

Jingzhi Pu

List of Publications by Citations

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44
papers

7,805
citations

24
h-index

46
g-index

46
ext. papers

8,786
ext. citations

7.9
avg, IF

5.08
L-index

#	Paper	IF	Citations
44	CHARMM: the biomolecular simulation program. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1545-614	3.5	5515
43	Mechanisms and free energies of enzymatic reactions. <i>Chemical Reviews</i> , 2006 , 106, 3188-209	68.1	321
42	Multidimensional tunneling, recrossing, and the transmission coefficient for enzymatic reactions. <i>Chemical Reviews</i> , 2006 , 106, 3140-69	68.1	302
41	Tests of second-generation and third-generation density functionals for thermochemical kinetics. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 673	3.6	217
40	Generalized Hybrid Orbital (GHO) Method for Combining Ab Initio Hartree-Fock Wave Functions with Molecular Mechanics. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 632-650	2.8	127
39	How subunit coupling produces the gamma-subunit rotary motion in F1-ATPase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008 , 105, 1192-7	11.5	104
38	Small temperature dependence of the kinetic isotope effect for the hydride transfer reaction catalyzed by Escherichia coli dihydrofolate reductase. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 8551-6	3.4	104
37	Development of a polarizable intermolecular potential function (PIPF) for liquid amides and alkanes. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1878-1889	6.4	102
36	Combining Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) with Molecular Mechanics by the Generalized Hybrid Orbital (GHO) Method. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 5454-5463	2.8	87
35	Hydride transfer reaction catalyzed by hyperthermophilic dihydrofolate reductase is dominated by quantum mechanical tunneling and is promoted by both inter- and intramonomeric correlated motions. <i>Journal of the American Chemical Society</i> , 2006 , 128, 8015-23	16.4	71
34	Parametrized direct dynamics study of rate constants of H with CH4 from 250 to 2400 K. <i>Journal of Chemical Physics</i> , 2002 , 116, 1468-1478	3.9	71
33	Validation of variational transition state theory with multidimensional tunneling contributions against accurate quantum mechanical dynamics for H+CH4-H2+CH3 in an extended temperature interval. <i>Journal of Chemical Physics</i> , 2002 , 117, 1479-1481	3.9	70
32	Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 2475-2486	2.8	63
31	Generalized hybrid-orbital method for combining density functional theory with molecular mechanicals. <i>ChemPhysChem</i> , 2005 , 6, 1853-65	3.2	62
30	Nonperfect synchronization of reaction center rehybridization in the transition state of the hydride transfer catalyzed by dihydrofolate reductase. <i>Journal of the American Chemical Society</i> , 2005 , 127, 14875-86	16.4	54
29	Test of variational transition state theory with multidimensional tunneling contributions against an accurate full-dimensional rate constant calculation for a six-atom system. <i>Journal of Chemical Physics</i> , 2001 , 115, 6266-6267	3.9	50
28	Benchmark calculations of reaction energies, barrier heights, and transition-state geometries for hydrogen abstraction from methanol by a hydrogen atom. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 773-8	2.8	49

