaaw9298.	10.3	43
36	What factors tune the chemical equilibrium between metal-iodosylarene oxidants and high-valent metal-oxo ones?. Physical Chemistry Chemical Physics, 2019, 21, 1271-1276.	2.8	6

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37	Catalytic hydrogen atom transfer from hydrosilanes to vinylarenes for hydrosilylation and polymerization. Nature Catalysis, 2019, 2, 164-173.	34.4	33
38	Why Can Normal Palladium Catalysts Efficiently Mediate Aerobic Câ€“H Hydroxylation of Arylpyridines by Intercepting Aldehyde Autoxidation? A Nascent Palladium(III)â€“Peracid Intermediate Makes a Difference. Inorganic Chemistry, 2019, 58, 4376-4384.	4.0	7
39	Active-Site Heterogeneity of Lactate Dehydrogenase. ACS Catalysis, 2019, 9, 4236-4246.	11.2	10
40	Molecular-bond breaking induced by interatomic decay processes. Physical Review A, 2019, 100, .	2.5	2
41	Conformational Landscape of the PRKACA-DNAJB1 Chimeric Kinase, the Driver for Fibrolamellar Hepatocellular Carcinoma. Scientific Reports, 2018, 8, 720.	3.3	23
42	Comment on â€œSubstrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivityâ€• ACS Catalysis, 2018, 8, 1371-1375.	11.2	17
43	The charger transfer electronic coupling in diabatic perspective: A multi-state density functional theory study. Chemical Physics Letters, 2018, 691, 91-97.	2.6	11
44	Dual QM and MM Approach for Computing Equilibrium Isotope Fractionation Factor of Organic Species in Solution. Molecules, 2018, 23, 2644.	3.8	3
45	Diabatic States at Construction (DAC) through Generalized Singular Value Decomposition. Journal of Physical Chemistry Letters, 2018, 9, 6038-6046.	4.6	13
46	Probing Protein-Protein Interactions Using Asymmetric Labeling and Carbonyl-Carbon Selective Heteronuclear NMR Spectroscopy. Molecules, 2018, 23, 1937.	3.8	9
47	Combined Multistate and Kohn-Sham Density Functional Theory Studies of the Elusive Mechanism of N-Dealkylation of N,N-Dimethylanilines Mediated by the Biomimetic Nonheme Oxidant FeIV(O)(N4Py)(ClO4)2. Frontiers in Chemistry, 2018, 6, 406.	3.6	7
48	The Stories Tryptophans Tell: Exploring Protein Dynamics of Heptosyltransferase I from Escherichia coli. Biochemistry, 2017, 56, 886-895.	2.5	20
49	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.	5.3	49
50	Chemical Control in the Battle against Fidelity in Promiscuous Natural Product Biosynthesis: The Case of Trichodiene Synthase. ACS Catalysis, 2017, 7, 812-818.	11.2	48
51	Enhanced vibrational solvatochromism and spectral diffusion by electron rich substituents on small molecule silanes. Journal of Chemical Physics, 2017, 147, 124302.	3.0	10
52	Spin-Multiplet Components and Energy Splittings by Multistate Density Functional Theory. Journal of Physical Chemistry Letters, 2017, 8, 4838-4845.	4.6	37
53	Perturbation Approach for Computing Infrared Spectra of the Local Mode of Probe Molecules. Journal of Chemical Theory and Computation, 2017, 13, 191-201.	5.3	10
54	Oxidation increases the strength of the methionine-aromatic interaction. Nature Chemical Biology, 2016, 12, 860-866.	8.0	53

