Junming Ho

List of Publications by Year
in descending order

79 papers	3,714 citations	159525 30 h-index	138417 58 g-index
88 all docs	88 docs citations	88 times ranked	4595 citing authors

#	Article	IF	Citations
1	Comment on the Correct Use of Continuum Solvent Models. Journal of Physical Chemistry A, 2010, 114, 13442-13444.	1.1	432
2	A universal approach for continuum solvent pK a calculations: are we there yet?. Theoretical Chemistry Accounts, 2010, 125, 3-21.	0.5	408
3	Computational electrochemistry: prediction of liquid-phase reduction potentials. Physical Chemistry Chemical Physics, 2014, 16, 15068-15106.	1.3	407
4	Are thermodynamic cycles necessary for continuum solvent calculation of pK_as and reduction potentials?. Physical Chemistry Chemical Physics, 2015, 17, 2859-2868.	1.3	166
5	Eigenvector centrality for characterization of protein allosteric pathways. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E12201-E12208.	3.3	145
6	Calculating Free Energy Changes in Continuum Solvation Models. Journal of Physical Chemistry B, 2016, 120, 1319-1329.	1.2	140
7	pK_a Calculation of Some Biologically Important Carbon Acids - An Assessment of Contemporary Theoretical Procedures. Journal of Chemical Theory and Computation, 2009, 5, 295-306.	2.3	131
8	Firstâ€principles prediction of acidities in the gas and solution phase. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 649-660.	6.2	94
9	Tryptamine Synthesis by Iron Porphyrin Catalyzed Câ˜H Functionalization of Indoles with Diazoacetonitrile. Angewandte Chemie - International Edition, 2019, 58, 3630-3634.	7.2	92
10	Predicting pKa in Implicit Solvents: Current Status and Future Directions. Australian Journal of Chemistry, 2014, 67, 1441.	0.5	91
11	Structureâ€“function relationships of donorâ€“acceptor Stenhouse adduct photochromic switches. Chemical Science, 2018, 9, 8242-8252.	3.7	89
12	Photoinduced Protonâ€Transfer Reactions for Mild Oâ€H Functionalization of Unreactive Alcohols. Angewandte Chemie - International Edition, 2020, 59, 5562-5566.	7.2	81
13	pH-Regulated Nonelectrogenic Anion Transport by Phenylthiosemicarbazones. Journal of the American Chemical Society, 2016, 138, 8301-8308.	6.6	75
14	Tropylium-promoted carbonylâ€“olefin metathesis reactions. Chemical Science, 2018, 9, 5145-5151.	3.7	68
15	Just add sugar forÂcarbohydrate induced self-assembly of curcumin. Nature Communications, 2019, 10, 582.	5.8	57
16	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
17	Harnessing entropy to direct the bonding/debonding of polymer systems based on reversible chemistry. Chemical Science, 2013, 4, 2752.	3.7	49
18	Accurate Line Shapes from Sub-1 cm^{â€“1} Resolution Sum Frequency Generation Vibrational Spectroscopy of Î±-Pinene at Room Temperature. Journal of Physical Chemistry A, 2015, 119, 1292-1302.	1.1	49

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19	Accuracy of DLPNO-CCSD(T): Effect of Basis Set and System Size. Journal of Physical Chemistry A, 2021, 125, 1553-1563.	1.1	48
20	First-Principles Prediction of the pK_as of Anti-inflammatory Oxicams. Journal of Physical Chemistry A, 2010, 114, 11992-12003.	1.1	44
21	N-Heterocyclic Olefin Catalyzed Silylation and Hydrosilylation Reactions of Hydroxyl and Carbonyl Compounds. Organic Letters, 2017, 19, 1398-1401.	2.4	43
22	Electron Transfer Assisted by Vibronic Coupling from Multiple Modes. Journal of Chemical Theory and Computation, 2017, 13, 6000-6009.	2.3	41
23	Quantum Chemical Prediction of Equilibrium Acidities of Ureas, Deltamides, Squaramides, and Croconamides. Journal of Organic Chemistry, 2017, 82, 10732-10736.	1.7	40
24	Chloroform as a Hydrogen Atom Donor in Barton Reductive Decarboxylation Reactions. Journal of Organic Chemistry, 2013, 78, 6677-6687.	1.7	39
25	Coreyâ€“Chaykovsky Reactions of Nitro Styrenes Enable cis-Configured Trifluoromethyl Cyclopropanes. Journal of Organic Chemistry, 2017, 82, 8220-8227.	1.7	39
26	Predicting Octanolâ€“Water Partition Coefficients: Are Quantum Mechanical Implicit Solvent Models Better than Empirical Fragment-Based Methods?. Journal of Physical Chemistry B, 2019, 123, 6810-6822.	1.2	38
27	Rhenium(I) tricarbonyl complexes of salicylaldehyde semicarbazones: Synthesis, crystal structures and cytotoxicity. Journal of Inorganic Biochemistry, 2013, 119, 10-20.	1.5	35
28	Deltamides and Croconamides: Expanding the Range of Dual Hâ€bond Donors for Selective Anion Recognition. Chemistry - A European Journal, 2018, 24, 1140-1150.	1.7	34
29	Tropylium Ion Catalyzes Hydration Reactions of Alkynes. European Journal of Organic Chemistry, 2018, 2018, 3974-3981.	1.2	33
30	â€œWaterâ€•nâ€Sugarâ€•Electrolytes Enable Ultrafast and Stable Electrochemical Naked Proton Storage. Small, 2021, 17, e2102375.	5.2	33
31	Nanosecond Dynamics Regulate the MIFâ€Induced Activity of CD74. Angewandte Chemie - International Edition, 2018, 57, 7116-7119.	7.2	32
32	Visibleâ€Light Photoswitching by Azobenzazoles. Chemistry - A European Journal, 2020, 26, 1103-1110.	1.7	32
33	Resolution and Improved Synthesis of (Â±)-Arsenicin A: A Natural Adamantane-Type Tetraarsenical Possessing Strong Anti-Acute Promelocytic Leukemia Cell Line Activity. Organometallics, 2012, 31, 1808-1816.	1.1	30
34	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
35	Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of Î±-Pinene on Silica. Journal of Physical Chemistry C, 2016, 120, 12578-12589.	1.5	29
36	Are Explicit Solvent Models More Accurate than Implicit Solvent Models? A Case Study on the Menschutkin Reaction. Journal of Physical Chemistry A, 2019, 123, 5580-5589.	1.1	26

