Grace Hsiao-Han Chuang

CONTACT INFORMATION

Max-Planck Institute for the Physics of Complex Systems
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RESEARCH INTERESTS

Light-Matter Interaction | Open Quantum Systems | Electronic Excited State|
Non-Adiabatic Molecular Dynamics | Selectivity of Chemical Reactions |

EDUCATION

Doctor of Philosophy in Physical Chemistry *Sept. 2013 – July 2020*
Department of Chemistry, National Taiwan University Taipei, Taiwan
Taiwan International Graduate Program, Academia Sinica
Supervisor: Dr. Chao-Ping Hsu
Dissertation: "Two-Dimensional Potential Energy Surfaces of the Reactions with Post-Transition-State Bifurcation" doi:10.6342/NTU202001503

Master of Science in Physical Chemistry *Sept. 2010 – July 2012*
Department of Chemistry and Biochemistry, National Chung-Cheng University
Supervisor: Dr. Wei-Ping Hu Chiayi, Taiwan
Thesis: "Theoretical Study on the Excited-State Proton Transfer Reactions and on the Prebiotic Synthesis of α-Amino Acids" (in Chinese) NDLTD ID: 099CCU00065056

Bachelor of Science in Chemistry *Sept. 2005 – June 2009*
Department of Chemistry, Chung-Yuan Christian University Zhongli, Taiwan
Supervisor: Dr. Hsi-Wei Jia

RESEARCH EXPERIENCE

Guest Scientist *Feb. 2023 – Present*
Finite System Department Dresden, Germany
Max Planck Institute for the Physics of Complex Systems (MPIPKS)
Principal Investigator: Dr. Alexander Eisfeld

- Investigated the impact of transition current density in the strong-coupling regime (coherent dynamics) for confined 2D materials to enhance the understanding of excitonic interactions.

Research Associate *Aug. 2021 – Feb. 2023*
School of Chemistry, University of Leeds Leeds, UK
Principal Investigator: Dr. Dmitry Shalashilin

- Studied the reaction dynamics of electron-impact processes using conventional trajectory-based methods in the field of non-adiabatic molecular dynamics.

Research Associate *Dec. 2020 – July 2021*
School of Applied Mathematics, University of Bristol Bristol, UK
Principal Investigator: Dr. Stephen R. Wiggins

- Applied Lagrangian descriptors to analyse phase space structures in general reaction dynamics.

Postdoctoral Researcher *Sept. 2020 – Oct. 2020*
Institute of Chemistry, Academia Sinica Taipei, Taiwan
Principal Investigator: Dr. Chao-Ping Hsu

- Investigated electronic correlation effects in interstellar glycine formation using high-level electronic excited-state structure methods.

Visiting Scholar *May 2018 – Apr. 2019*
Department of Chemistry, University of California, Davis California, USA
Supervisor: Dr. Dean J. Tantillo

- Investigated dynamics and and built tools to generate potential energy surfaces for reactions with post-transition state bifurcation.

Doctoral Research *Aug. 2015 – Apr. 2018*
Institute of Chemistry, Academia Sinica Taipei, Taiwan
Supervisor: Dr. Chao-Ping (Cherri) Hsu

- Used Q-Chem and diabatic Hamiltonians for constructing potential energy curves of proton-coupled electron transfer (PCET) reactions.
- Studied sugar chemistry with experimentalists.

Doctoral Research *Aug. 2013 – Jul. 2015*
Institute of Atomic and Molecular Sciences, Academia Sinica Taipei, Taiwan
Supervisor: Dr. Jer-Lai Kuo

- Derived the analytical expression up to the 4^{th}-body term of anharmonic oscillators.

Research Assistant *Aug. 2012 – Jul. 2013*
Institute of Atomic and Molecular Science, Academia Sinica Taipei, Taiwan
Supervisor: Dr. Jer-Lai Kuo

- Understand the anharmonicity of the O−H bond in molecular clusters using IR spectrum for their predissociation reactions.

Masters Research *Aug. 2010 – Jul. 2012*
Department of Chemistry and Biochemistry Chiayi, Taiwan
National Chung-Cheng University
Supervisor: Dr. Wei-Ping Hu

- Found the barrierless intramolecular proton transfer mechanism and confirmed by time-resolved femtosecond spectroscopy.

