Kaito Takahashi

List of Publications by Year
in descending order

90 papers	2,233 citations	201385 27 h-index	253896 43 g-index
90 all docs	90 docs citations	90 times ranked	1501 citing authors

#	Article	IF	Citations
1	Molecular dynamics simulations of sulfone derivatives in complex with DNA topoisomerase IIÎ± ATPase domain. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1692-1701.	2.0	3
2	Theoretical analysis on reactions between synâ€methyl Criegee intermediate and amino alcohols. Journal of the Chinese Chemical Society, 2022, 69, 184-192.	0.8	3
3	Understanding the effect of transition metals and vacancy boron nitride catalysts on activity and selectivity for CO2 reduction reaction to valuable products: A DFT-D3 study. Fuel, 2022, 319, 123808.	3.4	13
4	Absolute photodissociation cross sections of thermalized methyl vinyl ketone oxide and methacrolein oxide. Physical Chemistry Chemical Physics, 2022, 24, 10439-10450.	1.3	11
5	Understanding the interaction between transition metal doping and ligand atoms of ZnS and ZnO monolayers to promote the CO₂ reduction reaction. Physical Chemistry Chemical Physics, 2022, 24, 12909-12921.	1.3	3
6	Theoretical insight on why N-vacancy promotes the selective CO2 reduction to ethanol on NiMn doped graphitic carbon nitride sheets. Applied Surface Science, 2022, 595, 153527.	3.1	15
7	Co-embedded sulfur vacant MoS₂ monolayer as a promising catalyst for formaldehyde oxidation: a theoretical evaluation. New Journal of Chemistry, 2021, 45, 17407-17417.	1.4	2
8	Surprisingly long lifetime of methacrolein oxide, an isoprene derived Criegee intermediate, under humid conditions. Communications Chemistry, 2021, 4, .	2.0	32
9	Substrate binding mechanism of glycerophosphodiesterase towards organophosphate pesticides. Journal of Molecular Liquids, 2021, 329, 115526.	2.3	1
10	PEG-stabilized coaxial stacking of two-dimensional covalent organic frameworks for enhanced photocatalytic hydrogen evolution. Nature Communications, 2021, 12, 3934.	5.8	111
11	Effect of 3d-transition metals doped in ZnO monolayers on the CO2 electrochemical reduction to valuable products: first principles study. Applied Surface Science, 2021, 550, 149380.	3.1	21
12	Substituent Effect in the Reactions between Criegee Intermediates and 3-Aminopropanol. Journal of Physical Chemistry A, 2021, 125, 6580-6590.	1.1	5
13	Experimental and Computational Studies of Criegee Intermediate syn-CH₃CHOO Reaction with Hydrogen Chloride. Journal of Physical Chemistry A, 2021, 125, 8587-8594.	1.1	10
14	Evaluation of Ar tagging toward the vibrational spectra and zero point energy of Xâ‹¯HOH, Xâ‹¯DOH, and Xâ‹¯HOD, for X = F, Cl, Br. Physical Chemistry Chemical Physics, 2021, 23, 9492-9499.	1.3	2
15	Source of oseltamivir resistance due to single E119D and double E119D/H274Y mutations in pdm09H1N1 influenza neuraminidase. Journal of Computer-Aided Molecular Design, 2020, 34, 27-37.	1.3	15
16	Theoretical study on direction of vibrational transition dipole moment of XH stretching vibration in HXD. Chinese Journal of Chemical Physics, 2020, 33, 13-22.	0.6	0
17	Reactions of Criegee Intermediates are Enhanced by Hydrogenâ€Atom Relay Through Molecular Design. ChemPhysChem, 2020, 21, 2056-2059.	1.0	7
18	Kinetics of Unimolecular Decay of Methyl Vinyl Ketone Oxide, an Isoprene-Derived Criegee Intermediate, under Atmospherically Relevant Conditions. Journal of Physical Chemistry A, 2020, 124, 9375-9381.	1.1	12

