

Kaito Takahashi

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PROFESSIONAL EXPERIENCE:

Lecturer, 2024 July

School of Bio-Chemical Engineering and Technology
Sirindhorn International Institute of Technology, Thammasat University
Pathum Thani, Thailand

Research Fellow, 2024 February-2024 July

Institute of Atomic and Molecular Sciences, Academia Sinica
Taipei, Taiwan (R.O.C.)

Associate Research Fellow, 2017 January-

Institute of Atomic and Molecular Sciences, Academia Sinica
Taipei, Taiwan (R.O.C.)

Assistant Research Fellow, 2009 June-2017, January

Institute of Atomic and Molecular Sciences, Academia Sinica
Taipei, Taiwan (R.O.C.)

Postdoctoral Fellow, 2006 October-2009 April

Department of Chemistry and Biochemistry, University of Colorado at Boulder,
Boulder, Colorado, U. S. A.

Postdoctoral Fellow, 2005 April-2006 September

Institute of Atomic and Molecular Sciences, Academia Sinica
Taipei, Taiwan (R. O. C.)

Research Assistant, 2003 April-2005 March

Keio University, Yokoyama, Japan

ACADEMIC BACKGROUND:

Ph.D. in Science (Chemistry), Graduate School of Science and Technology, Keio University,
Yokohama, 2005

Advisor: Dr. Satoshi Yabushita

M.S., in Science (Chemistry) Graduate School of Science and Technology, Keio University, Yokohama, 2002

Advisor: Dr. Satoshi Yabushita

B.S., in Chemistry, Department of Chemistry, Keio University, Yokohama, 2002

Advisor: Dr. Satoshi Yabushita

CURRENT RESEARCH INTERESTS:

Theoretical calculation of vibrational spectra

Rate calculation with anharmonic corrections

Modelling of reactions on metal surface

Photoinduced reactions

Electronic structure calculation for couple electronic states

RESEARCH SKILLS:

Quantum chemistry calculation using the ACES II, COLUMBUS, GAMESS, Gaussian, and MOLPRO programs

Quantum dynamics calculation using ABC and MCTDH programs

Programming using FORTRAN and *Mathematica*

Fond with using Linux, Unix, Windows, and Macintosh machines

LANGUAGES:

Fluent in English and Japanese, beginner in Chinese and Thai

PUBLICATIONS:

Lecturer SIIT 2026

1. Yoshiyuki Matsuda,* Tomoya Endo, Ryo Yasumoto, Asuka Fujii, **Kaito Takahashi***, “Covalent-bonded pentane dimer cation: A reaction intermediate of H₂ elimination”, preparation.
2. Pradeep Kumar Pal, Supawadee Namuangruk, **Kaito Takahashi*** “Competition of proton and hydride tunneling in the reaction between Criegee intermediates and hydrogen molecule” preparation

3. Chia-Hsuan Hsieh, Hui-Ming Hung,* Ching-Wei Chu, and **Kaito Takahashi**, May 2026 “Anthropogenic–Biogenic Interactions: Influence of SO₂ on Early-Stage Secondary Organic Aerosol Formation from α -Pinene Ozonolysis” ACS Earth and Space Chemistry <https://doi.org/10.1021/acsearthspacechem.6c00062>
4. Natthakrij Nipanutiyan, Daisuke Yoshida, **Kaito Takahashi***, January 2026, “Can single reference density functional theory methods describe spin state crossing for 3d transition metal carbonyl association?”, Physical Chemistry Chemical Physics, 28, 6099-6110 DOI: <https://doi.org/10.1039/D5CP04203H>

Lecturer SIIT 2025

5. Poobodin Mano, Klichchupong Dabsamut, Ching-Ming Wei, Siriporn Kosawatthanakun, Bunyarat Rungtaweeveranit, Supawadee Namuangruk* and **Kaito Takahashi*** December 2025, “Unraveling the Humidity-induced Phase Transition in CALF-20 via Machine Learning Potentials”, Journal of American Chemical Society, 147, 51, 47824–47834 <https://pubs.acs.org/doi/10.1021/jacs.5c18944>
6. Wayu Takemura, **Kaito Takahashi*** September 2025, “Can Electric Field Modulate the Formaldehyde Hydration Reactivity?” Science & Technology Asia, 30, 3, 128-134 doi:10.14456/scitechasia.2025.55
7. Natthakrij Nipanutiyan, **Kaito Takahashi***, September 2025, “Is Change of Spin State Critical for 3d Transition Metal Carbon Monoxide Bonding?” Science & Technology Asia, 30, 3, 120-127 doi:10.14456/scitechasia.2025.54
8. Kaewalee Vesysirindra, **Kaito Takahashi***, September 2025, “Does Water Clustering Accelerate Acetylacetone Tautomerization Reaction?” Science & Technology Asia, 30, 3, 112-119 doi:10.14456/scitechasia.2025.53
9. Sodara Thao, Poobodin Mano, **Kaito Takahashi**, Luckhana Lawtrakul, Supawadee Namuangruk* June 2025, “Effect of ligand substitution on CO₂ localization and pressure responsive adsorption in CALF-20 derivatives”, Microporous and Mesoporous Materials 396, 113745. <https://doi.org/10.1016/j.micromeso.2025.113745>

Lecturer SIIT 2024

10. Daisuke Yoshida* and **Kaito Takahashi***, December 2024, “Multistate Transition Metal Carbonyl Bonding Beyond Minimum Energy Pathway: Nonlocality of Spin-Orbit Interaction”, Inorganic Chemistry, 64, 1, 286–294. <https://doi.org/10.1021/acs.inorgchem.4c04568> (Q1, 4.4)
11. Poobodin Mano, Thanadol Jitwatanasirikul, Thantip Roongcharoen, **Kaito Takahashi***,

Supawadee Namuangruk* December 2024 “Tuning covalent bonding of single transition metal atom doped in S vacant MoS₂ for catalytic CO₂ reduction reaction product selectivity” Applied Surface Science, 688, 162339, <https://doi.org/10.1016/j.apsusc.2025.162339> (Q1, 6.3)

12. Poobodin Mano, **Kaito Takahashi***, Chularat Wattanakit, Supawadee Namuangruk* December 2024, “Spillover Promoted Dual CO₂ Reduction to Ethanol via Low C–C Coupling Barrier on Co-Embedded γ -Graphyne with d– π Orbital Centers” ACS Applied Energy Materials, 8, 1060–1068. <https://doi.org/10.1021/acsaem.4c02563> (Q1, 5.5)

