Junming Ho

List of Publications by Year in Descending Order

76 papers	2,695 citations	25 h-index	51 g-index
88 ext. papers	3,237 ext. citations	5.4 avg, IF	5.81 L-index

#	Paper	IF	Citations
76	Hydrogen-Bond Disrupting Electrolytes for Fast and Stable Proton Batteries.. *Small*, **2022**, e2201449	11	4
75	Accurate Quantum Chemical Prediction of Gas-Phase Anion Binding Affinities and Their Structure-Binding Relationships. *Journal of Physical Chemistry A*, **2021**, 125, 9838-9851	2.8	2
74	Diaminomethylenemalononitriles and Diaminomethyleneindanediones as Dual Hydrogen Bond Donors for Anion Recognition. *Journal of Organic Chemistry*, **2021**, 86, 4957-4964	4.2	5
73	Explanation of Substituent Effects on the Enolization of -Diketones and -Ketoesters. *Journal of Chemical Education*, **2021**, 98, 1043-1048	2.4	1
72	Accuracy of DLPNO-CCSD(T): Effect of Basis Set and System Size. *Journal of Physical Chemistry A*, **2021**, 125, 1553-1563	2.8	12
71	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	3.4	1
70	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
69	"Water-in-Sugar" Electrolytes Enable Ultrafast and Stable Electrochemical Naked Proton Storage. *Small*, **2021**, 17, e2102375	11	5
68	Anion Binding Affinity: Acidity versus Conformational Effects. *Journal of Organic Chemistry*, **2020**, 85, 8074-8084	4.2	12
67	How accurate are approximate quantum chemical methods at modelling solute-solvent interactions in solvated clusters?. *Physical Chemistry Chemical Physics*, **2020**, 22, 3855-3866	3.6	13
66	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	2.1	1
65	Predicting Octanol–Water Partition Coefficients of Fluorinated Drug-Like Molecules: A Combined Experimental and Theoretical Study. *Australian Journal of Chemistry*, **2020**, 73, 677	1.2	4
64	Halide Anion Triggered Reactions of Michael Acceptors with Tropylium Ion. *Angewandte Chemie*, **2020**, 132, 1471-1475	3.6	2
63	Halide Anion Triggered Reactions of Michael Acceptors with Tropylium Ion. *Angewandte Chemie - International Edition*, **2020**, 59, 1455-1459	16.4	18
62	Photoinduced Proton-Transfer Reactions for Mild O-H Functionalization of Unreactive Alcohols. *Angewandte Chemie - International Edition*, **2020**, 59, 5562-5566	16.4	50
61	Photoinduzierte Protonentransferreaktionen für milde O-H-Funktionalisierungsreaktionen unreaktiver Alkohole. *Angewandte Chemie*, **2020**, 132, 5608-5613	3.6	4
60	Visible-Light Photoswitching by Azobenzazoles. *Chemistry - A European Journal*, **2020**, 26, 1103-1110	4.8	16

