

Junming Ho

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	A universal approach for continuum solvent pK _a calculations: are we there yet?. <i>Theoretical Chemistry Accounts</i> , 2010 , 125, 3-21	1.9	359
75	Comment on the correct use of continuum solvent models. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 13442-4	2.8	326
74	Computational electrochemistry: prediction of liquid-phase reduction potentials. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 15068-106	3.6	311
73	Are thermodynamic cycles necessary for continuum solvent calculation of pK _a s and reduction potentials?. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 2859-68	3.6	138
72	pK _a Calculation of Some Biologically Important Carbon Acids - An Assessment of Contemporary Theoretical Procedures. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 295-306	6.4	121
71	Calculating Free Energy Changes in Continuum Solvation Models. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 1319-29	3.4	108
70	First-principles prediction of acidities in the gas and solution phase. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011 , 1, 649-660	7.9	80
69	Eigenvector centrality for characterization of protein allosteric pathways. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E12201-E12208	11.5	72
68	Predicting pK _a in Implicit Solvents: Current Status and Future Directions. <i>Australian Journal of Chemistry</i> , 2014 , 67, 1441	1.2	71
67	Structure-function relationships of donor-acceptor Stenhouse adduct photochromic switches. <i>Chemical Science</i> , 2018 , 9, 8242-8252	9.4	60
66	Tryptamine Synthesis by Iron Porphyrin Catalyzed C-H Functionalization of Indoles with Diazoacetonitrile. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 3630-3634	16.4	59
65	pH-Regulated Nonelectrogenic Anion Transport by Phenylthiosemicarbazones. <i>Journal of the American Chemical Society</i> , 2016 , 138, 8301-8	16.4	58
64	Tropylium-promoted carbonyl-olefin metathesis reactions. <i>Chemical Science</i> , 2018 , 9, 5145-5151	9.4	50
63	Photoinduced Proton-Transfer Reactions for Mild O-H Functionalization of Unreactive Alcohols. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 5562-5566	16.4	50
62	Accurate line shapes from sub-1 cm ⁻¹ resolution sum frequency generation vibrational spectroscopy of β -pinene at room temperature. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1292-302	2.8	42
61	Harnessing entropy to direct the bonding/debonding of polymer systems based on reversible chemistry. <i>Chemical Science</i> , 2013 , 4, 2752	9.4	41
60	First-principles prediction of the pK _a (s) of anti-inflammatory oxicams. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 11992-2003	2.8	38

59	Rhenium(I) tricarbonyl complexes of salicylaldehyde semicarbazones: synthesis, crystal structures and cytotoxicity. <i>Journal of Inorganic Biochemistry</i> , 2013 , 119, 10-20	4.2	34
58	Corey-Chaykovsky Reactions of Nitro Styrenes Enable cis-Configured Trifluoromethyl Cyclopropanes. <i>Journal of Organic Chemistry</i> , 2017 , 82, 8220-8227	4.2	32
57	Chloroform as a hydrogen atom donor in Barton reductive decarboxylation reactions. <i>Journal of Organic Chemistry</i> , 2013 , 78, 6677-87	4.2	31
56	Just add sugar for carbohydrate induced self-assembly of curcumin. <i>Nature Communications</i> , 2019 , 10, 582	17.4	30
55	N-Heterocyclic Olefin Catalyzed Silylation and Hydrosilylation Reactions of Hydroxyl and Carbonyl Compounds. <i>Organic Letters</i> , 2017 , 19, 1398-1401	6.2	29
54	Quantum Chemical Prediction of Equilibrium Acidities of Ureas, Deltamides, Squaramides, and Croconamides. <i>Journal of Organic Chemistry</i> , 2017 , 82, 10732-10736	4.2	29
53	Electron Transfer Assisted by Vibronic Coupling from Multiple Modes. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 6000-6009	6.4	28
52	Resolution and Improved Synthesis of (E)-Arsenicin A: A Natural Adamantane-Type Tetraarsenical Possessing Strong Anti-Acute Promyelocytic Leukemia Cell Line Activity. <i>Organometallics</i> , 2012 , 31, 1808-1816	3.8	26
51	Tropylium Ion Catalyzes Hydration Reactions of Alkynes. <i>European Journal of Organic Chemistry</i> , 2018 , 2018, 3974-3981	3.2	24
50	Nanosecond Dynamics Regulate the MIF-Induced Activity of CD74. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 7116-7119	16.4	23
49	Predicting Octanol-Water Partition Coefficients: Are Quantum Mechanical Implicit Solvent Models Better than Empirical Fragment-Based Methods?. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 6810-6822	3.4	22
48	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
47	Deltamides and Croconamides: Expanding the Range of Dual H-bond Donors for Selective Anion Recognition. <i>Chemistry - A European Journal</i> , 2018 , 24, 1140-1150	4.8	20
46	Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulations Reveal a Rotationally Fluid Adsorption State of β -Pinene on Silica. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 12578-12589	2.8	18
45	Protonated alcohols are examples of complete charge-shift bonds. <i>Journal of Organic Chemistry</i> , 2014 , 79, 9998-10001	4.2	18
44	Halide Anion Triggered Reactions of Michael Acceptors with Tropylium Ion. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 1455-1459	16.4	18
43	Are Explicit Solvent Models More Accurate than Implicit Solvent Models? A Case Study on the Menschutkin Reaction. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 5580-5589	2.8	17
42	Triplet-triplet energy transfer in artificial and natural photosynthetic antennas. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, E5513-E5521	11.5	17