Research Fellow (AS) 2024

13. Nuttapon Yodsin, Poobodin Mano, **Kaito Takahashi** and Supawadee Namuangruk*, July 2024, “Dual Electron Donating Metal-Boron Reaction Center Boosts Electrocatalytic Urea Synthesis from N₂ and CO₂”, ChemCatChem, e202400304 <https://doi.org/10.1002/cctc.202400304>
14. Klichchupong Dabsamut, **Kaito Takahashi**, and Walter R. L. Lambrecht June 2024, “Native defects and their complexes in spinel LiGa₅O₈” Journal of Applied Physics, 135, 235707. <https://doi.org/10.1063/5.0209774>
15. Klichchupong Dabsamut and **Kaito Takahashi*** March 2024, “Theoretical calculations for modeling carbon-carbon coupling reactions on copper surface: A comprehensive review” ScienceAsia 50, 1-11. [10.2306/scienceasia1513-1874.2024.029](https://doi.org/10.2306/scienceasia1513-1874.2024.029)
16. Klichchupong Dabsamut and **Kaito Takahashi***, January 2024 “Controlling C–C coupling reactivity through pore shape engineering of B-doped graphyne family” Carbon, 218, 118672 <https://doi.org/10.1016/j.carbon.2023.118672>

Associate Research Fellow 2023

17. Yen-Hsiu Lin, **Kaito Takahashi**, and Jim Jr-Min Lin* November 2023, “Comment on “UV Absorption Spectroscopy of the Conformer-Dependent Reactivity of the Four Carbon Criegee Intermediate of Methyl Vinyl Ketone Oxide: An Ab initio Quantum Dynamics Study””, Journal of Physical Chemistry A, 127, 10091-10103. <https://doi.org/10.1021/acs.jpca.4c00105>
18. Sarinya Hadsadee, Thantip Rooncharoen, **Kaito Takahashi**, Siriporn Jungstittiwong, Supawadee Namuangruk*, October 2023, “Enhanced electrocatalytic CO₂ reduction reactivity by S and N doping to Fe-embedded graphene”, ChemPlusChem, e202300306. <https://doi.org/10.1002/cplu.202300306>

19. Yen-Ju Wu, **Kaito Takahashi**, and Jim Jr-Min Lin, September 2023 “Kinetics of the simplest Criegee intermediate reaction with water vapor: Revisit and isotope effect”, *Journal of Physical Chemistry A*, 127, 8059-8072.
<https://doi.org/10.1021/acs.jpca.3c03418>
20. **Kaito Takahashi*** August 2023 “Substituent Dependence on the Reactions of Criegee Intermediates with Carbon Dioxide and Carbon Monoxide” *ChemPlusChem*, 88, e2002300354. <https://doi.org/10.1002/cplu.202300354>
21. Poobodin Mano, Supawadee Namuangruk, **Kaito Takahashi*** April 2023 “Origin of strong CO binding and low C-C coupling barrier for ethanol synthesis on non-metal doped graphyne: Bond order conservation and flexible orbital hybridization” *Journal of Physical Chemistry C*, 127, 7683-7894. <https://doi.org/10.1021/acs.jpcc.3c00946>
22. Thanadol Jitwatanasirikul, Thantip Roongcharoen, Pornsawan Sikam, **Kaito Takahashi**, Thanyada Rungrotmongkol, and Supawadee Namuangruk* January 2023 “The Screening of Homo- and Hetero-Dual Atoms Anchored Graphdiyne for Boosting Electrochemical CO₂ Reduction” *Advanced Material Interfaces*, 2201904 DOI: 10.1002/admi.202201904

Associate Research Fellow (AS) 2022

23. Jake Tan and **Kaito Takahashi*** November 2022 “Vibrational Spectrum of a 1D Oscillator: The Quantum, the Wigner, and the Classical Ways” *Journal of Chinese Chemical Society*, 70, 495-510 <https://doi.org/10.1002/jccs.202200398>
24. Jie-Ning Yang, **Kaito Takahashi**, Jim Jr-Min Lin*, August 2022, “Reaction Kinetics of Criegee Intermediates with Nitric Acid”, *Journal of Physical Chemistry A*, 126, 6160-6170 <https://doi.org/10.1021/acs.jpca.2c04596>
25. **Kaito Takahashi*** August 2022 “Wave Packet Calculation of Absolute UV Cross Sections of Criegee Intermediates” *Journal of Physical Chemistry A*, 126, 6080-6090 <https://doi.org/10.1021/acs.jpca.2c04141>
26. Bedabyas Behera, **Kaito Takahashi*** and Yuan-Pern Lee*, July 23, 2022 “Mechanism and kinetics of the reaction of Criegee intermediate CH₂OO with acetic acid studied with a step-scan Fourier-transform IR spectrometer”, *Physical Chemistry Chemical Physics*, 24, 18568-18581 DOI: 10.1039/D2CP01053D
27. Thantip Roongcharoen, Poobodin Mano, Thanadol Jitwatanasirikul, Pornsawan Sikam, Teera Butburee, **Kaito Takahashi***, Supawadee Namuangruk* April 2022 “Synergic Cooperation of Ni, Mn and N-vacancy in Graphitic Carbon Nitride Sheets for Boosting

- Carbon Dioxide Electrochemical Reduction to Ethanol” Applied Surface Science 595, 153527 <https://doi.org/10.1016/j.apsusc.2022.153527>
28. Pornsawan Sikam, Thanadol Jitwatanasirikul, Thantip Roongcharoen, Nuttapon Yodsin, Jittima Meeprasert, **Kaito Takahashi**,* Supawadee Namuangruk* April 2022, “Understanding the interaction between transition metal doping and ligand atoms of ZnS and ZnO monolayers to promote CO₂ reduction reaction”, Physical Chemistry Chemical Physics 24, 12909-12921 DOI: 10.1039/D2CP00878E
 29. Yen-Hsiu Lin **Kaito Takahashi*** and Jim Jr-Min Lin*, April 2022, “Absolute photodissociation cross sections of thermalized methyl vinyl ketone oxide and methacrolein oxide”, Physical Chemistry Chemical Physics 24, 10439-10450 doi:10.1039/d2cp00476c
 30. Tanabat Mudchimo, **Kaito Takahashi**, Poobodin Mano, Vannajan Sanghiran Lee, Thanyada Rungrotmongkol,* Supawadee Namuangruk*, March 2022 “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 319, 123808 doi.org/10.1016/j.fuel.2022.123808