59	Nontargeted Identification of Plasma Proteins O-, N-, and S-Transmethylated by O-Methyl Organophosphates. *Analytical Chemistry*, **2020**, 92, 15420-15428	7.8	2
58	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
57	Accelerating the Calculation of Solute-Solvent Interaction Energies through Systematic Molecular Fragmentation. *Journal of Physical Chemistry A*, **2019**, 123, 8476-8484	2.8	2
56	Substituent effects in solid-state assembly of activated benzotriazoles. *CrystEngComm*, **2019**, 21, 835-842	3.3	4
55	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	2.8	17
54	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	2.2	3
53	Just add sugar for carbohydrate induced self-assembly of curcumin. *Nature Communications*, **2019**, 10, 582	17.4	30
52	Electronic Structure and Triplet-Triplet Energy Transfer in Artificial Photosynthetic Antennas. *Photochemistry and Photobiology*, **2019**, 95, 211-219	3.6	6
51	Predicting Octanol-Water Partition Coefficients: Are Quantum Mechanical Implicit Solvent Models Better than Empirical Fragment-Based Methods?. *Journal of Physical Chemistry B*, **2019**, 123, 6810-6822	3.4	22
50	Eisenporphyrin-katalysierte C-H-Funktionalisierung von Indol mit Diazoacetonitril für die Synthese von Tryptaminen. *Angewandte Chemie*, **2019**, 131, 3669-3673	3.6	11
49	Tryptamine Synthesis by Iron Porphyrin Catalyzed C-H Functionalization of Indoles with Diazoacetonitrile. *Angewandte Chemie - International Edition*, **2019**, 58, 3630-3634	16.4	59
48	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	4.8	5
47	Tropylium Ion Catalyzes Hydration Reactions of Alkynes. *European Journal of Organic Chemistry*, **2018**, 2018, 3974-3981	3.2	24
46	Nanosecond Dynamics Regulate the MIF-Induced Activity of CD74. *Angewandte Chemie - International Edition*, **2018**, 57, 7116-7119	16.4	23
45	Tropylium-promoted carbonyl-olefin metathesis reactions. *Chemical Science*, **2018**, 9, 5145-5151	9.4	50
44	Nanosecond Dynamics Regulate the MIF-Induced Activity of CD74. *Angewandte Chemie*, **2018**, 130, 7234-7237	3.6	2
43	Deltamides and Croconamides: Expanding the Range of Dual H-bond Donors for Selective Anion Recognition. *Chemistry - A European Journal*, **2018**, 24, 1140-1150	4.8	20
42	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	11.5	72

41	Do Better Quality Embedding Potentials Accelerate the Convergence of QM/MM Models? The Case of Solvated Acid Clusters. *Molecules*, **2018**, 23,	4.8	7
40	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	4.2	4
39	Structure-function relationships of donor-acceptor Stenhouse adduct photochromic switches. *Chemical Science*, **2018**, 9, 8242-8252	9.4	60
38	N-Heterocyclic Olefin Catalyzed Silylation and Hydrosilylation Reactions of Hydroxyl and Carbonyl Compounds. *Organic Letters*, **2017**, 19, 1398-1401	6.2	29
37	NHC-Catalyzed Metathesis and Phosphorylation Reactions of Disulfides: Development and Mechanistic Insights. *Chemistry - A European Journal*, **2017**, 23, 6259-6263	4.8	12
36	Assessment of several machine learning methods towards reliable prediction of hormone receptor binding affinity. *Chemical Data Collections*, **2017**, 9-10, 114-124	2.1	4
35	Corey-Chaykovsky Reactions of Nitro Styrenes Enable cis-Configured Trifluoromethyl Cyclopropanes. *Journal of Organic Chemistry*, **2017**, 82, 8220-8227	4.2	32
34	Probing the remarkable thermal kinetics of visual rhodopsin with E181Q and S186A mutants. *Journal of Chemical Physics*, **2017**, 146, 215104	3.9	6
33	Unanticipated Stickiness of β-Pinene. *Journal of Physical Chemistry A*, **2017**, 121, 3239-3246	2.8	11
32	Quantum Chemical Prediction of Equilibrium Acidities of Ureas, Deltamides, Squaramides, and Croconamides. *Journal of Organic Chemistry*, **2017**, 82, 10732-10736	4.2	29
31	Electron Transfer Assisted by Vibronic Coupling from Multiple Modes. *Journal of Chemical Theory and Computation*, **2017**, 13, 6000-6009	6.4	28
30	Triplet-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	11.5	17
29	pH-Regulated Nonelectrogenic Anion Transport by Phenylthiosemicarbazones. *Journal of the American Chemical Society*, **2016**, 138, 8301-8	16.4	58
28	Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of β-Pinene on Silica. *Journal of Physical Chemistry C*, **2016**, 120, 12578-12589	4.8	18
27	Calculating Free Energy Changes in Continuum Solvation Models. *Journal of Physical Chemistry B*, **2016**, 120, 1319-29	3.4	108
26	Peptidomimetic Star Polymers for Targeting Biological Ion Channels. *PLoS ONE*, **2016**, 11, e0152169	3.7	5
25	The MOD-QM/MM Method: Applications to Studies of Photosystem II and DNA G-Quadruplexes. *Methods in Enzymology*, **2016**, 577, 443-81	1.7	4
24	Are thermodynamic cycles necessary for continuum solvent calculation of pKas and reduction potentials?. *Physical Chemistry Chemical Physics*, **2015**, 17, 2859-68	3.6	138