41	Visible-Light Photoswitching by Azobenzazoles. <i>Chemistry - A European Journal</i> , 2020 , 26, 1103-1110	4.8	16
40	The distal effect of electron-withdrawing groups and hydrogen bonding on the stability of peptide enolates. <i>Journal of the American Chemical Society</i> , 2010 , 132, 5515-21	16.4	15
39	MoD-QM/MM Structural Refinement Method: Characterization of Hydrogen Bonding in the Oxytricha nova G-Quadruplex. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 5125-35	6.4	14
38	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
37	How accurate are approximate quantum chemical methods at modelling solute-solvent interactions in solvated clusters?. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 3855-3866	3.6	13
36	NHC-Catalyzed Metathesis and Phosphorylation Reactions of Disulfides: Development and Mechanistic Insights. <i>Chemistry - A European Journal</i> , 2017 , 23, 6259-6263	4.8	12
35	Anion Binding Affinity: Acidity versus Conformational Effects. <i>Journal of Organic Chemistry</i> , 2020 , 85, 8074-8084	4.2	12
34	Accuracy of DLPNO-CCSD(T): Effect of Basis Set and System Size. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 1553-1563	2.8	12
33	Unanticipated Stickiness of β -Pinene. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 3239-3246	2.8	11
32	Synthesis of (β)-Panduratin A and Related Natural Products Using the High Pressure Diels-Alder Reaction. <i>Asian Journal of Organic Chemistry</i> , 2013 , 2, 60-63	3	11
31	Eisenporphyrin-katalysierte C-H-Funktionalisierung von Indol mit Diazoacetonitril ff die Synthese von Tryptaminen. <i>Angewandte Chemie</i> , 2019 , 131, 3669-3673	3.6	11
30	Techniques For Studies Of Electrochemical Reactions In Solution 2015 , 117-188		8
29	Evaluation of a chiral cubane-based Schiff base ligand in asymmetric catalysis reactions. <i>Beilstein Journal of Organic Chemistry</i> , 2012 , 8, 1814-8	2.5	8
28	Rigid body Brownian dynamics as a tool for studying ion channel blockers. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 1933-41	3.4	8
27	The Distal Effect of N-Electron-withdrawing Groups on the Stability of Peptide Carbon Radicals. <i>Australian Journal of Chemistry</i> , 2011 , 64, 403	1.2	8
26	Reversible cyclopropane ring-cleavage reactions within etheno-bridged [4.3.1]propelladiene frameworks leading to aza- and oxa-[5.6.5.6]fenestratetraenes. <i>Chemistry - A European Journal</i> , 2012 , 18, 13585-8	4.8	7
25	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. <i>Journal of Organic Chemistry</i> , 2011 , 76, 5907-14	4.2	7
24	Do Better Quality Embedding Potentials Accelerate the Convergence of QM/MM Models? The Case of Solvated Acid Clusters. <i>Molecules</i> , 2018 , 23,	4.8	7