Associate Research Fellow (AS) 2021

31. Siyue Liu, Xiaohu Zhou, Yang Chen, Yiqiang Liu,* Shengrui Yu, **Kaito Takahashi**,* Hongbin Ding, Zhenfeng Ding, Xueming Yang* and Wenrui Dong*, September, 2021 “Experimental and Computational Studies of Criegee Intermediate *syn*-CH₃CHOO reaction with Hydrogen chloride”, Journal of Physical Chemistry A. 125, 8587-8594. <https://doi.org/10.1021/acs.jpca.1c05578>
32. **Kaito Takahashi***, September 2021 “Theoretical calculation on the reaction between *syn*-CH₃CHOO and different amino alcohols”, Journal of Chinese Chemical Society, 69, 184-192 <https://doi.org/10.1002/jccs.202100249>.
33. Thanadol Jitwatanasirikul, Thantip Roongcharoen, Chirawat Chitpakdee, Siriporn Jungsuttiwong, Preeyaporn Poldorn, **Kaito Takahashi** and S. Namuangruk*, August 2021 “Theoretical evaluation of low-temperature formaldehyde oxidation on Co-embedded sulfur vacant MoS₂ monolayer”, New Journal of Chemistry 45, 17407-17417. DOI: 10.1039/D1NJ02869C.
34. Mei-Tsan Kuo, Jie-Ning Yang, Jim Jr-Min Lin*, and **Kaito Takahashi*** July 2021. “Substituent Effect in the Reactions between Criegee Intermediates and 3-Aminopropanol”, Journal of Physical Chemistry A, 125, 6580-6590

<https://doi.org/10.1021/acs.jpca.1c03737>

35. Ting Zhou, Lei Wang, Xingye Huang, Junjuda Unruangsri, Rong Wang, Qingyuan Yang, Changchun Wang, **Kaito Takahashi**,* Hangxun Xu,* and Jia Guo*, June, 2021, “PEG-stabilized coaxial stacking of two-dimensional covalent organic frameworks for enhanced photocatalytic hydrogen evolution”, *Nature Communications*, 12, 3934. <https://doi.org/10.1038/s41467-021-24179-5>
36. Wikorn Punyain, and **Kaito Takahashi*** March 2021, “Evaluation of Ar tagging toward the vibrational spectra and zero point energy of X-HOH, X-DOH, and X-HOD, for X=F, Cl, Br”, *Physical Chemistry Chemical Physics*, 23, 9492-9499. DOI: 10.1039/D0CP06339H
37. Pornsawan Sikam, **Kaito Takahashi**, Thantip Roongcharoen, Thanadol Jitwatanasirikul, Chirawat Chitpakdee, Kajornsak Faungnawakij, Supawadee Namuangruk* Februruay 2021 “Effect of 3d-transition metals doped in ZnO monolayers on the CO₂ electrochemical reduction to valuable products: First Principles study”, *Applied Surface Science*, 550, 149380. <https://doi.org/10.1016/j.apsusc.2021.149380>
38. Yen-Hsiu Lin, Cangtao Yin, **Kaito Takahashi**, and Jim Jr-Min Lin* January 2021, “Surprisingly long lifetime of methacrolein oxide, an isoprene derived Criegee intermediate, under humid conditions”, *Communications Chemistry*, 4, 12. <https://doi.org/10.1038/s42004-021-00451-z>
39. Nayana Bhat, Bodee Nutho, Alisa Vangnai, **Kaito Takahashi**, Thanyada Rungrotmongkol*, January 2021 “Substrate binding mechanism of glycerophosphodiesterase towards organophosphate pesticides”, *Journal of Molecular Liquids*, 329, 115526. <https://doi.org/10.1016/j.molliq.2021.115526>

Associate Research Fellow (AS) 2020

40. Kanika Verma, Panupong Mahalapbutr, Atima Auepattanapong, Onnicha Khaikate , Chutima Kuhakarn, **Kaito Takahashi**, and Thanyada Rungrotmongkol* October 2020, “Molecular dynamics simulations of sulfone derivatives in complex with DNA topoisomerase II α ATPase domain “, *Journal of Biomolecular Structure and Dynamics*, 34, 27-37. <https://doi.org/10.1080/07391102.2020.1831961>
41. Sheng Yuan Tzeng, **Kaito Takahashi**, Wen Bih Tzeng*, November 2020, “Two-color resonant two-photon mass-analyzed threshold ionization of 2,4-difluoroanisole and the additivity rule on ionization energy”, *Journal of Physical Chemistry A*, 124, 10517-10526. <https://dx.doi.org/10.1021/acs.jpca.0c08272>

42. Yen-Hsiu Lin, Chung-Hsin Yang, **Kaito Takahashi**, and Jim Jr-Min Lin*, October 2020, “Kinetics of Unimolecular Decay of Methyl Vinyl Ketone Oxide, an Isoprene-Derived Criegee Intermediate, under Atmospherically Relevant Conditions”, *Journal of Physical Chemistry A*, 124, 9375-9381. <https://doi.org/10.1021/acs.jpca.0c07928>
43. Mei-Tsan Kuo, **Kaito Takahashi**,* and Jim Jr-Min Lin*, August 2020, “Reactions of Criegee Intermediates are Enhanced by Hydrogen-atom Relay Through Molecular Design”, *ChemPhysChem*, 21, 2056-2059. <https://doi.org/10.1002/cphc.202000585>
44. Yen-Hsiu Lin, Yu-Lin Li, Wen Chao, **Kaito Takahashi** and Jim Jr-Min Lin*, June 2020, “The role of the iodine-atom adduct in the synthesis and kinetics of methyl vinyl ketone oxide— a resonance-stabilized Criegee intermediate”, *Physical Chemistry Chemical Physics*, 22, 13603-13612. DOI: 10.1039/d0cp02085k
45. **Kaito Takahashi*** February 2020, “Theoretical Study on the Direction of the Vibrational Transition Dipole Moment of XH Stretching Vibration in HXD”, *Chinese Journal of Chemical Physics*, 33. 13-22. DOI:10.1063/1674-0068/cjcp1910191

Associate Research Fellow (AS) 2019

46. Chonnikan Hanpaibool, Matina Leelawiwat, **Kaito Takahashi**, Thanyada Rungrotmongkol* November 2019, “Source of oseltamivir resistance due to single E119D and double E119D/H274Y mutations in pdm09H1N1 influenza neuraminidase” *Journal of Computer-Aided Molecular Design*, 34, 27-37. <https://doi.org/10.1007/s10822-019-00251-7>
47. Wen Chao, Cangtao Yin, **Kaito Takahashi**, Jim Jr-Min Lin* Sept 2019, “Effects of Water Vapor on the Reaction of CH₂OO with NH₃”, *Physical Chemistry Chemical Physics*, 21, 22589. DOI: 10.1039/c9cp04682h
48. Wen Chao, Cangtao Yin, **Kaito Takahashi**, Jim Jr-Min Lin* Sept 2019, “Hydrogen-Bonding Mediated Reactions of Criegee Intermediates — The Competition between Bimolecular and Termolecular Reactions and the Catalytic Role of Water”, *Journal of Physical Chemistry A*, 123, 8336-8348. DOI: 10.1021/acs.jpca.9b071
49. Sheng Yuan Tzeng, Changwu Dong, **Kaito Takahashi**, Wen Bih Tzeng* July 2019, “Cation spectra of p-chloroanisole and heavy atom effect on ionization energy”, *Chemical Physics Letter*, 731, 136626. <https://doi.org/10.1016/j.cplett.2019.136626>
50. **Kaito Takahashi*** July 2019, “The effect of pinning the lone pair on the direction of the OH stretching transition moment of water”, *Journal of Molecular Spectroscopy* 139, 111171. <https://doi.org/10.1016/j.jms.2019.07.002>

