Jingzhi Pu

List of Publications by Year in Descending Order

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	Doubly Polarized QM/MM with Machine Learning Chaperone Polarizability. *Journal of Chemical Theory and Computation*, **2021**,	6.4	2
43	Interligand communication in a metal mediated LLCT system - a case study. *RSC Advances*, **2021**, 11, 24381-24386	3.7	3
42	Reaction Path-Force Matching in Collective Variables: Determining Ab Initio QM/MM Free Energy Profiles by Fitting Mean Force. *Journal of Chemical Theory and Computation*, **2021**, 17, 4961-4980	6.4	6
41	Machine-Learning-Assisted Free Energy Simulation of Solution-Phase and Enzyme Reactions. *Journal of Chemical Theory and Computation*, **2021**, 17, 5745-5758	6.4	14
40	Identifying Thermal Decomposition Products of Nitrate Ester Explosives Using Gas Chromatography-Vacuum Ultraviolet Spectroscopy: An Experimental and Computational Study. *Applied Spectroscopy*, **2020**, 74, 1486-1495	3.1	5
39	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. *Physical Chemistry Chemical Physics*, **2019**, 21, 20595-20605	3.6	20
38	Exploring Cycloreversion Reaction of Cyclobutane Pyrimidine Dimers Quantum Mechanically. *Journal of Physical Chemistry A*, **2019**, 123, 2025-2039	2.8	1
37	Mapping Free Energy Pathways for ATP Hydrolysis in the ABC Transporter HlyB by the String Method. *Molecules*, **2018**, 23,	4.8	3
36	Elucidating the role of surface passivating ligand structural parameters in hole wave function delocalization in semiconductor cluster molecules. *Nanoscale*, **2017**, 9, 14127-14138	7.7	10
35	Toward Determining ATPase Mechanism in ABC Transporters: Development of the Reaction Path-Force Matching QM/MM Method. *Methods in Enzymology*, **2016**, 577, 185-212	1.7	11
34	Treating electrostatics with Wolf summation in combined quantum mechanical and molecular mechanical simulations. *Journal of Chemical Physics*, **2015**, 143, 174111	3.9	5
33	Isotropic Periodic Sum Treatment of Long-Range Electrostatic Interactions in Combined Quantum Mechanical and Molecular Mechanical Calculations. *Journal of Chemical Theory and Computation*, **2014**, 10, 134-45	6.4	22
32	Reaction Path Force Matching: A New Strategy of Fitting Specific Reaction Parameters for Semiempirical Methods in Combined QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 3038-54	6.4	36
31	Trapping the ATP binding state leads to a detailed understanding of the F1-ATPase mechanism. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 17851-6	11.5	38
30	Assessing the accuracy of the isotropic periodic sum method through Madelung energy computation. *Journal of Chemical Physics*, **2014**, 140, 164106	3.9	12
29	H-loop histidine catalyzes ATP hydrolysis in the E. coli ABC-transporter HlyB. *Physical Chemistry Chemical Physics*, **2013**, 15, 15811-5	3.6	21
28	Replica exchange molecular dynamics simulations of an α-type small acid soluble protein (SASP). *Biophysical Chemistry*, **2013**, 184, 17-21	3.5	2

