Taro Udagawa

List of Publications by Year
in descending order

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56	793	623734	552781
papers	citations	14 h-index	26 g-index

58	58	58	817
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Constrained sialic acid donors enable selective synthesis of Î±-glycosides. Science, 2019, 364, 677-680.	12.6	74
2	HâˆD isotope effect on porphine and porphycene molecules with multicomponent hybrid density functional theory. Journal of Chemical Physics, 2006, 125, 244105.	3.0	72
3	A gas-plastic elastomer that quickly self-heals damage with the aid of CO2 gas. Nature Communications, 2019, 10, 1828.	12.8	57
4	Geometric Isotope Effect of Various Intermolecular and Intramolecular Câ”HÂ·Â·Â·O Hydrogen Bonds, Using the Multicomponent Molecular Orbital Method. Journal of Physical Chemistry A, 2006, 110, 7279-7285.	2.5	53
5	The Origin of High Stereoselectivity in Di-tert-butylsilylene-Directed Î±-Galactosylation. Journal of Organic Chemistry, 2016, 81, 9086-9104.	3.2	52
6	Electron-nucleus correlation functional for multicomponent density-functional theory. Physical Review A, 2014, 89, .	2.5	45
7	Synthesis of thieno[2,3-b]quinoline and selenopheno[2,3-b]quinoline derivativesviaiodocyclization reaction and a DFT mechanistic study. Organic and Biomolecular Chemistry, 2018, 16, 245-255.	2.8	37
8	Quantum Treatment of Hydrogen Nuclei in Primary Kinetic Isotope Effects in a Thermal [1,5]-Sigmatropic Hydrogen (or Deuterium) Shift from (Z)-1,3-Pentadiene. Journal of Physical Chemistry A, 2007, 111, 261-267.	2.5	33
9	Neutral Molecular Iron(II) Complexes Showing Tunable Bistability at Above, Below, and Just Room Temperature by a Crystal Engineering Approach: Ligand Mobility into a Three-Dimensional Flexible Supramolecular Network. Crystal Growth and Design, 2017, 17, 6006-6019.	3.0	26
10	Toward strong self-healing polyisoprene elastomers with dynamic ionic crosslinks. Soft Matter, 2020, 16, 3384-3394.	2.7	25
11	Multicomponent Molecular Orbitalâ€“Climbing Imageâ€“Nudged Elastic Band Method to Analyze Chemical Reactions Including Nuclear Quantum Effect. ChemPhysChem, 2015, 16, 3156-3160.	2.1	19
12	Theoretical Study of H/D Isotope Effects on Nuclear Magnetic Shieldings Using an ab initio Multi-Component Molecular Orbital Method. Molecules, 2013, 18, 5209-5220.	3.8	17
13	H/D isotope effect on charge-inverted hydrogen-bonded systems: Systematic classification of three different types in H₃XH^{â€¦}YH₃(X = C, Si, or Ge, and Y = B, Al, or Ga) with multicomponent calculation. Journal of Computational Chemistry, 2015, 36, 1647-1654.	3.3	16
14	Synthesis and photophysical properties of selenopheno[2,3-b]quinoxaline and selenopheno[2,3-b]pyrazine heteroacenes. Organic and Biomolecular Chemistry, 2020, 18, 4063-4070.	2.8	16
15	Metal-doped carbon nanocones as highly efficient catalysts for hydrogen storage: Nuclear quantum effect on hydrogen spillover mechanism. Molecular Catalysis, 2021, 504, 111486.	2.0	15
16	Synthesis of carbazoloquinone derivatives and their antileukemic activity via modulating cellular reactive oxygen species. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 2243-2247.	2.2	14
17	Design and synthesis of quinoxaline-1,3,4-oxadiazole hybrid derivatives as potent inhibitors of the anti-apoptotic Bcl-2 protein. Bioorganic Chemistry, 2020, 104, 104245.	4.1	14
18	Unusual H/D isotope effect in isomerization and ketoâ€“enol tautomerism reactions of pyruvic acid: nuclear quantum effect restricts some rotational isomerization reactions. RSC Advances, 2017, 7, 9328-9337.	3.6	11