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55	Beyond Kohnâ€“Sham Approximation: Hybrid Multistate Wave Function and Density Functional Theory. Journal of Physical Chemistry Letters, 2016, 7, 5143-5149.	4.6	66
56	Multistate Density Functional Theory for Effective Diabatic Electronic Coupling. Journal of Physical Chemistry Letters, 2016, 7, 2286-2293.	4.6	59
57	Two Aromatic Rings Coupled a Sulfur-Containing Group to Favor Protein Electron Transfer by Instantaneous Formations of Ï€âˆ˜S:Ï€â†”Ï€:Sâˆ Ï€ or Ï€âˆ Ï€:Sâ†”Ï€:Ï€âˆ˜S Five-Electron Bindings. Journal of Physical Chemistry C, 2015, 119, 9149-9158.	3.1	7
58	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.	7.1	43
59	Quantum mechanical force field for hydrogen fluoride with explicit electronic polarization. Journal of Chemical Physics, 2014, 140, 204501.	3.0	10
60	NMR mapping of protein conformational landscapes using coordinated behavior of chemical shifts upon ligand binding. Physical Chemistry Chemical Physics, 2014, 16, 6508-6518.	2.8	54
61	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.	7.1	15
62	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. Israel Journal of Chemistry, 2014, 54, 1250-1263.	2.3	45
63	Explicit Polarization: A Quantum Mechanical Framework for Developing Next Generation Force Fields. Accounts of Chemical Research, 2014, 47, 2837-2845.	15.6	82
64	Beyond QM/MM: Fragment Quantum Mechanical Methods. Accounts of Chemical Research, 2014, 47, 2711-2711.	15.6	14
65	AM1/d-CB1: A Semiempirical Model for QM/MM Simulations of Chemical Glycobiology Systems. Journal of Chemical Theory and Computation, 2014, 10, 4694-4707.	5.3	32
66	Quantum mechanical force field for water with explicit electronic polarization. Journal of Chemical Physics, 2013, 139, 054503.	3.0	36
67	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	15.6	262
68	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.	3.0	30
69	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.	2.8	23
70	Multilevel X-Pol: A Fragment-Based Method with Mixed Quantum Mechanical Representations of Different Fragments. Journal of Physical Chemistry B, 2012, 116, 6781-6788.	2.6	32
71	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.	5.3	30
72	The Methionine-aromatic Motif Plays a Unique Role in Stabilizing Protein Structure. Journal of Biological Chemistry, 2012, 287, 34979-34991.	3.4	261

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73	Optimization of the explicit polarization (X-Pol) potential using a hybrid density functional. Theoretical Chemistry Accounts, 2012, 131, 1161.	1.4	15
74	Polarized Molecular Orbital Model Chemistry. 2. The PMO Method. Journal of Chemical Theory and Computation, 2011, 7, 857-867.	5.3	27
75	Kinetic Isotope Effects of <scp>L</scp>-Dopa Decarboxylase. Journal of the American Chemical Society, 2011, 133, 4398-4403.	13.7	29
76	Energy decomposition analysis based on a block-localized wavefunction and multistate density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 6760.	2.8	203
77	Incorporation of charge transfer into the explicit polarization fragment method by grand canonical density functional theory. Journal of Chemical Physics, 2011, 135, 084107.	3.0	16
78	Insight into the phosphodiesterase mechanism from combined QM/MM free energy simulations. FEBS Journal, 2011, 278, 2579-2595.	4.7	25
79	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.	1.4	10
80	Computation of kinetic isotope effects for enzymatic reactions. Science China Chemistry, 2011, 54, 1841-1850.	8.2	8
81	The opsin shift and mechanism of spectral tuning in rhodopsin. Journal of Computational Chemistry, 2011, 32, 854-865.	3.3	44
82	Dipole preserving and polarization consistent charges. Journal of Computational Chemistry, 2011, 32, 2127-2139.	3.3	27
83	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.	7.1	129
84	Generalized X-Pol Theory and Charge Delocalization States. Journal of Chemical Theory and Computation, 2010, 6, 2402-2410.	5.3	26
85	A Non-Orthogonal Block-Localized Effective Hamiltonian Approach for Chemical and Enzymatic Reactions. Journal of Chemical Theory and Computation, 2010, 6, 2242-2251.	5.3	18
86	On the Interfragment Exchange in the X-Pol Method. Journal of Chemical Theory and Computation, 2010, 6, 2469-2476.	5.3	27
87	Internal Proton Transfer in the External Pyridoxal 5â€²-Phosphate Schiff Base in Dopa Decarboxylase. Biochemistry, 2010, 49, 84-94.	2.5	37
88	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.	7.1	69
89	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.	5.3	110
90	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.	2.5	18