23	Techniques For Studies Of Electrochemical Reactions In Solution **2015**, 117-188		8
22	Accurate line shapes from sub-1 cm(-1) resolution sum frequency generation vibrational spectroscopy of □-pinene at room temperature. *Journal of Physical Chemistry A*, **2015**, 119, 1292-302	2.8	42
21	Protonated alcohols are examples of complete charge-shift bonds. *Journal of Organic Chemistry*, **2014**, 79, 9998-10001	4.2	18
20	MoD-QM/MM Structural Refinement Method: Characterization of Hydrogen Bonding in the Oxytricha nova G-Quadruplex. *Journal of Chemical Theory and Computation*, **2014**, 10, 5125-35	6.4	14
19	Computational electrochemistry: prediction of liquid-phase reduction potentials. *Physical Chemistry Chemical Physics*, **2014**, 16, 15068-106	3.6	311
18	Predicting pKa in Implicit Solvents: Current Status and Future Directions. *Australian Journal of Chemistry*, **2014**, 67, 1441	1.2	71
17	Rhenium(I) tricarbonyl complexes of salicylaldehyde semicarbazones: synthesis, crystal structures and cytotoxicity. *Journal of Inorganic Biochemistry*, **2013**, 119, 10-20	4.2	34
16	Synthesis of (□)-Panduratin A and Related Natural Products Using the High Pressure Diels□Alder Reaction. *Asian Journal of Organic Chemistry*, **2013**, 2, 60-63	3	11
15	Harnessing entropy to direct the bonding/debonding of polymer systems based on reversible chemistry. *Chemical Science*, **2013**, 4, 2752	9.4	41
14	Chloroform as a hydrogen atom donor in Barton reductive decarboxylation reactions. *Journal of Organic Chemistry*, **2013**, 78, 6677-87	4.2	31
13	Resolution and Improved Synthesis of (□)-Arsenicin A: A Natural Adamantane-Type Tetraarsenical Possessing Strong Anti-Acute Promelocytic Leukemia Cell Line Activity. *Organometallics*, **2012**, 31, 1808-1816	3.8	26
12	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, 13585-8	4.8	7
11	Evaluation of a chiral cubane-based Schiff base ligand in asymmetric catalysis reactions. *Beilstein Journal of Organic Chemistry*, **2012**, 8, 1814-8	2.5	8
10	Rigid body Brownian dynamics as a tool for studying ion channel blockers. *Journal of Physical Chemistry B*, **2012**, 116, 1933-41	3.4	8
9	The Distal Effect of N-Electron-withdrawing Groups on the Stability of Peptide Carbon Radicals. *Australian Journal of Chemistry*, **2011**, 64, 403	1.2	8
8	First-principles prediction of acidities in the gas and solution phase. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 649-660	7.9	80
7	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, 5907-14	4.2	7
6	The distal effect of electron-withdrawing groups and hydrogen bonding on the stability of peptide enolates. *Journal of the American Chemical Society*, **2010**, 132, 5515-21	16.4	15

5	First-principles prediction of the pK(a)s of anti-inflammatory oxicams. *Journal of Physical Chemistry A*, **2010**, 114, 11992-2003	2.8	38
4	Comment on the correct use of continuum solvent models. *Journal of Physical Chemistry A*, **2010**, 114, 13442-4	2.8	326
3	A universal approach for continuum solvent pK a calculations: are we there yet?. *Theoretical Chemistry Accounts*, **2010**, 125, 3-21	1.9	359
2	pKa Calculation of Some Biologically Important Carbon Acids - An Assessment of Contemporary Theoretical Procedures. *Journal of Chemical Theory and Computation*, **2009**, 5, 295-306	6.4	121
1	Approximating coupled cluster level vibrational frequencies with composite methods. *Journal of Physical Chemistry A*, **2006**, 110, 2796-800	2.8	3