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19	The role of the iodine-atom adduct in the synthesis and kinetics of methyl vinyl ketone oxideâ€"a resonance-stabilized Criegee intermediate. Physical Chemistry Chemical Physics, 2020, 22, 13603-13612.	1.3	12
20	Two-Color Resonant Two-Photon Mass-Analyzed Threshold Ionization of 2,4-Difluoroanisole and the Additivity Relation of Ionization Energy. Journal of Physical Chemistry A, 2020, 124, 10517-10526.	1.1	2
21	The effect of pinning the lone pair on the direction of the OH stretching transition moment of water. Journal of Molecular Spectroscopy, 2019, 363, 111171.	0.4	1
22	Hydrogen-Bonding Mediated Reactions of Criegee Intermediates in the Gas Phase: Competition between Bimolecular and Termolecular Reactions and the Catalytic Role of Water. Journal of Physical Chemistry A, 2019, 123, 8336-8348.	1.1	15
23	Cation spectra of p-chloroanisole and the heavy atom effect on ionization energy. Chemical Physics Letters, 2019, 731, 136626.	1.2	6
24	Synergy of Water and Ammonia Hydrogen Bonding in a Gas-Phase Reaction. Journal of Physical Chemistry A, 2019, 123, 1337-1342.	1.1	16
25	Oddâ€"Even Reactivity Variation Due to Dynamical Effects around the Roaming Saddle Points of the Reaction Between C_n^{â€"} Chain (n = 2â€"8) and H₂. Journal of Physical Chemistry A, 2019, 123, 5300-5308.	1.1	0
26	Temperature and isotope effects in the reaction of CH₃CHOO with methanol. Physical Chemistry Chemical Physics, 2019, 21, 13633-13640.	1.3	25
27	Temperature-Dependent Rate Coefficient for the Reaction of CH₃SH with the Simplest Criegee Intermediate. Journal of Physical Chemistry A, 2019, 123, 4096-4103.	1.1	20
28	Water Vapor Does Not Catalyze the Reaction between Methanol and OH Radicals. Angewandte Chemie, 2019, 131, 5067-5071.	1.6	3
29	Water Vapor Does Not Catalyze the Reaction between Methanol and OH Radicals. Angewandte Chemie - International Edition, 2019, 58, 5013-5017.	7.2	16
30	Effects of water vapor on the reaction of CH₂OO with NH₃. Physical Chemistry Chemical Physics, 2019, 21, 22589-22597.	1.3	22
31	How Does Vibrational Excitation Affect the X-Ray Absorption Spectra of Monohydrated Halide and Alkali Metal Clusters?. Advances in Quantum Chemistry, 2019, , 57-81.	0.4	0
32	Reactivity of Criegee Intermediates toward Carbon Dioxide. Journal of Physical Chemistry Letters, 2018, 9, 184-188.	2.1	22
33	Kinetics of the reaction of the simplest Criegee intermediate with ammonia: a combination of experiment and theory. Physical Chemistry Chemical Physics, 2018, 20, 29669-29676.	1.3	27
34	Criegee Intermediate Reaction with Alcohol Is Enhanced by a Single Water Molecule. Journal of Physical Chemistry Letters, 2018, 9, 7040-7044.	2.1	37
35	How big is the substituent dependence of the solar photolysis rate of Criegee intermediates?. Physical Chemistry Chemical Physics, 2018, 20, 16247-16255.	1.3	13
36	Effect of unsaturated substituents in the reaction of Criegee intermediates with water vapor. Physical Chemistry Chemical Physics, 2018, 20, 20217-20227.	1.3	14