23	Probing the remarkable thermal kinetics of visual rhodopsin with E181Q and S186A mutants. <i>Journal of Chemical Physics</i> , 2017 , 146, 215104	3.9	6
22	Electronic Structure and Triplet-Triplet Energy Transfer in Artificial Photosynthetic Antennas. <i>Photochemistry and Photobiology</i> , 2019 , 95, 211-219	3.6	6
21	Peptidomimetic Star Polymers for Targeting Biological Ion Channels. <i>PLoS ONE</i> , 2016 , 11, e0152169	3.7	5
20	Diaminomethylenemalononitriles and Diaminomethyleneindanediones as Dual Hydrogen Bond Donors for Anion Recognition. <i>Journal of Organic Chemistry</i> , 2021 , 86, 4957-4964	4.2	5
19	Origin and Prediction of Highly Specific Bond Cleavage Sites in the Thermal Activation of Intact Protein Ions. <i>Chemistry - A European Journal</i> , 2019 , 25, 823-834	4.8	5
18	"Water-in-Sugar" Electrolytes Enable Ultrafast and Stable Electrochemical Naked Proton Storage. <i>Small</i> , 2021 , 17, e2102375	11	5
17	Assessment of several machine learning methods towards reliable prediction of hormone receptor binding affinity. <i>Chemical Data Collections</i> , 2017 , 9-10, 114-124	2.1	4
16	Substituent effects in solid-state assembly of activated benzotriazoles. <i>CrystEngComm</i> , 2019 , 21, 835-843	3.3	4
15	Predicting Octanol/Water Partition Coefficients of Fluorinated Drug-Like Molecules: A Combined Experimental and Theoretical Study. <i>Australian Journal of Chemistry</i> , 2020 , 73, 677	1.2	4
14	Photoinduzierte Protonentransferreaktionen ff milde O-H-Funktionalisierungsreaktionen unreaktiver Alkohole. <i>Angewandte Chemie</i> , 2020 , 132, 5608-5613	3.6	4
13	The MOD-QM/MM Method: Applications to Studies of Photosystem II and DNA G-Quadruplexes. <i>Methods in Enzymology</i> , 2016 , 577, 443-81	1.7	4
12	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. <i>Journal of Organic Chemistry</i> , 2018 , 83, 13678-13690	4.2	4
11	Hydrogen-Bond Disrupting Electrolytes for Fast and Stable Proton Batteries.. <i>Small</i> , 2022 , e2201449	11	4
10	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. <i>Analytica Chimica Acta: X</i> , 2019 , 1, 100004	2.2	3
9	Approximating coupled cluster level vibrational frequencies with composite methods. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 2796-800	2.8	3
8	Accelerating the Calculation of Solute-Solvent Interaction Energies through Systematic Molecular Fragmentation. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 8476-8484	2.8	2
7	Nanosecond Dynamics Regulate the MIF-Induced Activity of CD74. <i>Angewandte Chemie</i> , 2018 , 130, 7234-7237	3.2	2
6	Accurate Quantum Chemical Prediction of Gas-Phase Anion Binding Affinities and Their Structure-Binding Relationships. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 9838-9851	2.8	2

5	Halide Anion Triggered Reactions of Michael Acceptors with Tropylium Ion. <i>Angewandte Chemie</i> , 2020 , 132, 1471-1475	3.6	2
4	Nontargeted Identification of Plasma Proteins O-, N-, and S-Transmethylated by O-Methyl Organophosphates. <i>Analytical Chemistry</i> , 2020 , 92, 15420-15428	7.8	2
3	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. <i>Journal of Fluorine Chemistry</i> , 2020 , 236, 109536	2.1	1
2	Explanation of Substituent Effects on the Enolization of β -Diketones and β -Ketoesters. <i>Journal of Chemical Education</i> , 2021 , 98, 1043-1048	2.4	1
1	On the Accuracy of QM/MM Models: A Systematic Study of Intramolecular Proton Transfer Reactions of Amino Acids in Water. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 9304-9316	3.4	1