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37	Hydrogenâ€Bond Disrupting Electrolytes for Fast and Stable Proton Batteries. Small, 2022, 18, e2201449.	5.2	26
38	Tripletâ€“triplet energy transfer in artificial and natural photosynthetic antennas. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5513-E5521.	3.3	24
39	How accurate are approximate quantum chemical methods at modelling soluteâ€“solvent interactions in solvated clusters?. Physical Chemistry Chemical Physics, 2020, 22, 3855-3866.	1.3	24
40	NHCâ€Catalyzed Metathesis and Phosphorylation Reactions of Disulfides: Development and Mechanistic Insights. Chemistry - A European Journal, 2017, 23, 6259-6263.	1.7	22
41	Halide Anion Triggered Reactions of Michael Acceptors with Tropylium Ion. Angewandte Chemie - International Edition, 2020, 59, 1455-1459.	7.2	22
42	Anion Binding Affinity: Acidity versus Conformational Effects. Journal of Organic Chemistry, 2020, 85, 8074-8084.	1.7	20
43	The Distal Effect of Electron-Withdrawing Groups and Hydrogen Bonding on the Stability of Peptide Enolates. Journal of the American Chemical Society, 2010, 132, 5515-5521.	6.6	19
44	Protonated Alcohols Are Examples of Complete Charge-Shift Bonds. Journal of Organic Chemistry, 2014, 79, 9998-10001.	1.7	19
45	Synthesis of (Â±)â€Panduratin A and Related Natural Products Using the High Pressure Dielsâ€“Alder Reaction. Asian Journal of Organic Chemistry, 2013, 2, 60-63.	1.3	17
46	MoD-QM/MM Structural Refinement Method: Characterization of Hydrogen Bonding in the Oxytricha nova G-Quadruplex. Journal of Chemical Theory and Computation, 2014, 10, 5125-5135.	2.3	16
47	Eisenporphyrinâ€katalysierte Câ€Hâ€Funktionalisierung von Indol mit Diazoacetonitril fÃ¼r die Synthese von Tryptaminen. Angewandte Chemie, 2019, 131, 3669-3673.	1.6	16
48	Unanticipated Stickiness of Î±-Pinene. Journal of Physical Chemistry A, 2017, 121, 3239-3246.	1.1	14
49	Do Better Quality Embedding Potentials Accelerate the Convergence of QM/MM Models? The Case of Solvated Acid Clusters. Molecules, 2018, 23, 2466.	1.7	11
50	Techniques For Studies Of Electrochemical Reactions In Solution. , 2015, , 117-188.		10
51	Photoinduzierte Protonentransferreaktionen fÃ¼r milde Oâ€Hâ€Funktionalisierungsreaktionen unreaktiver Alkohole. Angewandte Chemie, 2020, 132, 5608-5613.	1.6	10
52	Validation of the Distal Effect of Electron-Withdrawing Groups on the Stability of Peptide Enolates and Its Exploitation in the Controlled Stereochemical Inversion of Amino Acid Derivatives. Journal of Organic Chemistry, 2011, 76, 5907-5914.	1.7	9
53	Evaluation of a chiral cubane-based Schiff base ligand in asymmetric catalysis reactions. Beilstein Journal of Organic Chemistry, 2012, 8, 1814-1818.	1.3	9
54	Explanation of Substituent Effects on the Enolization of Î²-Diketones and Î²-Ketoesters. Journal of Chemical Education, 2021, 98, 1043-1048.	1.1	9