27	Tests of potential energy surfaces for H+CH ₄ ←CH ₃ +H ₂ : Deuterium and muonium kinetic isotope effects for the forward and reverse reaction. <i>Journal of Chemical Physics</i> , 2002 , 117, 10675-10687	3.9	43
26	Trapping the ATP binding state leads to a detailed understanding of the F1-ATPase mechanism. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 17851-6	11.5	38
25	Reaction Path Force Matching: A New Strategy of Fitting Specific Reaction Parameters for Semiempirical Methods in Combined QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3038-54	6.4	36
24	Lateral confinement of image electron wave function by an interfacial dipole lattice. <i>Journal of Chemical Physics</i> , 2003 , 118, 4337-4340	3.9	34
23	Efficient Molecular Mechanics for Chemical Reactions: Multiconfiguration Molecular Mechanics Using Partial Electronic Structure Hessians. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 4112-4124	2.8	32
22	Multicoefficient Gaussian-3 calculation of the rate constant for the OH + CH ₄ reaction and its ¹² C/ ¹³ C kinetic isotope effect with emphasis on the effects of coordinate system and torsional treatment. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 11706-17	2.8	28
21	Searching for Saddle Points by Using the Nudged Elastic Band Method: An Implementation for Gas-Phase Systems. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 895-904	6.4	28
20	Isotropic Periodic Sum Treatment of Long-Range Electrostatic Interactions in Combined Quantum Mechanical and Molecular Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 134-45	6.4	22
19	H-loop histidine catalyzes ATP hydrolysis in the E. coli ABC-transporter HlyB. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 15811-5	3.6	21
18	Accelerated computation of free energy profile at ab initio quantum mechanical/molecular mechanical accuracy via a semi-empirical reference potential. II. Recalibrating semi-empirical parameters with force matching. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 20595-20605	3.6	20
17	Temperature dependence of carbon-13 kinetic isotope effects of importance to global climate change. <i>Journal of the American Chemical Society</i> , 2005 , 127, 2830-1	16.4	20
16	Chemical synthesis, crystal structure and enzymatic evaluation of a dinucleotide spore photoproduct analogue containing a formacetal linker. <i>Chemistry - A European Journal</i> , 2011 , 17, 9658-68	4.8	19
15	Machine-Learning-Assisted Free Energy Simulation of Solution-Phase and Enzyme Reactions. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5745-5758	6.4	14
14	A coupled polarization-matrix inversion and iteration approach for accelerating the dipole convergence in a polarizable potential function. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 2109-16	2.8	13
13	Assessing the accuracy of the isotropic periodic sum method through Madelung energy computation. <i>Journal of Chemical Physics</i> , 2014 , 140, 164106	3.9	12
12	Toward Determining ATPase Mechanism in ABC Transporters: Development of the Reaction Path-Force Matching QM/MM Method. <i>Methods in Enzymology</i> , 2016 , 577, 185-212	1.7	11
11	Elucidating the role of surface passivating ligand structural parameters in hole wave function delocalization in semiconductor cluster molecules. <i>Nanoscale</i> , 2017 , 9, 14127-14138	7.7	10
10	Reaction Path-Force Matching in Collective Variables: Determining Ab Initio QM/MM Free Energy Profiles by Fitting Mean Force. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 4961-4980	6.4	6

9	Identifying Thermal Decomposition Products of Nitrate Ester Explosives Using Gas Chromatography-Vacuum Ultraviolet Spectroscopy: An Experimental and Computational Study. <i>Applied Spectroscopy</i> , 2020 , 74, 1486-1495	3.1	5
8	Treating electrostatics with Wolf summation in combined quantum mechanical and molecular mechanical simulations. <i>Journal of Chemical Physics</i> , 2015 , 143, 174111	3.9	5
7	Expanding the horizon of the thymine isostere biochemistry: unique cyclobutane dimers formed by photoreaction between a thymine and a toluene residue in the dinucleotide framework. <i>Chemistry - A European Journal</i> , 2012 , 18, 7823-33	4.8	5
6	Use of Block Hessians for the Optimization of Molecular Geometries. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 54-60	6.4	4
5	Mapping Free Energy Pathways for ATP Hydrolysis in the ABC Transporter HlyB by the String Method. <i>Molecules</i> , 2018 , 23,	4.8	3
4	Replica exchange molecular dynamics simulations of an α -type small acid soluble protein (SASP). <i>Biophysical Chemistry</i> , 2013 , 184, 17-21	3.5	2
3	Doubly Polarized QM/MM with Machine Learning Chaperone Polarizability. <i>Journal of Chemical Theory and Computation</i> , 2021 ,	6.4	2
2	Exploring Cycloreversion Reaction of Cyclobutane Pyrimidine Dimers Quantum Mechanically. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 2025-2039	2.8	1
1	Interligand communication in a metal mediated LLCT system - a case study. <i>RSC Advances</i> , 2021 , 11, 24381-24386	3.7	1