Chin-Hui Yu

List of Publications by Year
in descending order

38	513	759233 12	713466 21
papers	citations	h-index	g-index

38	38	38	663
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Extended ab initio studies of the vinylideneâ€“acetylene rearrangement. Journal of Chemical Physics, 1997, 106, 3237-3242.	3.0	88
2	Enantiodivergent Steglich rearrangement of O-carboxylazlactones catalyzed by a chirality switchable helicene containing a 4-aminopyridine unit. Chemical Science, 2017, 8, 524-529.	7.4	54
3	Density Functional Study of Bergman Cyclization of Enediynes. Journal of Physical Chemistry A, 1998, 102, 2584-2593.	2.5	43
4	Computations in Treating Fullerenes and Carbon Aggregates. Reviews in Computational Chemistry, 2007, , 1-62.	1.5	42
5	THE COOPERATIVITY BETWEEN HYDROGEN AND HALOGEN BONDS. Journal of Theoretical and Computational Chemistry, 2008, 07, 13-35.	1.8	33
6	A computational study of unique properties of pillar[n]quinones: Selfâ€assembly to tubular structures and potential applications as electron acceptors and anion recognizers. Journal of Computational Chemistry, 2011, 32, 2716-2726.	3.3	30
7	A MNDO study of carbon clusters with specifically fitted parameters. Theoretica Chimica Acta, 1995, 92, 269-280.	0.8	19
8	A computational study of the activation of allenoates by Lewis bases and the reactivity of intermediate adducts. Organic and Biomolecular Chemistry, 2014, 12, 7297.	2.8	19
9	Production of HCO from propenal photolyzed at 193 nm: Relaxation of excited states and distribution of internal states of fragment HCO. Journal of Chemical Physics, 2001, 114, 8964-8970.	3.0	18
10	Photoionization efficiency spectrum and ionization energy of HSO studied by discharge flow-photoionization mass spectrometry. Journal of Chemical Physics, 1997, 106, 9727-9733.	3.0	14
11	Stereochemical Course of Wittig Rearrangements of Dihydropyran Allyl Propargyl Ethers. Journal of Organic Chemistry, 2015, 80, 6222-6237.	3.2	14
12	Intermediate oxiranes in the base-catalyzed depolymerisation of lignin. Green Chemistry, 2016, 18, 1590-1596.	9.0	14
13	Ionization energy of HSSH. Journal of Chemical Physics, 1997, 107, 5273-5274.	3.0	11
14	The potential energy surface of excited states by time-dependent density functional theory: The reaction of sulfur atom and nitrogen dioxide. Journal of Chemical Physics, 2001, 115, 7495-7502.	3.0	11
15	The relationship between the energy of activation for the proton-movement and the difference in proton affinities of bonded partners in double well hydrogen bonds. Chemical Physics Letters, 2006, 424, 264-267.	2.6	11
16	The relationship between the bond length and the difference in proton affinities for the observation of heteronuclear low barrier hydrogen bonds. Chemical Physics Letters, 2007, 433, 275-278.	2.6	10
17	Stereocontrolled Synthesis of Functionalized Bicyclic Î±-Methylene Butyrolactones via Tungsten-Mediated Intramolecular Allylation of Aldehydes. Journal of Organic Chemistry, 1999, 64, 7552-7558.	3.2	9
18	Photoionization efficiency spectrum and ionization energy of C2H5SO. Journal of Chemical Physics, 1997, 107, 8794-8799.	3.0	7

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19	Computational Study of the Degradation of S-Adenosyl Methionine in Water. Journal of Physical Chemistry A, 2017, 121, 505-514.	2.5	7
20	Photoionization spectrum and ionization energy of CH3SCl. Journal of Chemical Physics, 1999, 110, 4757-4762.	3.0	6
21	Analytical fittings for the global potential energy surface of the ground state of methylene. Journal of Chemical Physics, 2003, 118, 582-594.	3.0	6
22	A theoretical study of the nornicotine-catalyzed Mannich reaction in wet solvents and water. Green Chemistry, 2014, 16, 3999-4008.	9.0	6
23	Photoionization study of CH3SCH2Cl formed in the reaction system Cl/Cl2/CH3SCH3. Journal of Chemical Physics, 2001, 114, 4817-4823.	3.0	5
24	Solvent effects on the intramolecular conversion of trimethylsulfonium chloride to dimethyl sulfide and methyl chloride. Physical Chemistry Chemical Physics, 2014, 16, 26658-26671.	2.8	5
25	The NHN⁺ hydrogen bridge between 4,5â€dihydroâ€1Hâ€imidazole and various amines. International Journal of Quantum Chemistry, 2009, 109, 2286-2296.	2.0	4
26	Turning Low Barrier Hydrogen Bonds on and Off. Journal of the Chinese Chemical Society, 2010, 57, 671-676.	1.4	4
27	Benchmarks of the PC-UNIX Computer with Electronic Structure Calculation. Journal of Chemical Information and Computer Sciences, 1997, 37, 1111-1114.	2.8	3
28	Photoionization-efficiency spectrum and ionization energy of C2H5SCl. Journal of Chemical Physics, 1999, 111, 10093-10098.	3.0	3
29	A model study of the efficiency of the Aspâ€“Hisâ€“Ser triad. Journal of Computational Chemistry, 2010, 31, 1853-1859.	3.3	3
30	Substituent effects in the Nicholas epimerization of glycosides. Journal of Physical Organic Chemistry, 2018, 31, e3780.	1.9	3
31	Computational Evidence for Homonuclear Ge^IGe^I Dative Bonds. Journal of Physical Chemistry A, 2020, 124, 3795-3804.	2.5	3
32	A Computational Study of the Promiscuity of the SAM-Dependent Methyltransferase AtHTMT1. ACS Omega, 2022, 7, 12753-12764.	3.5	3
33	A Multiâ€Center Energy Analysis of the Tunable Proton Affinity of Hydrogen Bonded Cluster Ions. Journal of the Chinese Chemical Society, 2009, 56, 80-88.	1.4	2
34	Interstitial water and the formation of low barrier hydrogen bonds: A computational model study. International Journal of Quantum Chemistry, 2012, 112, 1460-1472.	2.0	2
35	Evaluation of Vibrational Energies by Means of Neural Networks. Journal of the Chinese Chemical Society, 1993, 40, 113-119.	1.4	1
36	Effect of Orbital Overlap in Thermal Reverse Homoâ€Dielsâ€Alder Reaction and Intramolecular Reverse Ene Reaction. Journal of the Chinese Chemical Society, 1994, 41, 631-634.	1.4	0

#	Article	IF	Citations
37	THE ESTIMATIONS OF INNER-SHELL IONIZATION ENERGIES FOR ALKYL HALIDES: A DESIGNATED SINGLE-CONFIGURATION CASSCF APPROACH AND ADVANCED CORRECTION. Journal of Theoretical and Computational Chemistry, 2004, 03, 103-115.	1.8	0
38	Reply to â€œComment on â€˜Time-Dependent Density Functional Study of Electroluminescent Polymers'â€. Journal of Physical Chemistry A, 2004, 108, 9318-9318.	2.5	0