51. Daisuke Yoshida*, and **Kaito Takahashi*** June 2019, “Odd-Even Reactivity Variation due to Dynamical Effects around the Roaming Saddle Point of the Reaction Between C_n^- Chain ($n = 2-8$) and H_2 ”, *Journal of Physical Chemistry A*, 123, 5300-5308. DOI: 10.1021/acs.jpca.9b03435
52. Wen Chao, Yen-Hsiu Lin, Cangtao Yin, Wei-Hong Lin, **Kaito Takahashi,*** and Jim Jr-Min Lin* June 2019, “Temperature and Isotope Effects in the Reaction of CH_3CHO with methanol”, *Physical Chemistry Chemical Physics*, 21, 13633-13640. DOI: 10.1039/c9cp02534k
53. Yu-Lin Li, Yen-Hsiu Lin, Che-Yu Chiang, Cangtao Yin, Yuan-Pin Chang,* **Kaito Takahashi,*** Jim Jr-Min Lin April 2019, “Temperature-dependent Rate Coefficients for the Reaction of CH_3SH with Simplest Criegee intermediates”, *Journal of Physical Chemistry A* 123, 4096-4103. DOI: 10.1021/acs.jpca.8b12553
54. Wen Chao, Jim Jr-Min Lin, **Kaito Takahashi**, Alexandre Tomas, Lu Yu, Yoshizumi Kajii, Sebastien Batut, Coralie Schoemaeker, and Christa Fittschen* February 2019, “Water Vapor Does Not Catalyze the Reaction between Methanol and OH Radicals”, *Angewandte Chemie International Edition*, 58, 5013-5017. <https://doi.org/10.1002/anie.201900711>
55. Wen Chao, Cangtao Yin, Yu-Lin Li, **Kaito Takahashi***, Jim Jr-Min Lin* January 2019, “Synergy of water and ammonia hydrogen bonding in a gas-phase reaction”, *Journal of Physical Chemistry A*, 123, 1337-1342. DOI: 10.1021/acs.jpca.9b00672
56. **Kaito Takahashi*** January 2019, “How does vibrational excitation affect the X-ray absorption spectra of monohydrated halide and alkali metal clusters?”, chapter in *Quantum Systems in Physics, Chemistry and Biology, Theory, Interpretation, and Results* Volume 78, 57-81. <https://doi.org/10.1016/bs.aiq.2018.06.007>

Associate Research Fellow (AS) 2018

57. Yen-Hsiu Lin, Cangtao Yin, Wei-Hong Lin, Yu-Lin Li, **Kaito Takahashi***, Jim Jr-Min Lin* December 2018, “Criegee Intermediate Reaction with Alcohol Is Enhanced by a Single Water Molecule”, *Journal of Physical Chemistry Letters*, 9, 7040-7044. DOI: 10.1021/acs.jpcelett.8b03349
58. Yiqiang Liu, Cangtao Yin, Mica C. Smith, Siyue Liu, Xiaohu Zhou, Chunlei Xiao, **Kaito Takahashi,*** Jim Jr-Min Lin,* Wenrui Dong* and Xueming Yang* November 2018, “Kinetics of the simplest Criegee intermediate reaction with ammonia: a combination of experiment and theory”, *Physical Chemistry Chemical Physics*, 20, 29669-29676. DOI:

10.1039/c8cp05920a

59. Cangtao Yin, and **Kaito Takahashi***, July 2018, “Effect of unsaturated substituents in the reaction of Criegee intermediates with water vapor”, *Physical Chemistry Chemical Physics* 20, 20217-20227. DOI: 10.1039/c8cp02064g
60. Cangtao Yin, and **Kaito Takahashi***, May 2018, “How big is the substituent dependence of the solar photolysis rate of Criegee intermediates?”, *Physical Chemistry Chemical Physics*, 20, 16247-16255. DOI: 10.1039/c8cp02015a
61. Yen-Hsiu Lin **Kaito Takahashi**, and Jim Jr-Min Lin*, January 2018, “The reactivity of Criegee intermediates towards carbon dioxide”, *Journal of Physical Chemistry Letters*, 9, 184-188. DOI: 10.1021/acs.jpcclett.7b03154

Associate Research Fellow (AS) 2017

62. Do Ngoc Son, Pham Ngoc Thanh, Nguyen Dinh Quang, **Kaito Takahashi**, My Phuong Pham-Ho, April 2017, “First-principles study of Pd-skin/Pd3Fe(111) electrocatalyst for oxygen reduction reaction”, *Journal of Applied Electrochemistry*, 47, 747-754. DOI 10.1007/s10800-017-1077-y
63. Cangtao Yin, and **Kaito Takahashi***, May 2017, “How does substitution affect the unimolecular reaction rates of Criegee intermediates?”, *Physical Chemistry Chemical Physics*, 19, 12075 - 12084. DOI: 10.1039/c7cp01091e
64. Seongin Hong, Geonwook Yoo, Dong Hak Kim Won Geun Song, Ong Kim Le, Young Ki Hong, **Kaito Takahashi**, Inturu Omkaram, Do Ngoc Son, and Sunkook Kim, February 2017, “The doping mechanism and electrical performance of polyethylenimine-doped MoS₂ transistor”, *Physica Status Solidi C*, 14, 1600262. DOI 10.1002/pssc.201600262
65. Mica C. Smith, Wen Chao, Manoj Kumar, Joseph S. Francisco, **Kaito Takahashi***, Jim Jr-Min Lin*, January 2017, “Temperature-Dependent Rate Coefficients for the Reaction of CH₂OO with Hydrogen Sulfide”, *Journal of Physical Chemistry A*, 121, 938-945. DOI: 10.1021/acs.jpca.6b12303

Assistant Research Fellow (AS) 2016

66. Liang-Chun Lin, Wen Chao, Chun-Hung Chang, **Kaito Takahashi*** and Jim Jr-Min Lin*, September 2016, “Temperature dependence of the reaction of *anti*-CH₃CHOO with water vapor”, *Physical Chemistry Chemical Physics*, 18, 28189 - 28197. DOI: 10.1039/c6cp05171e
67. Wikorn Punyain, and **Kaito Takahashi***, September 2016, “Theoretical analysis on vibrational and photodetachment spectra of X⁻H₂O, X=F, Cl, Br”, *Physical Chemistry*