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37	Temperature-Dependent Rate Coefficients for the Reaction of CH2OO with Hydrogen Sulfide. Journal of Physical Chemistry A, 2017, 121, 938-945.	1.1	30
38	How does substitution affect the unimolecular reaction rates of Criegee intermediates?. Physical Chemistry Chemical Physics, 2017, 19, 12075-12084.	1.3	42
39	First-principles study of Pd-skin/Pd3Fe(111) electrocatalyst for oxygen reduction reaction. Journal of Applied Electrochemistry, 2017, 47, 747-754.	1.5	8
40	The doping mechanism and electrical performance of polyethylenimineâ€doped MoSÂ-₂ transistor. Physica Status Solidi C: Current Topics in Solid State Physics, 2017, 14, 1600262.	0.8	12
41	Will (CH₃)₂COO Survive in Humid Conditions?. Journal of the Chinese Chemical Society, 2016, 63, 472-479.	0.8	5
42	Theoretical calculation of the vibrational state dependent photodetachment spectra of X^{â^'}H₂O, X = F, Cl, Br. Physical Chemistry Chemical Physics, 2016, 18, 26970-26979.	1.3	10
43	Dependence of Adenine Raman Spectrum on Excitation Laser Wavelength: Comparison between Experiment and Theoretical Simulations. Journal of Physical Chemistry A, 2016, 120, 8114-8122.	1.1	7
44	Temperature dependence of the reaction of anti-CH₃CHOO with water vapor. Physical Chemistry Chemical Physics, 2016, 18, 28189-28197.	1.3	61
45	Ab-initio study of surface oxide formation in Pt(111) electrocatalyst under influences of O2-containing intermediates of oxygen reduction reaction. Journal of Applied Electrochemistry, 2016, 46, 1031-1038.	1.5	4
46	Absolute UV absorption cross sections of dimethyl substituted Criegee intermediate (CH 3) 2 COO. Chemical Physics Letters, 2016, 653, 155-160.	1.2	35
47	Competition between H₂O and (H₂O)₂ reactions with CH₂OO/CH₃CHOO. Physical Chemistry Chemical Physics, 2016, 18, 4557-4568.	1.3	144
48	Unimolecular Decomposition Rate of the Criegee Intermediate (CH₃)₂COO Measured Directly with UV Absorption Spectroscopy. Journal of Physical Chemistry A, 2016, 120, 4789-4798.	1.1	75
49	Features in Vibrational Spectra Induced by Ar-Tagging for H₃O⁺Ar_m, m = 0â€“3. Journal of Physical Chemistry A, 2015, 119, 10887-10892.	1.1	27
50	Evenâ€“odd product variation of the Cn+ + D2 (n = 4â€“9) reaction: complexity of the linear carbon cation electronic states. Physical Chemistry Chemical Physics, 2015, 17, 24810-24819.	1.3	3
51	Is the structure of hydroxide dihydrate OHâ^'(H2O)2? An ab initio path integral molecular dynamics study. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	3
52	Interpretation of Semiclassical Transition Moments through Wave Function Expansion of Dipole Moment Functions with Applications to the OH Stretching Spectra of Simple Acids and Alcohols. Journal of Physical Chemistry A, 2015, 119, 4834-4845.	1.1	6
53	The Large Variation in Acidity of Diethyl Ether Cation Induced by Internal Rotation about a Single Covalent Bond. Journal of Physical Chemistry A, 2015, 119, 4885-4890.	1.1	11
54	Temperature dependent structural variations of OH^{â^'}(H₂O)_n, n = 4â€“7: effects on vibrational and photoelectron spectra. Physical Chemistry Chemical Physics, 2015, 17, 19162-19172.	1.3	16

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55	Strong Negative Temperature Dependence of the Simplest Criegee Intermediate CH₂OO Reaction with Water Dimer. Journal of Physical Chemistry Letters, 2015, 6, 2708-2713.	2.1	127
56	Identification of four rotamers of m-methoxystyrene by resonant two-photon ionization and mass analyzed threshold ionization spectroscopy. Journal of Chemical Physics, 2015, 142, 124314.	1.2	19
57	Effects of Co Content in Pd-Skin/PdCo Alloys for Oxygen Reduction Reaction: Density Functional Theory Predictions. Journal of Physical Chemistry C, 2015, 119, 24364-24372.	1.5	20
58	Theoretical vibrational spectra of OHâ^'(H2O)2: the effect of quantum distribution and vibrational coupling. Physical Chemistry Chemical Physics, 2015, 17, 25505-25515.	1.3	11
59	Hyperconjugation in diethyl ether cation versus diethyl sulfide cation. Physical Chemistry Chemical Physics, 2015, 17, 23602-23612.	1.3	3
60	Infrared spectroscopic investigations of cationic ethanol, propanol, and butanol. Chemical Physics Letters, 2015, 640, 215-218.	1.2	7
61	UV absorption spectrum of the C2 Criegee intermediate CH3CHOO. Journal of Chemical Physics, 2014, 141, 074302.	1.2	79
62	Why does the IR spectrum of hydroxide stretching vibration weaken with increase in hydration?. Physical Chemistry Chemical Physics, 2014, 16, 23143-23149.	1.3	19
63	Multidimensional local mode calculations for the vibrational spectra of OHâ^'(H2O)2 and OHâ^'(H2O)2Â·Ar. Physical Chemistry Chemical Physics, 2013, 15, 14973.	1.3	16
64	A study of resonance progressions in the F + HCl â†' Cl + HF reaction: A lifetime matrix analysis of pre-reactive and post-reactive collision complexes. Journal of Chemical Physics, 2013, 138, 024309.	1.2	10
65	Multidimensional OH local mode calculations for OH^{â^'}(H₂O)₃â€"Importance of intermode anharmonicity. Physical Chemistry Chemical Physics, 2013, 15, 114-124.	1.3	22
66	Will water act as a photocatalyst for cluster phase chemical reactions? Vibrational overtone-induced dehydration reaction of methanediol. Journal of Chemical Physics, 2012, 136, 164302.	1.2	30
67	Selectivity of Palladiumâ€"Cobalt Surface Alloy toward Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2012, 116, 6200-6207.	1.5	24
68	Theoretical study on the difference of OH vibrational spectra between OHâ^'(H2O)3 and OHâ^'(H2O)4. Physical Chemistry Chemical Physics, 2012, 14, 2797.	1.3	29
69	Assessment of density functional theory to calculate the phase transition pressure of ice. Physical Chemistry Chemical Physics, 2012, 14, 11484.	1.3	22
70	Theoretical Calculation of the OH Vibrational Overtone Spectra of 1,5-Pentanediol and 1,6-Hexanediol. Journal of Physical Chemistry A, 2011, 115, 14315-14324.	1.1	17
71	Theoretical Calculation of the OH Vibrational Overtone Spectra of 1-n Alkane Diols (n =) Tj ETQq1 1 0.784314 rgBT /Ov... 5641-5653.	1.1	37
72	Hydration of pyruvic acid to its geminal-diol, 2,2-dihydroxypropanoic acid, in a water-restricted environment. Chemical Physics Letters, 2011, 513, 184-190.	1.2	50