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55	Accurate Quantum Chemical Prediction of Gas-Phase Anion Binding Affinities and Their Structure-Binding Relationships. Journal of Physical Chemistry A, 2021, 125, 9838-9851.	1.1	9
56	The Distal Effect of N-Electron-withdrawing Groups on the Stability of Peptide Carbon Radicals. Australian Journal of Chemistry, 2011, 64, 403.	0.5	8
57	Rigid Body Brownian Dynamics as a Tool for Studying Ion Channel Blockers. Journal of Physical Chemistry B, 2012, 116, 1933-1941.	1.2	8
58	On the mechanism of protein supercharging in electrospray ionisation mass spectrometry: Effects on charging of additives with short- and long-chain alkyl constituents with carbonate and sulphite terminal groups. Analytica Chimica Acta: X, 2019, 1, 100004.	2.8	8
59	Diaminomethylenemalononitriles and Diaminomethyleneindanediones as Dual Hydrogen Bond Donors for Anion Recognition. Journal of Organic Chemistry, 2021, 86, 4957-4964.	1.7	8
60	On the Accuracy of QM/MM Models: A Systematic Study of Intramolecular Proton Transfer Reactions of Amino Acids in Water. Journal of Physical Chemistry B, 2021, 125, 9304-9316.	1.2	8
61	Reversible Cyclopropane Ring-Cleavage Reactions within Etheno-Bridged [4.3.1]Propelladiene Frameworks Leading to Aza- and Oxa-[5.6.5.6]fenestratetraenes. Chemistry - A European Journal, 2012, 18, 13585-13588.	1.7	7
62	Mechanistic Studies on the Base-Promoted Conversion of Alkoxy-Substituted, Ring-Fused gem-Dihalocyclopropanes into Furans: Evidence for a Process Involving Electrocyclic Ring Closure of a Carbonyl Ylide Intermediate. Journal of Organic Chemistry, 2018, 83, 13678-13690.	1.7	7
63	Electronic Structure and Tripletâ€“Triplet Energy Transfer in Artificial Photosynthetic Antennas. Photochemistry and Photobiology, 2019, 95, 211-219.	1.3	7
64	Nontargeted Identification of Plasma Proteins O-, N-, and S-Transmethylated by O-Methyl Organophosphates. Analytical Chemistry, 2020, 92, 15420-15428.	3.2	7
65	Approximating Coupled Cluster Level Vibrational Frequencies with Composite Methods. Journal of Physical Chemistry A, 2006, 110, 2796-2800.	1.1	6
66	Assessment of several machine learning methods towards reliable prediction of hormone receptor binding affinity. Chemical Data Collections, 2017, 9-10, 114-124.	1.1	6
67	Probing the remarkable thermal kinetics of visual rhodopsin with E181Q and S186A mutants. Journal of Chemical Physics, 2017, 146, 215104.	1.2	6
68	Origin and Prediction of Highly Specific Bond Cleavage Sites in the Thermal Activation of Intact Protein Ions. Chemistry - A European Journal, 2019, 25, 823-834.	1.7	6
69	Polyphenylglyoxamide-Based Amphiphilic Small Molecular Peptidomimetics as Antibacterial Agents with Anti-Biofilm Activity. International Journal of Molecular Sciences, 2021, 22, 7344.	1.8	6
70	Predicting Octanolâ€“Water Partition Coefficients of Fluorinated Drug-Like Molecules: A Combined Experimental and Theoretical Study. Australian Journal of Chemistry, 2020, 73, 677.	0.5	6
71	Peptidomimetic Star Polymers for Targeting Biological Ion Channels. PLoS ONE, 2016, 11, e0152169.	1.1	5
72	The MOD-QM/MM Method. Methods in Enzymology, 2016, 577, 443-481.	0.4	4

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73	Substituent effects in solid-state assembly of activated benzotriazoles. CrystEngComm, 2019, 21, 835-842.	1.3	4
74	Halide Anion Triggered Reactions of Michael Acceptors with Tropylium Ion. Angewandte Chemie, 2020, 132, 1471-1475.	1.6	4
75	Accelerating the Calculation of Soluteâ€“Solvent Interaction Energies through Systematic Molecular Fragmentation. Journal of Physical Chemistry A, 2019, 123, 8476-8484.	1.1	3
76	Sugar-substituted fluorous 1,2,3-triazoles: Helical twists in fluoroalkyl chains and their molecular association in the solid state and correlations with physicochemical properties. Journal of Fluorine Chemistry, 2020, 236, 109536.	0.9	3
77	Nanosecond Dynamics Regulate the MIFâ€Induced Activity of CD74. Angewandte Chemie, 2018, 130, 7234-7237.	1.6	2
78	The Effect of Vicinal Difluorination on the Conformation and Potency of Histone Deacetylase Inhibitors. Molecules, 2021, 26, 3974.	1.7	1
79	Development of an Albuminâ€“Polymer Bioconjugate via Covalent Conjugation and Supramolecular Interactions. Bioconjugate Chemistry, 2022, 33, 321-332.	1.8	1