27	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. *Chemistry - A European Journal*, **2012**, 18, 7823-33	4.8	5
26	Chemical synthesis, crystal structure and enzymatic evaluation of a dinucleotide spore photoproduct analogue containing a formacetal linker. *Chemistry - A European Journal*, **2011**, 17, 9658-68	4.8	19
25	CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614	3.5	5515
24	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, 2109-16	2.8	13
23	How subunit coupling produces the gamma-subunit rotary motion in F1-ATPase. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 1192-7	11.5	104
22	Development of a polarizable intermolecular potential function (PIPF) for liquid amides and alkanes. *Journal of Chemical Theory and Computation*, **2007**, 3, 1878-1889	6.4	102
21	Multicoefficient Gaussian-3 calculation of the rate constant for the OH + CH4 reaction and its 12C/13C kinetic isotope effect with emphasis on the effects of coordinate system and torsional treatment. *Journal of Physical Chemistry A*, **2007**, 111, 11706-17	2.8	28
20	Multidimensional tunneling, recrossing, and the transmission coefficient for enzymatic reactions. *Chemical Reviews*, **2006**, 106, 3140-69	68.1	302
19	Mechanisms and free energies of enzymatic reactions. *Chemical Reviews*, **2006**, 106, 3188-209	68.1	321
18	Hydride transfer reaction catalyzed by hyperthermophilic dihydrofolate reductase is dominated by quantum mechanical tunneling and is promoted by both inter- and intramonomeric correlated motions. *Journal of the American Chemical Society*, **2006**, 128, 8015-23	16.4	71
17	Searching for Saddle Points by Using the Nudged Elastic Band Method: An Implementation for Gas-Phase Systems. *Journal of Chemical Theory and Computation*, **2006**, 2, 895-904	6.4	28
16	Small temperature dependence of the kinetic isotope effect for the hydride transfer reaction catalyzed by Escherichia coli dihydrofolate reductase. *Journal of Physical Chemistry B*, **2005**, 109, 8551-6	3.4	104
15	Benchmark calculations of reaction energies, barrier heights, and transition-state geometries for hydrogen abstraction from methanol by a hydrogen atom. *Journal of Physical Chemistry A*, **2005**, 109, 773-8	2.8	49
14	Temperature dependence of carbon-13 kinetic isotope effects of importance to global climate change. *Journal of the American Chemical Society*, **2005**, 127, 2830-1	16.4	20
13	Nonperfect synchronization of reaction center rehybridization in the transition state of the hydride transfer catalyzed by dihydrofolate reductase. *Journal of the American Chemical Society*, **2005**, 127, 14879-86	16.4	54
12	Use of Block Hessians for the Optimization of Molecular Geometries. *Journal of Chemical Theory and Computation*, **2005**, 1, 54-60	6.4	4
11	Generalized hybrid-orbital method for combining density functional theory with molecular mechanicals. *ChemPhysChem*, **2005**, 6, 1853-65	3.2	62
10	Tests of second-generation and third-generation density functionals for thermochemical kinetics. *Physical Chemistry Chemical Physics*, **2004**, 6, 673	3.6	217

9	Efficient Molecular Mechanics for Chemical Reactions: Multiconfiguration Molecular Mechanics Using Partial Electronic Structure Hessians. *Journal of Physical Chemistry A*, **2004**, 108, 4112-4124	2.8	32
8	Generalized Hybrid Orbital (GHO) Method for Combining Ab Initio Hartree–Fock Wave Functions with Molecular Mechanics. *Journal of Physical Chemistry A*, **2004**, 108, 632-650	2.8	127
7	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	2.8	87
6	Benchmark Results for Hydrogen Atom Transfer between Carbon Centers and Validation of Electronic Structure Methods for Bond Energies and Barrier Heights. *Journal of Physical Chemistry A* , **2004**, 108, 2475-2486	2.8	63
5	Lateral confinement of image electron wave function by an interfacial dipole lattice. *Journal of Chemical Physics*, **2003**, 118, 4337-4340	3.9	34
4	Parametrized direct dynamics study of rate constants of H with CH4 from 250 to 2400 K. *Journal of Chemical Physics*, **2002**, 116, 1468-1478	3.9	71
3	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. *Journal of Chemical Physics*, **2002**, 117, 1479-1481	3.9	70
2	Tests of potential energy surfaces for H+CH4<–CH3+H2: Deuterium and muonium kinetic isotope effects for the forward and reverse reaction. *Journal of Chemical Physics*, **2002**, 117, 10675-10687	3.9	43
1	Test of variational transition state theory with multidimensional tunneling contributions against an accurate full-dimensional rate constant calculation for a six-atom system. *Journal of Chemical Physics*, **2001**, 115, 6266-6267	3.9	50