Publications

Peer-Reviewed Journals

W. Quapp, **G.H.-H. Chuang**, J.M. Bofill, "Exploring potential energy surfaces around a valley bifurcation"
Theor. Chem. Acc. **2025**, *144*, 67. 10.1007/s00214-025-03225-1

D.V. Makhov, G. Armstrong, **G.H.-H. Chuang**, H. Ambalampitiya, K. Lemishko, S. Mohr, A. Nelson, J. Tennyson, D. Shalashilin, "Dissociation of hydrofluorocarbon molecules after electron impact in plasma"
J. Phys. Chem. Lett. **2024**, *15*, 3404. 10.1021/acs.jpclett.4c00348

B. Chen, R.Y. He, H.M. Chien, C.C. Lee, **G.H.-H. Chuang**, C.P. Hsu, J. Chan, J.T. Huang, "Superresolution Imaging of Photochromic Acylhydrazone Moieties on Amyloid Nanofibrils: Implications for Photoswitchable Probes"
ACS Appl. Nano Mater. **2022**, *5*, 1734. 10.1021/acsanm.1c04004

G.H.-H. Chuang, D.J. Tantillo, C.P. Hsu, "Construction of Two-Dimensional Potential Energy Surfaces of Reactions with Post-Transition-State Bifurcations"
J. Chem. Theory Comput. **2020**, *16*, 4050. 10.1021/acs.jctc.0c00172

C.W. Chang, C.H. Wu, M.H. Line, P.H. Liao, C.C. Chang, **G.H.-H. Chuang**, S.C. Lin, S. Lam, V.P. Verma, C.P. Hsu, C.C. Wang, "Establishment of Guidelines for the Control of Glycosylation Reactions and Intermediates by Quantitative Assessment of Reactivity.",
Angew. Chem. Int. Ed. **2019**, *58*, 16775. 10.1002/anie.201906297

K.C. Tang, C.L. Cheng, **G.H.-H. Chuang**, J.L. Chen, Y.J. Lin, J.Y. Shen, W.P. Hu, P.T. Chou, "A Genuine Intramolecular Proton Relay System Undergoing Excited-State Double Proton Transfer Reaction",
J. Phys. Chem. Lett. **2011**, *2*, 3063. 10.1021/jz201439w

Under Review

G.H.-H. Chuang, A. Pendse, "Capturing spin chain dynamics with periodically projected time-dependent basis " **2025**
- Submitted to Journal of Computational Physics (Referee report received: July 2025)
arXiv:2306.07407v3

In Preparation

G.H.-H. Chuang, U. Saalmann, A. Eisfeld, "Calculating Excitonic Interactions using Transition Currents with Application to PTCDA" **2025**

Thesis & Dissertation

G.H.-H. Chuang, "Two-Dimensional Potential Energy Surfaces of the Reactions with Post-Transition-State Bifurcation",
PhD dissertation, National Taiwan University **2020**
10.6342/NTU202001503

G.H.-H. Chuang, "Theoretical Study on the Excited-State Proton Transfer Reactions and on the Prebiotic Synthesis of α-amino acids",
Master's thesis, National Chung-Cheng University **2012**
NDLTD ID: 099CCU00065056

Academic Service

Reviewer for Scientific Journals

Theoretical Chemistry Accounts *Mar. 2025*
Reviewed a theoretical chemistry manuscript involving reaction mechanisms and astrochemical relevance.

Organisation of Conferences, Seminars & Workshops

Co-organiser - Finite Systems Department Seminar *Feb. 2025*
Max Planck Institute for the Physics of Complex Systems Germany
Organised a departmental seminar, managed speaker invitations, coordinated schedules, and facilitated collaboration and knowledge exchange.

Co-organiser - 1^{st} Taiwan–Philippines Workshop *Oct. 2017*
Institute of Chemistry, Academia Sinica Taiwan
Managed overall event organisation, including scheduling, speaker coordination, and participant engagement.

Coordinator - Growing Career Workshop *Feb. 2017*
Institute of Chemistry, Academia Sinica Taiwan
Handled programme logistics and planning, supporting career development and enhancing professional skills for graduate students.

Volunteer & Leadership Roles

Volunteer - 10^{th} Woman in Physical and Chemical Science Workshop *Oct. 2017*
The Society of Taiwan Women in Science and Technology Taiwan
Coordinated speaker sessions, facilitated networking, and promoted visibility for women in science. [Event Link]

Volunteer - 8^{th} Asian Consortium on Computational Material Science *June 2015*
Institute of Atomic and Molecular Sciences, Academia Sinica Taiwan
Assisted in organising and coordinating the event, designed promotional materials, and supported logistical activities. [Event Link]

Outreach & Public Speaking

Distinguished Speaker - Lecture on Scientific Conference Planning *May 2024*
Junior Chemist Society, Institute of Chemistry, Academia Sinica Taiwan
Delivered presentations on effective scientific conference planning, sharing academic and cultural experiences from the US, UK, and Germany. [Event Link]

Speaker - Taiwan Academic Talents Overseas Advancement Program *Dec. 2019*
National Sciences and Technology Council Taiwan
Spoke on pursuing academic careers abroad, offering insights on research opportunities, cultural adaptation, and international collaboration.