- Chemical Physics, 18, 26970-26979. DOI: 10.1039/c6cp04886b
68. Navchtsetseg Nergui, Miin-Jang Chen, Juen-Kai Wang, Yuh-Lin Wang, Cheng-Rong Hsing, Ching-Ming Wei and **Kaito Takahashi***, September 2016, “Dependence of Adenine Raman Spectrum on Excitation Laser Wavelength: Comparison between Experiment and Theoretical Simulations”, *Journal of Physical Chemistry A* 120, 8114-8122. DOI: 10.1021/acs.jpca.6b08311
69. Do Ngoc Son*, Nguyen Thi Gam, **Kaito Takahashi**, July 2016, “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*, 46, 1031-1038. DOI 10.1007/s10800-016-0982-9
70. Masato Morita, **Kaito Takahashi***, June 2016, “Ionic hydrogen bonding vibration in OH⁻(H₂O)₂₋₄” *Journal of Computational Chemistry Japan*, 15, 192-198. DOI 10.1007/s10800-016-0982-9
71. Yuan-Pin Chang*, Chun-Hung Chang, **Kaito Takahashi** and Jim Jr-Min Lin, April 2016, “Absolute UV absorption cross sections of dimethyl substituted Criegee intermediate (CH₃)₂COO”, *Chemical Physics Letters* 653, 155-160. <http://dx.doi.org/10.1016/j.cplett.2016.04.082>
72. Liang-Chun Lin, **Kaito Takahashi*** March 2016, “Will (CH₃)₂COO survive humidity?”, *Journal of Chinese Chemical Society*, 63, 472-479.
73. Liang-Chun Lin, Wen Chao, Mica Smith, Jim Jr-Min Lin*, **Kaito Takahashi***, Jan 2016, “Competition between H₂O and (H₂O)₂ reactions with H₂COO/CH₃CHOO”, *Physical Chemistry Chemical Physics*, 18, 4557-4568. DOI: 10.1039/c5cp06446e
74. Mica C. Smith, Wen Chao, **Kaito Takahashi**, Kristie A. Boering, and Jim Jr-Min Lin*, March 2016, “Unimolecular Decomposition Rate of the Criegee Intermediate (CH₃)₂COO Measured Directly with UV Absorption Spectroscopy”, *Journal of Physical Chemistry A*, 120, 4789-4798. DOI: 10.1021/acs.jpca.5b12124

Assistant Research Fellow (AS) 2015

75. Yoshiyuki Matsuda,* Hiroyuki Harigaya, Xie Min, **Kaito Takahashi**, Asuka Fujii*, October 2015, “Infrared spectroscopic investigations of cationic ethanol, propanol, and butanol”, *Chemical Physics Letter*, 640, 215-218. <http://dx.doi.org/10.1016/j.cplett.2015.10.044>
76. Do Ngoc Son*, Ong Kim Le, Chihai Viorel, **Kaito Takahashi**, September 2015, “Effects of Co Content in Pd-skin/PdCo Alloys for Oxygen Reduction Reaction:

- Prediction from Density Functional Theory Calculations”, *Journal of Physical Chemistry C*, 119, 24364-24372. DOI: 10.1021/acs.jpcc.5b06439
77. Jheng-Wei Li, Masato Morita, **Kaito Takahashi***, Jer-Lai Kuo*, October 2015, “Features in Vibrational Spectra Induced by Ar-Tagging for $\text{H}_3\text{O}^+ - \text{Ar}_m$ $m=0-3$ ”, *Journal of Physical Chemistry A*, 119, 10887-10892. DOI: 10.1021/acs.jpca.5b08898
78. Yudai Ogata, Yukio Kawashima, **Kaito Takahashi***, and Masanori Tachikawa*, September 2015, “Theoretical vibrational spectra of $\text{OH}^-(\text{H}_2\text{O})_2$: the effect of quantum distribution and vibrational coupling”, *Physical Chemistry Chemical Physics*, 17, 25505-25515. DOI: 10.1039/c5cp03632a
79. Kiichiro Koyasu, Tomohiro Ohtaki, **Kaito Takahashi***, and Fuminori Misaizu*, September 2015, “Even-Odd Product Variation of the $\text{C}_n^+ + \text{D}_2$ ($n=4-9$) Reaction: Complexity of the Linear Carbon Cation Electronic States”, *Physical Chemistry Chemical Physics*, 17, 24810-24819. DOI: 10.1039/c5cp04480d
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81. Ren-Jie Lin, Quoc Chinh Nguyen, Yew-Soon Ong, **Kaito Takahashi*** and Jer-Lai Kuo*, July 2015, “Temperature dependent structural variations of $\text{OH}^-(\text{H}_2\text{O})_n$ $n=4-7$: Effects on Vibrational and Photoelectron Spectra”, *Physical Chemistry Chemical Physics*, 17, 19162-19172. DOI: 10.1039/c5cp02604k
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83. Hirokazu Takahashi, **Kaito Takahashi**, and Satoshi Yabushita*, April 2015, “Interpretation of Semiclassical Transition Moments through Wavefunction Expansion of Dipole Moment Function with Application to the OH Stretching Spectra of Simple Acids and Alcohols”, *Journal of Physical Chemistry A*, 119, 4834-4845. DOI: 10.1021/acs.jpca.5b02050
84. Yoshiyuki Matsuda*, Tomoya Endo, Naohiko Mikami, Asuka Fujii, Masato Morita, and **Kaito Takahashi***, April 2015, “The large variation in acidity of diethylether cation induced by internal rotation around a single covalent bond”, *Journal of Physical*

Chemistry A, 119, 4885-4890. DOI: 10.1021/acs.jpca.5b02604

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Assistant Research Fellow (AS) 2014

87. Masato Morita, Hirokazu Takahashi, Satoshi Yabushita*, and **Kaito Takahashi***, October 2014, “Why does the IR Spectra of Hydroxide Stretching Vibration weaken with increase in hydration?”, *Physical Chemistry Chemical Physics*, 16, 23143-23149. DOI: 10.1039/c4cp03623a
88. Mica C. Smith, Wei-Lun Ting, Chun-Hung Chang, **Kaito Takahashi**, Kristie A. Boering, Jim Jr-Min Lin, August 2014, “UV Absorption Spectrum of the C2 Criegee Intermediate CH_3CHOO ”, *Journal of Chemical Physics*, 141, 074302. <http://dx.doi.org/10.1063/1.4892582>