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19	Systematic exploitation of thermotropic bicontinuous cubic phase families from 1,2-bis(aryloyl)hydrazine-based molecules. Physical Chemistry Chemical Physics, 2018, 20, 7953-7961.	2.8	11
20	Selenolactams as Synthetic Intermediates for the Synthesis of Polycyclic Amines via Seleno-Claisen Rearrangements. Journal of Organic Chemistry, 2018, 83, 3078-3089.	3.2	10
21	Nuclear quantum effect and H/D isotope effect on ClÂ· + (H2O)n â†' HCl + OHÂ·(H2O)nâ^'1 (n = 1â€“3) reactions. RSC Advances, 2018, 8, 17191-17201.	3.6	10
22	Alternative Route Triggering Multistep Spin Crossover with Hysteresis in an Iron(II) Family Mediated by Flexible Anion Ordering. Inorganic Chemistry, 2020, 59, 9866-9880.	4.0	10
23	Theoretical analysis of H/D geometric isotope effect on adenineâ€“thymine base pair using multi-component molecular orbital method. Computational and Theoretical Chemistry, 2009, 912, 63-66.	1.5	9
24	Analysis of exponent values of Gaussian-type functions on quantum protons and deuterons in charged or polarized systems. International Journal of Quantum Chemistry, 2016, 116, 961-970.	2.0	9
25	Nuclear quantum effect and H/D isotope effect on F + (H2O)n â†' FH + (H2O)nâ^'1OH (n = 1-3) reactions. Journal of Chemical Physics, 2016, 145, 164310.	3.0	9
26	Multicomponent QM study on the reaction of HOSOâ€‰+â€‰NO₂ with H₂O: Nuclear quantum effect on structure and reaction energy profile. International Journal of Quantum Chemistry, 2019, 119, e25895.	2.0	9
27	Why is NÂ·Â·Â·Be distance of NH₃H⁺Â·Â·Â·DBeH shorter than that of NH₃D⁺Â·Â·Â·HBeH? paradoxical geometrical isotope effects for partially isotopeâ€substituted dihydrogenâ€bonded isotopomers. Journal of Computational Chemistry, 2014, 35, 271-274.	3.3	8
28	Why does deuterium substitution lead to the contraction of XÂ·Â·Â·Ï€ distance? Origin of the reverse Ubbelohde effect in XHÂ·Â·Â·Ï€ interaction. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
29	Self-organization of dipyridylcalix[4]pyrrole into a supramolecular cage for dicarboxylates. RSC Advances, 2016, 6, 19794-19796.	3.6	7
30	A 1,2â€transâ€Selective Glycosyl Donor Bearing Cyclic Protection at the Câ€2 and Câ€3 Hydroxy Groups. European Journal of Organic Chemistry, 2017, 2017, 4778-4785.	2.4	7
31	Synthesis of thieno[2,3-c]acridine and furo[2,3-c]acridine derivatives via an iodocyclization reaction and their fluorescence properties and DFT mechanistic studies. New Journal of Chemistry, 2018, 42, 15315-15324.	2.8	7
32	H/D isotope effect on structures, binding energies, and basis set superposition errors in Fâ^'(H2O) (n=) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.9	6
33	Theoretical analysis on the aromaticity of uracil: Important electronic configurations and solvent effect on the aromaticity. Chemical Physics Letters, 2015, 637, 115-119.	2.6	6
34	Effect of heteroatoms on aromaticity analyzed by geometric, magnetic, and electronic criteria. Chemical Physics Letters, 2020, 745, 137271.	2.6	6
35	H/D Isotope Effects in Keto-Enol Tautomerism of Î²-Dicarbonyl Compounds â€"Importance of Nuclear Quantum Effects of Hydrogen Nucleiâ€". Bulletin of the Chemical Society of Japan, 2021, 94, 1954-1962.	3.2	6
36	Theoretical studies on [2â€‰+â€‰2â€‰+â€‰2] reaction mechanisms of three ethynes. More accurate estimation of activation energy. Journal of Physical Organic Chemistry, 2013, 26, 517-522.	1.9	5