Speaker - Chemical Society National Meeting *Dec. 2016*
Taiwan
Delivered a talk focused on motivating graduate students through effective mentorship, goal-setting, and supportive research environments.

Public Lecturer - International Academic Competence Conference *Dec. 2013*
National Taiwan University Taiwan
Provided a public lecture simplifying complex quantum mechanics concepts using visual aids and relatable analogies. [Event Link]

Teaching Experience

International Max Planck Research School *Aug. 2025*
Exploring and Harnessing Non-Adiabatic Processes Germany

- Designed and delivered a three-hour lecture on Non-Adiabatic Molecular Dynamics (NAMD), using Mathematica to demonstrate three basic methods: Born–Oppenheimer Molecular Dynamics (BOMD), Ehrenfest dynamics, and Trajectory Surface Hopping (TSH).
- Combined analytical models with electronic structure theory (EST) concepts to illustrate the role of EST and energy near-degeneracy regions—such as avoided crossings—in model diatomic molecular systems. [IMPRS Summer School 2025]

University of Leeds *Oct. 2022*
Workshop for Physical Chemists UK

- Delivered specialised lectures on electronic structure theory (EST), with a rigorous theoretical derivation of EST models tailored to physical chemists.
- Emphasised the mathematical foundations and practical applications of quantum chemistry models, ensuring students grasped both conceptual and real-world aspects.

University of Bristol *June 2021*
Workshop for Mathematicians UK

- Designed and taught lectures on simplified Hartree-Fock theory, adapted for audiences with a formal mathematical background.
- Used a Jupyter Notebook-based implementation of the helium atom to illustrate computational workflows in EST.
- Promoted an understanding of numerical techniques underpinning quantum models via hands-on Python coding. [Teaching code on GitHub]

University of California, Davis *Aug. 2018 – Oct. 2018*
Workshop for Organic Chemists USA

- Conducted chalkboard lectures connecting electronic structure theory with practical applications in organic reaction mechanisms.
- Integrated examples from students' research to demonstrate how computational methods elucidate reaction pathways and molecular properties.
- Developed and provided mathematical exercises aligned with their chemical interests to foster interdisciplinary learning.

Chung-Yuan Christian University *Sept. 2007 – Feb. 2008*
Teaching Assistant of Quantum Chemistry Taiwan

- Supported undergraduate teaching by leading tutorials, explaining theoretical concepts, and answering student questions during office hours.
- Reinforced students' understanding of quantum mechanics fundamentals through applied problem-solving.

Advising Experience

School of Chemistry, University of Leeds *Feb. 2022 – Feb. 2023*
UK

- Supervised a first-year PhD student, offering guidance on her research project on the coupled-coherent state method and supporting her academic development.
- Held regular one-on-one meetings to discuss research progress and designed targeted tasks to strengthen her mathematical and programming skills.

Research Presentations

Invited Talks

The Mixed-Gen Lecture Series — *May 2025*
Taiwan Theoretical and Computational Molecular Sciences Association — Taiwan
National Center for Theoretical Sciences - Physics Division — (Online)
"Calculating excitonic interactions using transition currents with application to PTCDA"

The Finite Systems Department Seminar — *Feb. 2023*
Max Planck Institute for the Physics of Complex Systems — Germany
"From Physical Chemistry to More Physical Projects"

Atmospheric, Planetary and Theoretical Chemistry Seminar — *Jan. 2023*
School of Chemistry, University of Leeds — UK
"Electron-Molecule Collision of Hydrofluoroolefins"

11th International Meeting on Photodynamics and Related Aspects — *Nov. 2022*
"Using Coherent States to Study Dynamics of Rydberg Atom Chain" — Cuba

1st Symposium and Workshop on First-Principles Calculations — *Aug. 2022*
University of the Philippines Los Banos — Philippines
"*Using the Moving Grids in Both Chemistry and Physics*" — (Online)

Selected Oral Presentations

88th Deutsche Physikalische Gesellschaft — *Mar. 2025*
"Calculating excitonic interactions using transition currents with application to PTCDA" — Germany

