Jingzhi Pu

List of Publications by Year
in descending order

45 papers	9,649 citations	218381 26 h-index	233125 45 g-index
46 all docs	46 docs citations	46 times ranked	11965 citing authors

#	Article	IF	Citations
1	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	1.5	7,077
2	Mechanisms and Free Energies of Enzymatic Reactions. Chemical Reviews, 2006, 106, 3188-3209.	23.0	355
3	Multidimensional Tunneling, Recrossing, and the Transmission Coefficient for Enzymatic Reactions. Chemical Reviews, 2006, 106, 3140-3169.	23.0	328
4	Tests of second-generation and third-generation density functionals for thermochemical kineticsElectronic supplementary information (ESI) available: Mean errors for pure and hybrid DFT methods. See http://www.rsc.org/suppdata/cp/b3/b316260e/. Physical Chemistry Chemical Physics, 2004, 6, 673.	1.3	242
5	Generalized Hybrid Orbital (GHO) Method for Combining Ab Initio Hartreeâ^'Fock Wave Functions with Molecular Mechanics. Journal of Physical Chemistry A, 2004, 108, 632-650.	1.1	133
6	How subunit coupling produces the Î³-subunit rotary motion in F ₁ -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 1192-1197.	3.3	114
7	Small Temperature Dependence of the Kinetic Isotope Effect for the Hydride Transfer Reaction Catalyzed byEscherichiacoliDihydrofolate Reductase. Journal of Physical Chemistry B, 2005, 109, 8551-8556.	1.2	110
8	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
9	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
10	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, 8015-8023.	6.6	75
11	Parametrized direct dynamics study of rate constants of H with CH4 from 250 to 2400 K. Journal of Chemical Physics, 2002, 116, 1468-1478.	1.2	73
12	Validation of variational transition state theory with multidimensional tunneling contributions against accurate quantum mechanical dynamics for H+CH4â†'H2+CH3 in an extended temperature interval. Journal of Chemical Physics, 2002, 117, 1479-1481.	1.2	73
13	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.	1.1	70
14	Generalized Hybrid-Orbital Method for Combining Density Functional Theory with Molecular Mechanicals. ChemPhysChem, 2005, 6, 1853-1865.	1.0	67
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, 773-778.	1.1	57
16	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, 14879-14886.	6.6	56
17	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.	1.2	55
18	Machine-Learning-Assisted Free Energy Simulation of Solution-Phase and Enzyme Reactions. Journal of Chemical Theory and Computation, 2021, 17, 5745-5758.	2.3	55

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19	Trapping the ATP binding state leads to a detailed understanding of the F ₁ -ATPase mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17851-17856.	3.3	51
20	Tests of potential energy surfaces for H+CH4â†"CH3+H2: Deuterium and muonium kinetic isotope effects for the forward and reverse reaction. Journal of Chemical Physics, 2002, 117, 10675-10687.	1.2	43
21	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, 3038-3054.	2.3	40
22	Lateral confinement of image electron wave function by an interfacial dipole lattice. Journal of Chemical Physics, 2003, 118, 4337-4340.	1.2	35
23	Searching for Saddle Points by Using the Nudged Elastic Band Method:â€‰ An Implementation for Gas-Phase Systems. Journal of Chemical Theory and Computation, 2006, 2, 895-904.	2.3	33
24	Efficient Molecular Mechanics for Chemical Reactions:Â Multiconfiguration Molecular Mechanics Using Partial Electronic Structure Hessians. Journal of Physical Chemistry A, 2004, 108, 4112-4124.	1.1	32
25	Multicoefficient Gaussian-3 Calculation of the Rate Constant for the OH + CH4Reaction and Its12C/13C Kinetic Isotope Effect with Emphasis on the Effects of Coordinate System and Torsional Treatment. Journal of Physical Chemistry A, 2007, 111, 11706-11717.	1.1	30
26	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.	1.3	30
27	H-loop histidine catalyzes ATP hydrolysis in the E. coli ABC-transporter HlyB. Physical Chemistry Chemical Physics, 2013, 15, 15811.	1.3	24
28	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, 134-145.	2.3	23
29	Chemical Synthesis, Crystal Structure and Enzymatic Evaluation of a Dinucleotide Spore Photoproduct Analogue Containing a Formacetal Linker. Chemistry - A European Journal, 2011, 17, 9658-9668.	1.7	22
30	Temperature Dependence of Carbon-13 Kinetic Isotope Effects of Importance to Global Climate Change. Journal of the American Chemical Society, 2005, 127, 2830-2831.	6.6	21
31	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
32	Assessing the accuracy of the isotropic periodic sum method through Madelung energy computation. Journal of Chemical Physics, 2014, 140, 164106.	1.2	14
33	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.	2.3	14
34	Toward Determining ATPase Mechanism in ABC Transporters. Methods in Enzymology, 2016, 577, 185-212.	0.4	11
35	Elucidating the role of surface passivating ligand structural parameters in hole wave function delocalization in semiconductor cluster molecules. Nanoscale, 2017, 9, 14127-14138.	2.8	11
36	Mapping Free Energy Pathways for ATP Hydrolysis in the E. coli ABC Transporter HlyB by the String Method. Molecules, 2018, 23, 2652.	1.7	10

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37	Identifying Thermal Decomposition Products of Nitrate Ester Explosives Using Gas Chromatographyâ€“Vacuum Ultraviolet Spectroscopy: An Experimental and Computational Study. Applied Spectroscopy, 2020, 74, 1486-1495.	1.2	10
38	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, 7823-7833.	1.7	6
39	Treating electrostatics with Wolf summation in combined quantum mechanical and molecular mechanical simulations. Journal of Chemical Physics, 2015, 143, 174111.	1.2	6
40	Accelerating Ab Initio Quantum Mechanical and Molecular Mechanical (QM/MM) Molecular Dynamics Simulations with Multiple Time Step Integration and a Recalibrated Semiempirical QM/MM Hamiltonian. Journal of Physical Chemistry B, 2022, 126, 4226-4235.	1.2	6
41	Use of Block Hessians for the Optimization of Molecular Geometries. Journal of Chemical Theory and Computation, 2005, 1, 54-60.	2.3	5
42	Doubly Polarized QM/MM with Machine Learning Chaperone Polarizability. Journal of Chemical Theory and Computation, 2021, 17, 7682-7695.	2.3	5
43	Exploring Cycloreversion Reaction of Cyclobutane Pyrimidine Dimers Quantum Mechanically. Journal of Physical Chemistry A, 2019, 123, 2025-2039.	1.1	4
44	Replica exchange molecular dynamics simulations of an Î±/Î²-type small acid soluble protein (SASP). Biophysical Chemistry, 2013, 184, 17-21.	1.5	2
45	Interligand communication in a metal mediated LLâ€²CT system â€“ a case study. RSC Advances, 2021, 11, 24381-24386.	1.7	1