Assistant Research Fellow (AS) 2013

89. Masato Morita, and **Kaito Takahashi***, August 2013, “Multidimensional local mode calculations for the vibrational spectra of $\text{OH}^-(\text{H}_2\text{O})_2$ and $\text{OH}^-(\text{H}_2\text{O})_2\cdot\text{Ar}$ ”, *Physical Chemistry Chemical Physics*, 15, 14973-14985. DOI: 10.1039/c2cp42501g
90. **Kaito Takahashi***, Micheal Y. Hayes, and Rex T Skodje*, January 2013, “A study of resonance progressions in the $\text{F}+\text{HCl}\rightarrow\text{Cl}+\text{HF}$ reaction: A lifetime matrix analysis of pre-reactive and post-reactive collision complexes”, *Journal of Chemical Physics*, 138, 024309. <http://dx.doi.org/10.1063/1.4774057>
91. Masato Morita, and **Kaito Takahashi***, January 2013, “Multidimensional OH local mode calculations for $\text{OH}^-(\text{H}_2\text{O})_3 \sim$ Importance of intermode anharmonicity \sim ”, *Physical Chemistry Chemical Physics* 15, 114-124. DOI: 10.1039/c3cp51903a

Assistant Research Fellow (AS) 2012

92. Ohki Kambara, **Kaito Takahashi***, Michitoshi Hayashi, and Jer-Lai Kuo*, July 2012, “Assessment of density functional theory to calculate the phase transition pressure of ice at 0K”, *Physical Chemistry Chemical Physics* 14, 11484-11490. DOI:

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94. Do Ngoc Son, and **Kaito Takahashi***, February 2012, “Selectivity of Palladium-Cobalt Surface Alloy toward Oxygen Reduction Reaction”, *Journal of Physical Chemistry C*, 116, 6200-6207. dx.doi.org/10.1021/jp2094615
95. Masato Morita, and **Kaito Takahashi***, January 2012, “Theoretical Study on the difference of OH Vibrational spectra between $\text{OH}^-(\text{H}_2\text{O})_3$ and $\text{OH}^-(\text{H}_2\text{O})_4$ ”, *Physical Chemistry Chemical Physics* 14, 2797-2808. DOI: 10.1039/c2cp23203k

Assistant Research Fellow (AS) 2011

96. Hui-Yi Chen, Yu-Lung Cheng, and **Kaito Takahashi***, November 2011, “Theoretical Calculation of the OH Vibrational Overtone Spectra of 1,5-Pentanediol and 1,6-Hexanediol”, *Journal of Physical Chemistry A*, 115, 14315-14324. dx.doi.org/10.1021/jp206202u
97. I-Cheng Chen, Andrew F Chen, Wen-Tsung Huang, **Kaito Takahashi** and Jim J. Lin*, September 2011, “Photolysis Cross-Section of Ozone Dimer”, *Chemistry An Asian Journal*, 6, 2925-2930. DOI: 10.1002/asia.201100526
98. Marta Maron, Richard Shoemaker, **Kaito Takahashi**, and Veronica Vaida*, September 2011, “Hydration of Pyruvic Acid to its Geminal-Diol, 2,2-Dihydroxypropanoic Acid, in a Water-Restricted Environment”, *Chemical Physics Letters*, 513, 184-190. doi:10.1016/j.cplett.2011.07.090
99. Yu-Lung Cheng, Hui-Yi Chen, and **Kaito Takahashi***, May 2011, “Theoretical Calculation of the OH Vibrational Overtone Spectra of 1-n Alkane Diols (n=2-4): Origin of Disappearing Hydrogen-Bonded OH Peak”, *Journal of Physical Chemistry A*, 115, 5641-5653. dx.doi.org/10.1021/jp202030c

Assistant Research Fellow (AS) 2010

100. Zeb C. Kramer, **Kaito Takahashi**, and Rex T. Skodje*, October 2010, “Water Catalysis and Anticatalysis in Photochemical Reactions: Observation of a Delayed Threshold Effect in the Reaction Quantum Yield”, *Journal of American Chemical Society*, 132, 15154-15157. [10.1021/ja107335t](http://dx.doi.org/10.1021/ja107335t)
101. **Kaito Takahashi***, July 2010, “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*, 12, 13950-13961. DOI: 10.1039/c0cp00788a
102. Jessica L. Axson, **Kaito Takahashi**, David O. De Haan, and Veronica Vaida*, April 2010, “Gas Phase water mediated equilibrium between methylglyoxal and its geminal diol”, *Proceedings of National Academy of Science*, 107, 6687-6692. www.pnas.org/cgi/doi/10.1073/pnas.0912121107
103. **Kaito Takahashi**, Kathryn Plath, Jessica Axson, Galen Nelson, Rex T. Skodje, and Veronica Vaida*, March 2010, “Dynamics and Spectroscopy of Vibrational Overtone Excited Glyoxylic Acid and 2,2-Dihydroxyacetic Acid in the Gas-Phase”, *Journal of Chemical Physics*, 132, 094305. 10.1063/1.3327839
- Post-Doctoral Research with Prof. Skodje (2005-2009)**
104. Holger Schneider, **Kaito Takahashi**, Rex T. Skodje*, and J. Mathias Weber*, May 2009, “Infrared Spectra of $SF_6^-HCOOH...Ar_n$ (n=0-2): Infrared-Triggered Reaction and Ar-Induced Inhibition“, *Journal of Chemical Physics*, 130, 174302. <https://doi.org/10.1063/1.3125960>
105. Kathryn L. Plath, **Kaito Takahashi**, Rex. T. Skodje*, and Veronica Vaida*, March 2009, “Fundamental and Overtone Spectra of Gas-Phase Pyruvic Acid”, *Journal of Physical Chemistry A*, 113, 7294-7303. <https://doi.org/10.1021/jp810687t>
106. Kathryn L. Plath, Jessica L. Axson, Galen C. Nelson, **Kaito Takahashi**, Rex. T. Skodje, and Veronica Vaida*, February 2009, “Gas-phase vibrational spectra of glyoxylic acid and its gem diol monohydrate. Implications for atmospheric chemistry”; *Reaction Kinetics and Catalysis Letters*, 96, 209-224. <https://doi.org/10.1007/s11144-009-5528-2>
107. Meghan E. Dunn, George C. Shields, **Kaito Takahashi**, Rex T. Skodje, and Veronica Vaida*, August 2008, “Experimental and theoretical study of the OH vibrational spectra and overtone chemistry of gas-phase vinylacetic acid”, *Journal of Physical Chemistry A*, 112, 10226-10235. <https://doi.org/10.1021/jp805746t>
108. **Kaito Takahashi**, Kathryn L. Plath, Rex. T. Skodje*, and Veronica Vaida*, June 2008, “Dynamics of Vibrational Overtone Excited Pyruvic Acid in the Gas Phase: Line Broadening through Hydrogen-Atom Chattering”, *Journal of Physical Chemistry A*, 112, 7321-7331. <https://doi.org/10.1021/jp803225c>
109. Veronica Vaida*, Karl J. Felerabend, Nabilah Rontu, and **Kaito Takahashi**, May