87th Deutsche Physikalische Gesellschaft — *Mar. 2024*
"Interaction Between Polyatomic Molecules on Layered Surfaces beyond the Dipole Approximation" — Germany

Kinetic Monte Carlo Modeling Workshop — *July 2017*
"How do we Design an Artificial Catalyst for Hydrogen Gas Production: Lessons from the Key Reaction Mechanism" — Taiwan

Theoretical and Computational Molecular Sciences Association — *Sept. 2014*
"Spectroscopic Study of the O–H Stretching Motions in $H^+(CH_3OH)_{1-3}X_{0-2}$, X=Ar and N_2" — Taiwan

69th International Symposium on Molecular Spectroscopy — *June 2014*
"The Free O–H Anharmonic Stretching Motions in $H^+(CH_3OH)_{1-3}$ with/ without Attached Argon" — USA

Selected Poster Presentations

Coherent Control with Modified Vacuum Fields — *Aug. 2024*
"Interaction between polyatomic molecules on layered surfaces - beyond the dipole approximation" — Sweden

Path Integral Quantum Mechanics Workshop — *June 2023*
"Preserve Non-Stationary Long-Term Dynamics via Selected Incomplete Dual Bases" — Israel

Spectroscopy and Dynamics Group Annual Conference — *Apr. 2022*
"Building a Many-Body Wave Function with Less Computational Cost: Coupled-Coherent State" — UK

NTU Graduate Student Poster Presentation — *June 2020*

"A General Method for Probing a Special Reaction with the Intrinsic Selectivity is Developed by Modifying one of the Reaction Coordinates" — Taiwan

Chemical Society National Meeting — *Feb. 2016*
"Interstellar Glycine Formation: Can O–H Dangling Bond on the Icy Grain Reduce the Barrier?" — Taiwan

8^{th} Asian Consortium on Computational Materials Science — *June 2015*
"Anharmonicity Calculation of O–H Stretching Motion in Small Methanol Clusters along Normal Coordinates" — Taiwan

Spring Symposium of Photochemistry — *Jan. 2014*
"Theoretical Investigation of $H^+(MeOH)_n$ Vibrational Spectroscopy with/without Argon Attachment, n=1-4" — Taiwan

Asian Core Winter School — *Jan. 2013*
"Theoretical study on proton transfer dynamics of $((CH_3)_3N)_2$–H^+–R" — South Korea

Grants

Graduate Student Study Abroad Program — *Nov. 2018*
Ministry of Science and Technology — EUR 17,000

Subsidy for Attending International Academic Conferences — *June 2013*
Ministry of Science and Technology — EUR 1,400

Fellowship of Taiwan International Graduate Program — *Sept. 2012*
Academic Sinica — EUR 37,000

AWARDS

Poster Award — *June 2023*
Path integral quantum mechanics workshop
"Preserve Non-Stationary Long-Term Dynamics via Selected Incomplete Dual Basis Sets"

Doctoral Dissertation Competition — *Mar. 2021*
Chemical Society National Meeting
"Two-Dimensional Potential Energy Surfaces of the Reactions with Post-Transition-State Bifurcation"

Poster Award — *June 2019*
Graduate Student Poster Exhibition, National Taiwan University
"The Construction of Two-Dimensional Potential Energy Surfaces of Reactions with Post-Transition State Bifurcations"

Certifications & Additional Training

Nano Science and Technology Program — June 2020
Taiwan International Graduate Program (TIGP) — Taiwan

Summer course of scientific computing on supercomputer — *July 2017*
National Center for Theoretical Sciences — Taiwan

Academic writing — *January 2015*
The Language Training and Testing Center (LTTC) — Taiwan

Conference of International Academic Competence — *December 2013*
National Taiwan University — Taiwan

Biochemical Technology Programme *June 2009*
Chung-Yuan Christian University Taiwan

Skill

Languages
Chinese Mandarin (native), English (fluent), German (basic) and Japanese (basic).

Programming Languages
Proficient: Python, Bash, LaTeX, Fortran
Familiar: C, Matlab, Mathematica

Software Development: Q-Chem 2015-2020

Experienced in quantum chemistry packages
Gaussian, Molpro, Q-Chem , Psi4 , Orca

REFEREES **Available Upon Request**
Dr. Alexander Eisfeld (Max Planck Institute) | Dr. Dean J. Tantillo (UC Davis) | Dr. Chao-Ping Hsu (Academia Sinica)