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73	Photolysis Crossâ€Section of Ozone Dimer. Chemistry - an Asian Journal, 2011, 6, 2925-2930.	1.7	2
74	Gas-phase water-mediated equilibrium between methylglyoxal and its geminal diol. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 6687-6692.	3.3	75
75	Dynamics and spectroscopy of vibrational overtone excited glyoxylic acid and 2,2-dihydroxyacetic acid in the gas-phase. Journal of Chemical Physics, 2010, 132, 094305.	1.2	22
76	Water Catalysis and Anticatalysis in Photochemical Reactions: Observation of a Delayed Threshold Effect in the Reaction Quantum Yield. Journal of the American Chemical Society, 2010, 132, 15154-15157.	6.6	19
77	Theoretical study on the effect of intramolecular hydrogen bonding on OH stretching overtone decay lifetime of ethylene glycol, 1,3-propanediol, and 1,4-butanediol. Physical Chemistry Chemical Physics, 2010, 12, 13950.	1.3	28
78	Gas-phase vibrational spectra of glyoxylic acid and its gem diol monohydrate. Implications for atmospheric chemistry. Reaction Kinetics and Catalysis Letters, 2009, 96, 209-224.	0.6	49
79	Fundamental and Overtone Vibrational Spectra of Gas-Phase Pyruvic Acid. Journal of Physical Chemistry A, 2009, 113, 7294-7303.	1.1	61
80	Infrared spectra of SF6â^'â‹…HCOOHâ‹…Arnâ€^(n=â€“2): Infrared triggered reaction and Ar-induced reactive inhibition. Journal of Chemical Physics, 2009, 130, 174302.	1.2	7
81	Dynamics of Vibrational Overtone Excited Pyruvic Acid in the Gas Phase: Line Broadening through Hydrogen-Atom Chattering. Journal of Physical Chemistry A, 2008, 112, 7321-7331.	1.1	74
82	Experimental and Theoretical Study of the OH Vibrational Spectra and Overtone Chemistry of Gas-Phase Vinylacetic Acid. Journal of Physical Chemistry A, 2008, 112, 10226-10235.	1.1	24
83	Sunlight-Initiated Photochemistry: Excited Vibrational States of Atmospheric Chromophores. International Journal of Photoenergy, 2008, 2008, 1-13.	1.4	26
84	Vibrational overtone induced elimination reactions within hydrogen-bonded molecular clusters: the dynamics of water catalyzed reactions in CH2FOHÂ·(H2O)n. Physical Chemistry Chemical Physics, 2007, 9, 3864-3871.	1.3	44
85	Experimental and Theoretical Investigation of Vibrational Overtones of Glycolic Acid and Its Hydrogen Bonding Interactions with Water. Journal of Physical Chemistry A, 2006, 110, 6439-6446.	1.1	41
86	A Simple Picture for the Rotational Enhancement of the Rate for the F + HCl â†' HF + Cl Reaction:Â A Dynamical Study Using a New ab initio Potential Energy Surfaceâ€. Journal of Physical Chemistry A, 2006, 110, 436-444.	1.1	43
87	Multireference configuration interaction calculations for the F(P2)+HClâ†'HF+Cl(P2) reaction: A correlation scaled ground state (1Aâ€²2) potential energy surface. Journal of Chemical Physics, 2006, 124, 224303.	1.2	49
88	Effective One-Dimensional Dipole Moment Function for the OH Stretching Overtone Spectra of Simple Acids and Alcohols. Journal of Physical Chemistry A, 2005, 109, 4242-4251.	1.1	33
89	Theoretical Analysis on the Fundamental and Overtone OH Stretching Spectra of Several Simple Acids and Alcohols. Journal of Physical Chemistry A, 2003, 107, 11092-11101.	1.1	42
90	Theoretical Analysis of the CH Stretching Overtone Vibration of 1,2-Dichloroethylene. Journal of Physical Chemistry A, 2002, 106, 2676-2684.	1.1	36