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37	Effect of alkali metal cations on network rearrangement in polyisoprene ionomers. Physical Chemistry Chemical Physics, 2022, 24, 17042-17049.	2.8	5
38	A multicomponent QM study of H 2 dissociation on small aluminum cluster. Procedia Computer Science, 2017, 108, 2275-2281.	2.0	4
39	Iron(II) Spin Crossover Complex with the 1,2,3-Triazole-Containing Linear Pentadentate Schiff-Base Ligand and the MeCN Monodentate Ligand. Crystals, 2019, 9, 276.	2.2	4
40	Supramolecular Lightâ€Harvesting Antennas of Metalâ€Coordinated Bis(8â€Hydroxyquinoline)â€Substituted Porphyrin Networks. Chemistry - an Asian Journal, 2019, 14, 2567-2572.	3.3	4
41	Theoretical Study on Hydrogen-Tritium Exchange Reactions between Several Organic and HTO Molecules: A Multicomponent QM Study. Bulletin of the Chemical Society of Japan, 2019, 92, 592-599.	3.2	4
42	Determining if Reaction Selectivity Can Be Controlled by the H/D Isotope Effect in CHÂ·Â·Â·O Interactions. Organic Letters, 2020, 22, 9439-9443.	4.6	4
43	Molecular design of anti-spindle-like molecules by use of siloxanyl terminals for a thermotropic bicontinuous cubic phase. Physical Chemistry Chemical Physics, 2020, 22, 10132-10141.	2.8	4
44	Geometric Isotope Effect on Low Barrier Hydrogen-Bonding Systems of Acetic Acid Dimer, Formic Acid Dimer, and Their Anionic Clusters by Using the Multi-Component Molecular Orbital Method. Journal of Computer Chemistry Japan, 2010, 9, 21-28.	0.1	4
45	Rapid Stretching Vibration at the Polymer Chain End. ACS Macro Letters, 2014, 3, 126-129.	4.8	3
46	Large amplitude motion in 9-methylanthracene: High-resolution spectroscopy and Ab Initio theoretical calculation. Chinese Journal of Chemical Physics, 2020, 33, 8-12.	1.3	3
47	Geometrical H/D Isotope Effect of Blue-shifting Dihydrogen-bonded Clusters. Chemistry Letters, 2020, 49, 745-748.	1.3	3
48	Stereoselective Transesterification of P â€Chirogenic Hydroxybinaphthyl Phosphinates. ChemistryOpen, 2022, , e202100294.	1.9	3
49	Reaction mechanism of hydrogen-tritium exchange reactions between several organic and HTO molecules: a role of the second HTO. RSC Advances, 2018, 8, 3878-3888.	3.6	2
50	Stabilization of Bicontinuous Cubic Phase and Its Twoâ€Sided Nature Produced by Use of Siloxane Tails and Introduction of Molecular Nonsymmetry. Chemistry - A European Journal, 2021, 27, 10293-10302.	3.3	2
51	Competitive nuclear quantum effect and H/D isotope effect on torsional motion of H2O2: An ab initio path integral molecular dynamics study. Computational and Theoretical Chemistry, 2022, 1208, 113542.	2.5	2
52	Low-Barrier Hydrogen Bond in Fujikurin Aâ€“D: A Computational Study. ACS Omega, 2022, 7, 14244-14251.	3.5	2
53	A New Electron-nucleus Correlation Functional forMulticomponent Density Functional Theory. Journal of Computer Chemistry Japan, 2016, 15, 143-147.	0.1	1
54	Nuclear quantum effect and H/D isotope effect in excited state intramolecular proton transfer and electronâ€induced intramolecular proton transfer reactions in 8â€hydroxyquinoline. International Journal of Quantum Chemistry, 0, , .	2.0	1

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55	Ab initio molecular dynamics of protonated water clusters by integrated multicenter molecularâ€orbital method. Journal of Computational Chemistry, 2011, 32, 2902-2908.	3.3	0
56	A path integral molecular dynamics study on the NH₄⁺ rotation in NH₄⁺â‹¯XH₂ (X = Be or Mg) dihydrogen bond systems. Physical Chemistry Chemical Physics, 0, , .	2.8	0