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	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
2	Stereoselective Transesterification of P â€Chirogenic Hydroxybinaphthyl Phosphinates. ChemistryOpen, 2022, , e202100294.	1.9	3
3	Low-Barrier Hydrogen Bond in Fujikurin Aâ€“D: A Computational Study. ACS Omega, 2022, 7, 14244-14251.	3.5	2
4	Effect of alkali metal cations on network rearrangement in polyisoprene ionomers. Physical Chemistry Chemical Physics, 2022, 24, 17042-17049.	2.8	5
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	Effect of heteroatoms on aromaticity analyzed by geometric, magnetic, and electronic criteria. Chemical Physics Letters, 2020, 745, 137271.	2.6	6
13	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
14	Geometrical H/D Isotope Effect of Blue-shifting Dihydrogen-bonded Clusters. Chemistry Letters, 2020, 49, 745-748.	1.3	3
15	Toward strong self-healing polyisoprene elastomers with dynamic ionic crosslinks. Soft Matter, 2020, 16, 3384-3394.	2.7	25
16	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
17	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
18	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

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19	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
20	Constrained sialic acid donors enable selective synthesis of Î±-glycosides. Science, 2019, 364, 677-680.	12.6	74
21	A gas-plastic elastomer that quickly self-heals damage with the aid of CO2 gas. Nature Communications, 2019, 10, 1828.	12.8	57
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	A multicomponent QM study of H 2 dissociation on small aluminum cluster. Procedia Computer Science, 2017, 108, 2275-2281.	2.0	4
31	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
32	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
33	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
34	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
35	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
36	The Origin of High Stereoselectivity in Di-tert-butylsilylene-Directed Î±-Galactosylation. Journal of Organic Chemistry, 2016, 81, 9086-9104.	3.2	52

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37	Self-organization of dipyridylcalix[4]pyrrole into a supramolecular cage for dicarboxylates. RSC Advances, 2016, 6, 19794-19796.	3.6	7
38	A New Electron-nucleus Correlation Functional forMulticomponent Density Functional Theory. Journal of Computer Chemistry Japan, 2016, 15, 143-147.	0.1	1
39	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
40	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
41	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
42	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
43	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
44	Rapid Stretching Vibration at the Polymer Chain End. ACS Macro Letters, 2014, 3, 126-129.	4.8	3
45	H/D isotope effect on structures, binding energies, and basis set superposition errors in Fâ^'(H2O) (n=) Tj ETQq1 1 0.784314 rgBT /Ov	1.9	6
46	Electron-nucleus correlation functional for multicomponent density-functional theory. Physical Review A, 2014, 89, .	2.5	45
47	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
48	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
49	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
50	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
51	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
52	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
53	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
54	Hâ^•D isotope effect on porphine and porphycene molecules with multicomponent hybrid density functional theory. Journal of Chemical Physics, 2006, 125, 244105.	3.0	72

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55	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
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