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91	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.	5.3	22
92	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.	13.7	18
93	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.	5.3	121
94	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.	5.3	45
95	Explicit Polarization (X-Pol) Potential Using ab Initio Molecular Orbital Theory and Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 11656-11664.	2.5	49
96	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.	3.3	45
97	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.	2.5	59
98	Incorporation of a QM/MM Buffer Zone in the Variational Double Self-Consistent Field Method. Journal of Physical Chemistry B, 2008, 112, 14124-14131.	2.6	31
99	Molecular Dynamics Simulations of Biotin Carboxylase. Journal of Physical Chemistry B, 2008, 112, 3149-3156.	2.6	12
100	The variational explicit polarization potential and analytical first derivative of energy: Towards a next generation force field. Journal of Chemical Physics, 2008, 128, 234108.	3.0	104
101	Hybrid Quantum and Classical Methods for Computing Kinetic Isotope Effects of Chemical Reactions in Solutions and in Enzymes. Methods in Molecular Biology, 2008, 443, 37-62.	0.9	5
102	Methods and Applications of Combined Quantum Mechanical and Molecular Mechanical Potentials. Reviews in Computational Chemistry, 2007, , 119-185.	1.5	189
103	Theoretical Analysis of the Rotational Barrier of Ethane. Accounts of Chemical Research, 2007, 40, 113-119.	15.6	172
104	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.	5.3	86
105	Development of a Polarizable Intermolecular Potential Function (PIPF) for Liquid Amides and Alkanes. Journal of Chemical Theory and Computation, 2007, 3, 1878-1889.	5.3	107
106	Synthetic Efficiency in Enzyme Mechanisms Involving Carbocations:â€‰ Aristolochene Synthase. Journal of the American Chemical Society, 2007, 129, 13008-13013.	13.7	61
107	Design of a Next Generation Force Field:â€‰ The X-POL Potential. Journal of Chemical Theory and Computation, 2007, 3, 1890-1900.	5.3	209
108	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.	5.3	138

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109	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.	5.3	53
110	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.	13.7	82
111	The Reaction Mechanism of Paraoxon Hydrolysis by Phosphotriesterase from Combined QM/MM Simulations. Biochemistry, 2007, 46, 13352-13369.	2.5	137
112	Potential energy functions for an intramolecular proton transfer reaction in the ground and excited state. Theoretical Chemistry Accounts, 2007, 118, 211-218.	1.4	8
113	Multidimensional Tunneling, Recrossing, and the Transmission Coefficient for Enzymatic Reactions. Chemical Reviews, 2006, 106, 3140-3169.	47.7	328
114	Mechanisms and Free Energies of Enzymatic Reactions. Chemical Reviews, 2006, 106, 3188-3209.	47.7	355
115	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.	5.3	57
116	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.	13.7	125
117	Implementation of the bisection sampling method in path integral simulations. Journal of Molecular Graphics and Modelling, 2005, 24, 121-127.	2.4	54
118	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.	5.3	258
119	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.	13.7	50
120	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.	2.6	34
121	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.	1.4	35
122	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.	2.0	122
123	The Magnitude of Hyperconjugation in Ethane: A Perspective from Ab Initio Valence Bond Theory. Angewandte Chemie - International Edition, 2004, 43, 1986-1990.	13.8	139
124	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.	2.5	94
125	How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations. Science, 2004, 303, 186-195.	12.6	1,048
126	Catalysis by enzyme conformational change as illustrated by orotidine 5â€²-monophosphate decarboxylase. Current Opinion in Structural Biology, 2003, 13, 184-192.	5.7	58