- 2008, “Review Article Sunlight-Initiated Photochemistry: Excited Vibrational States of Atmospheric Chromophore”, International Journal of Photoenergy, Article ID 138091. <https://doi.org/10.1155/2008/138091>
110. **Kaito Takahashi**, Zeb C. Kramer, Veronica Vaida, and Rex T. Skodje*, June 2007, “Vibrational overtone induced elimination reactions within hydrogen-bonded molecular clusters: the dynamics of water catalyzed reactions in $\text{CH}_2\text{FOH}(\text{H}_2\text{O})_n$ ”, Physical Chemistry Chemical Physics, 9, 3864-3871. <https://doi.org/10.1039/B705264B>
111. Michael P. Deskevich, Michael Y. Hayes, **Kaito Takahashi**, Rex T. Skodje, and David J. Nesbitt*, June 2006, “Multireference Configuration Interaction Calculations for the $F + \text{HCl} \rightarrow \text{HF} + \text{Cl}$ Reaction: A Correlation Scaled Ground State Potential Energy Surface”, Journal of Chemical Physics, 124, 224303. <https://doi.org/10.1063/1.2192505>
112. Daniel K. Havey, Karl J. Feierabend, **Kaito Takahashi**, Rex T. Skodje, and Veronica Vaida*, March 2006, “Experimental and Theoretical Investigation of Vibrational Overtones of Glycolic Acid and its Hydrogen Bonding Interactions with Water”, Journal of Physical Chemistry A, 110, 6439-6446. <https://doi.org/10.1021/jp060602q>
113. Michael Y. Hayes, Michael P. Deskevich, David J. Nesbitt, **Kaito Takahashi**, and Rex T. Skodje*, September 2005, “A Simple Picture for the Rotational Enhancement of the Rate for the $F + \text{HCl} \rightarrow \text{HF} + \text{Cl}$ Reaction: A Dynamical Study Using a New ab initio Potential Energy Surface”, Journal of Physical Chemistry A, 110, 436-444. <https://doi.org/10.1021/jp0535745>

PhD Study with Prof. Yabushita (2000-2005)

114. **Kaito Takahashi**, Michihiko Sugawara, and Satoshi Yabushita*, March 2005, “Effective One-Dimensional Dipole Moment Function for the OH Stretching Spectra of Simple Acids and Alcohols”, The Journal of Physical Chemistry A, 109, 4242-4251. <https://doi.org/10.1021/jp045041m>
115. **Kaito Takahashi**, Michihiko Sugawara, and Satoshi Yabushita*, September 2003, “Theoretical Analysis on the Fundamental and Overtone OH Stretching Spectra of Several Simple Acids and Alcohols”, The Journal of Physical Chemistry A, 107, 11092-11101. <https://doi.org/10.1021/jp0346965>
116. **Kaito Takahashi**, Michihiko Sugawara, and Satoshi Yabushita*, November 2001, “Theoretical Analysis of the CH Stretching Overtone Vibration of 1,2-Dichloroethylene”, The Journal of Physical Chemistry A, 106, 2676-2684. <https://doi.org/10.1021/jp0135252>

INVITED ORAL PRESENTATIONS AT CONFERENCES

1. **Kaito Takahashi** “Carbon anion chain meets hydrogen molecule: To roam or not“ at Pure and Applied Chemistry International Conference 2020, held in Impact Forum, Muangthong Thani, Bangkok, Thailand at February 13,14, 2020.
2. **Kaito Takahashi** “Theoretical view on gas phase water catalysis at room temperature” Asian Pacific Conference on Theoretical Chemistry, Sydney, Australia, September 30 to October 4, 2019.
3. **Kaito Takahashi** “How Big is the Substituent Dependence of the Solar Photolysis Rate of Criegee Intermediates?” at the 10th Asian Photochemistry Conference held at Taipei Taiwan Dec 16-20, 2018.
4. **Kaito Takahashi** “Theoretical Simulation of X-ray Absorption Spectra of Monohydrated Halide and Alkali Metal Clusters” Asian Consortium on Computational Materials Science – Theme Meeting on Multiscale Modelling of Materials for Sustainable Development” held at Vietnam National University Hanoi, from Sept 7 to 9, 2018.
5. **Kaito Takahashi** and Cangtao Yin “Theoretical Study on Criegee Intermediate Activity in the Atmosphere“, at the Pure and Applied Chemistry International Conference 2018, held at Had Yai, Thailand Feb 6-8, 2018.
6. **Kaito Takahashi** “How Does Vibrational Motion Effect the Electron Detachment from Monohydrated Halide Anion” at 9th Asian Consortium on Computational Materials Science held at Kuala Lumpur Aug 8-11, 2017.
7. **Kaito Takahashi** “Substitution effect in the reaction rate of Criegee Intermediates with Water Vapor” The 21st International Annual Symposium on Computational Science and Engineering, held at Bangkok Thailand Aug 3-4, 2017.
8. **Kaito Takahashi** “Theoretical modelling for reaction rates” at The 11th General Meeting of Asian Consortium on Computational Materials Science-Virtual Organization held at Sendai Japan, from December 19-21, 2016.
9. **Kaito Takahashi** “Theoretical analysis on electron detachment from small hydrated anion clusters”, at the third international conference on computation science and

- engineering held at Ho Chi Ming City Vietnam from November 28-30, 2015.
10. **Kaito Takahashi** “Theoretical rate coefficient calculation for C3Criegee intermediate water vapor reaction” at 7th Cross-strait Theoretical and Computational Chemistry, Changsha, Hunan, October 14-18, 2016.
 11. **Kaito Takahashi** “Some points to consider for theoretical simulation on oxygen reduction reaction catalysis” at Lecture Workshop on Advanced Materials Engineering in Madurai, India September 26, 2016.
 12. **Kaito Takahashi** “Ab Initio Modelling and Transient Absorption Measurement of Criegee Intermediate Water Vapor Reaction” at Theme meeting of Asian Consortium on Computational Materials Science in SRM University, Chennai India, September 21-24, 2016.
 13. **Kaito Takahashi** “Theoretical understanding on the Criegee intermediate decay process” at The 32nd symposium on Chemical Kinetics and Dynamics at Saitama University, Japan, June 1-3, 2016.
 14. **Kaito Takahashi** ”Theoretical analysis on electron detachment from small hydrated anion clusters” at the Seventh Aisa-Pacific Conference of Theoretical and Computational Chemistry held in Taiwan, January 25-28, 2016.
 15. **Kaito Takahashi** “What can we learn on hydroxide solvation from theoretical study on OH-(H₂O)_n n=0-7?” at The International Chemical Congress of Pacific Basin Societies 2015 at Sheraton Hotel Honolulu, from December 15-20, 2015.
 16. **Kaito Takahashi** “Theoretical Study on effect of water clustering on reactions: Dynamical and statistical aspects” at The International Chemical Congress of Pacific Basin Societies 2015 at Sheraton Hotel Honolulu, from December 15-20, 2015.
 17. **Kaito Takahashi** “Carbon Chain Ion Reaction with D₂: Differences between Cation and Anion” at Reaction Dynamics Symposium commemorating IAMS 20th Anniversary, Taiwan from Nov 10-11, 2015.
 18. **Kaito Takahashi** “Competition between H₂O and (H₂O)₂ reaction with H₂COO/CH₃CHOO” at The 10th General Meeting of Asian Consortium on Computational Materials Science-Virtual Organization held at Sendai Japan, from November 1-3, 2015.
 19. **Kaito Takahashi** “Is carbonyl oxide reaction with water vapor fast?” at 19th East Asia Workshop on Reaction Dynamics held at Australia, from October 4-8, 2015.
 20. **Kaito Takahashi** “How many water molecules contribute to atmospherically relevant