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127	Balancing Kinetic and Thermodynamic Control:Â the Mechanism of Carbocation Cyclization by Squalene Cyclase. Journal of the American Chemical Society, 2003, 125, 12768-12781.	13.7	91
128	Perturbation Approach to Combined QM/MM Simulation of Soluteâ˜Solvent Interactions in Solution. Journal of Physical Chemistry B, 2003, 107, 1664-1671.	2.6	30
129	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.	13.7	75
130	Free Energy Surface, Reaction Paths, and Kinetic Isotope Effect of Short-Chain Acyl-CoA Dehydrogenase. Journal of Physical Chemistry B, 2003, 107, 9567-9578.	2.6	75
131	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 /C	2.5	59
132	Reaction-Path Energetics and Kinetics of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase. Biochemistry, 2003, 42, 13558-13575.	2.5	202
133	Importance of Substrate and Cofactor Polarization in the Active Site of Dihydrofolate Reductase. Journal of Molecular Biology, 2003, 327, 549-560.	4.2	78
134	Hydrogen fluoride phase behavior and molecular structure: A QM/MM potential model approach. Journal of Chemical Physics, 2003, 119, 7365-7371.	3.0	26
135	The Incorporation of Quantum Effects in Enzyme Kinetics Modeling. Accounts of Chemical Research, 2002, 35, 341-349.	15.6	240
136	QUANTUMMECHANICALMETHODS FORENZYMEKINETICS. Annual Review of Physical Chemistry, 2002, 53, 467-505.	10.8	730
137	Cationâ˜Ï€ Interactions:â€‰ An Energy Decomposition Analysis and Its Implication in Î´-Opioid Receptorâ˜Ligand Binding. Journal of the American Chemical Society, 2002, 124, 4832-4837.	13.7	131
138	Combined QM/MM study of the opsin shift in bacteriorhodopsin. Journal of Computational Chemistry, 2002, 23, 96-105.	3.3	81
139	Polarization and Charge-Transfer Effects in Lewis Acidâ˜Base Complexes. Journal of Physical Chemistry A, 2001, 105, 6530-6536.	2.5	87
140	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.	2.6	184
141	Inclusion of quantum-mechanical vibrational energy in reactive potentials of mean force. Journal of Chemical Physics, 2001, 114, 9953-9958.	3.0	84
142	Hydrogen-bonding interactions in the active site of a low molecular weight protein-tyrosine phosphatase. Journal of Computational Chemistry, 2000, 21, 1192-1203.	3.3	16
143	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.	3.3	146
144	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.	1.4	110

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145	Perspective on "Theoretical studies of enzymic reactions: dielectric, electrostatic and steric stabilization of the carbonium ion in the reaction of lysozyme". Theoretical Chemistry Accounts, 2000, 103, 328-329.	1.4	3
146	An Ab Initio Molecular Orbitalâ^'Valence Bond (MOVB) Method for Simulating Chemical Reactions in Solution. Journal of Physical Chemistry A, 2000, 104, 3012-3020.	2.5	123
147	Quantum Dynamics of Hydride Transfer in Enzyme Catalysis. Journal of the American Chemical Society, 2000, 122, 8197-8203.	13.7	179
148	Energy decomposition analysis of intermolecular interactions using a block-localized wave function approach. Journal of Chemical Physics, 2000, 112, 5530-5538.	3.0	346
149	Ab initio QM/MM simulations with a molecular orbitalâ€valence bond (MOVB) method: application to an SN2 reaction in water. Journal of Computational Chemistry, 2000, 21, 1458-1469.	3.3	8
150	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.	13.7	111
151	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
152	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.	2.5	481
153	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.	2.5	16
154	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.	13.7	48
155	A molecular-orbital derived polarization potential for liquid water. Journal of Chemical Physics, 1998, 109, 2346-2354.	3.0	107
156	A hybrid semiempirical quantum mechanical and lattice-sum method for electrostatic interactions in fluid simulations. Journal of Chemical Physics, 1997, 107, 1212-1217.	3.0	48
157	Hybrid ab Initio QM/MM Simulation of N-Methylacetamide in Aqueous Solution. Journal of Physical Chemistry A, 1997, 101, 3182-3188.	2.5	103
158	Solvent Effects on the Bond Length Alternation and Absorption Energy of Conjugated Compounds. Journal of the American Chemical Society, 1997, 119, 2962-2963.	13.7	60
159	Toward a Molecular Orbital Derived Empirical Potential for Liquid Simulations. Journal of Physical Chemistry B, 1997, 101, 657-663.	2.6	207
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