- carbonyl oxide water reaction” at QSCP XX meeting held at Varna Bulgaria from September 14-20, 2015.
21. **Kaito Takahashi** “Understanding the reaction of atmospherically relevant carbonyl oxide with water vapor” at Symposium on The 2nd Advanced Materials for ASEAN Network held at Phitsanulok Naresuan University, on July 23, 2015.
 22. **Kaito Takahashi** “Tug of war between H_3O^+ versus Ar/OH ” at Asian Consortium on Computational Materials Science held at Taipei Taiwan, from June 16-18, 2015.
 23. **Kaito Takahashi** “Theoretical Study on photodissociation of ClOOCl at wavelength longer than 300nm” at 6th Cross Strait Theoretical and Computational Chemistry Conference held at Chong Zheng University in Taiwan from January 26-30, 2015.
 24. **Kaito Takahashi** “Coupling in electronic states and its imprint on reaction” at Asian Core Winter School held at Institute of Molecular Sciences Okazaki Japan, from January 13-16, 2015.
 25. **Kaito Takahashi** “Photodissociation dynamics of ClOOCl at wavelength longer than 300 nm” at The 9th General Meeting of Asian Consortium on Computational Materials Science-Virtual Organization held at Okinawa Institute of Science and Technology, from December 20-22, 2014.
 26. **Kaito Takahashi** “*What can we say to the condensed phase studies with detailed studies on clusters $\text{OH}(\text{H}_2\text{O})_n$, $n=2-4$* ” QSCP XIX meeting held at Taipei Taiwan from November 11-17, 2014.
 27. **Kaito Takahashi**, “Theoretical Study on the Broad Strongly Hydrogen Bonded OH Stretching Peaks of $\text{OH}^-(\text{H}_2\text{O})_n$, $n=2-4$ ” at The Seventh International Conference on Advanced Vibrational Spectroscopy held at Kobe, Japan from Aug 25-30, 2013.
 28. **Kaito Takahashi**, Masato Morita “Theoretical study on the broad strongly hydrogen bonded OH stretching peaks of small hydroxide water clusters” at 15th Asian Chemistry Congress held at Singapore from Aug 19-23, 2013.
 29. **Kaito Takahashi**, “Theoretical study on the effect of hydrogen bonding toward the observed OH vibrational spectra: Are red shift and width correlated?” at the 6th Asia-Pacific Conference of Theoretical and Computational Chemistry held at Gyeongju, Korea from Jul 10-13, 2013.
 30. **Kaito Takahashi** Masato Morita “Theoretical Study on OH Vibrational Spectra of Deprotonated Water Clusters $\text{OH}^-(\text{H}_2\text{O})_3$ and $\text{OH}^-(\text{H}_2\text{O})_4$ ” at 12th International Conference on Quantum Chemistry” held at Waseda University in Tokyo Japan from Sept

2 to 8 2011.

31. **Kaito Takahashi** “Theoretical study on OH stretching vibrational energy decay in protonated, deprotonated and neutral water clusters” Molecular & Ionic Cluster Conference 2010 held at Atema Kougen Hotel Bernatio, from Sept 5 to 11, 2010 (Poster, hot topic oral)
32. **Kaito Takahashi** “Theoretical Study on the effect of intramolecular hydrogen bonding on the width of OH stretching overtones” at the The International Chemical Congress of Pacific Basin Societies 2010 at Sheraton Hotel Honolulu, from Dec 15 to 20, 2010.

FUNDED PROPOSALS

1. “Spin State Control for Electrochemical Reactions” Sirindhorn International Institute of Technology Young Researcher Grant 2024 (SIIT-2024-YRG-KT02) 500,000 Baht
2. “Multireference calculation on metal atom interaction with gas molecules”, National Science and Technology Council NTD 1,800,000 per year, August 2022-July 2025.
3. “Theoretical Study on Water Catalyzed Reaction” Ministry of Science and Technology, NTD 1,700,000 per year, August 2019-July 2022.
4. “Development of Accurate Reaction Rate Calculations for Atmospheric Chemistry” Academia Sinica Career Development Award, NTD 3,500,000 per year, Jan 2017-Dec 2021.
5. “Accurate theoretical rates for carbonyl oxide and water vapor reaction” Ministry of Science and Technology, NTD 4,595,000 (total for 3 years), August 2016-July 2018.
6. “Spectroscopic Properties of Hydrated Anion Clusters: $X^-(H_2O)_n$ $X=OH, F, Cl, Br, I$; $n=2-5$ ” National Science Council of Taiwan, NTD 3,900,000 (total for 3 years), August 2013-July 2016.
7. “Vibrational Spectra of Condensed Phase Water: Beyond Fundamental Excitation” National Science Council of Taiwan, NTD 2,010,000 (total for 2 years), August 2011-July 2013.
8. “Dynamics Calculation on Photoinduced Processes of Importance in the Atmosphere” National Science Council of Taiwan, New Taiwan Dollars 2,925,000 (total for 2 years), October 2009-July 2011.

PROFESSIONAL MEMBERSHIPS:

Member of the Chemical Society of Japan
Member of the American Chemical Society
Member of the Chemical Society Located in Taiwan

AWARDS

2017 Academia Sinica Career Development Award
2017 QSCP Promising Scientist Prize of COMA

TEACHING EXPERIENCE (Graduate level)

2017 Fall (Half semester) National Taiwan Normal University “Special Topics in Physical Chemistry”

2013, 2015, 2017, 2019, 2021, 2023 Spring (Half semester) Taiwan International Graduate Program “Computational Materials Science”

2015, 2016, 2017, 2018 Spring (4 weeks) National Taiwan University “Introduction to recent trends in atomic and molecular physics”

2018, 2019, 2020, 2021, 2022 Spring and Fall (Full Semester) Taiwan International Graduate Program “Colloquium Course”