XVIII QUANTUM REACTIVE SCATTERING WORKSHOP

QRS 2026

22–26 JUNE 2026

NANOTECHNOLOGY CENTRE A,
GDAŃSK TECH, GDAŃSK, POLAND

GDAŃSK TECH

BOOK OF ABSTRACTS

NICOLAUS COPERNICUS
UNIVERSITY IN TORUŃ
Faculty of Chemistry

Honorary Patronage

The Workshop is held under the honorary patronage of His Magnificence,
the Rector of Gdańsk University of Technology,
Prof. Ph.D., D. Sc., Eng. Krzysztof Wilde,
Corresponding member of the PAS

GDAŃSK UNIVERSITY OF TECHNOLOGY

Contents

Welcome to QRS 2026 – the 18th Quantum Reactive Scattering Workshop!

On behalf of the Organizing Committee, we are delighted to invite the international community to Gdańsk. In this inspiring Baltic city, a distinguished historical legacy meets a dynamic landscape of contemporary science and innovation. QRS 2026 continues the long-standing tradition of excellence established by **David Clary in 1990**, offering a focused, intellectually rigorous forum dedicated to the theory and computation of molecular collisions and chemical reactivity.

The workshop brings together researchers working across quantum dynamics, reactive scattering, and computational chemistry more broadly, fostering deep scientific exchange, constructive debate, and the formation of new collaborations. In 2026, QRS reaches **Poland for the first time**, extending its global trajectory with new geographical and cultural perspectives. Hosting QRS 2026 in Gdańsk is particularly fitting. As a historic port city shaped by international exchange, Gdańsk embodies openness, pluralism, and a spirit of intellectual freedom. Its identity as a "free city" resonates with the workshop's values: curiosity-driven inquiry, cross-disciplinary dialogue, and an inclusive scientific community. At the same time, Gdańsk is firmly oriented toward the future - home to a thriving academic and technological ecosystem and a vibrant environment for research and innovation.

The venue, **Gdańsk University of Technology**, provides an outstanding academic setting for QRS 2026. The university combines a remarkable campus heritage with modern research infrastructure, offering an ideal atmosphere for intensive discussion, high-level presentations, and productive interactions among participants.

We warmly look forward to welcoming you to QRS 2026 in Gdańsk. Join us for an unforgettable workshop experience shaped by cutting-edge scientific dialogue, meaningful collaboration, and engaging social events - in a city that uniquely unites history, openness, and modern science.

QRS history

Since its inception in 1990 by David Clary, the Quantum Reactive Scattering (QRS) Workshop has evolved into a highly regarded forum for the international community studying molecular collisions and chemical reactivity. Across its successive editions, the QRS conference has consistently attracted leading scientists and emerging researchers alike including theoreticians, computational chemists and physicists, as well as experimentalists providing an environment that encourages open exchange, critical discussion, and the formation of lasting collaborations.

1. **1990** Cambridge, UK - David Clary
2. **1994** Cambridge, Massachusetts, USA - Yan Sun and Michael Baer
3. **1995** Nottingham, UK - David Clary and David Manolopoulos
4. **1997** Telluride, Colorado, USA - Joel Bowman
5. **1999** Perugia, Italy - Vincenzo Aquilanti and Antonio Laganà
6. **2001** Pasadena, California, USA - Aron Kuppermann
7. **2003** San Lorenzo de El Escorial, Spain - Javier Aoiz and Luis Bañares
8. **2005** Santa Cruz, California, USA - Millard Alexander and Anne McCoy
9. **2007** Cambridge, UK - Stuart Althorpe
10. **2009** Dalian, China - Dong-Hui Zhang and Ke-Li Han
11. **2011** Santa Fe, New Mexico, USA - Hua Guo
12. **2013** Bordeaux, France - Laurent Bonnet and Pascal Larregaray
13. **2015** Salamanca, Spain - Octavio Roncero, Tomás González-Lezana, Susana Gómez-Carrasco, Lola González-Sánchez
14. **2017** Trieste, Italy - Niyazi Bulut, Noelia Faginas Lago, Andrea Lombardi, Federico Palazzetti
15. **2019** Saitama, Japan - Toshiyuki Takayanagi
16. **2022** Balatonföldvár, Hungary - György Lendvay, Gabriella Lendvayné Győrik, Ákos Bencsura
17. **2024** Istanbul, Türkiye - Murat Kılıç, Niyazi Bulut

Venue

The lectures will take place at **Nanotechnology Centre A** on the Gdańsk University of Technology (Gdańsk Tech) campus, located at **Narutowicza 11/12, Gdańsk**. Gdańsk Tech is one of the leading technical universities in Poland, with a historic and well-connected campus situated close to the city centre. The conference activities will be held mainly within the central part of the campus, allowing participants to move easily between the lecture venue, poster session area, coffee break space, lunch venue, and conference dinner location.

Participants are encouraged to use the interactive Gdańsk Tech campus map to locate the relevant buildings and plan their movement around the campus.

Main Conference Locations

Nanotechnology Centre A – Building No. 4

This will be the main venue for the scientific programme. The lectures will be delivered in **Lecture Hall 3/11**, located inside Nanotechnology Centre A. The same building will also host the **poster sessions** and **coffee breaks**, making it the central meeting point for participants during the workshop.

Main Building – Building No. 1 Lunches and the conference dinner will take place in the historic Main Building of Gdańsk Tech. The conference dinner will be held in the Daniel Gabriel Fahrenheit Courtyard, an elegant and representative space within the university's main architectural landmark.

The close distance between Nanotechnology Centre A and the Main Building ensures convenient access between the scientific sessions and social activities. Clear signs and campus guidance will help participants find their way between the buildings during the workshop.

Accommodation

Hotels

A map with hotels located near the **Gdańsk Tech campus** (the center of this map - zoom in if needed).

Gdańsk offers a wide range of accommodation options, including hotels, aparthotels and private apartments. For QRS2026, the most convenient areas are Gdańsk Wrzeszcz and Gdańsk Aniołki, both located close to the Gdańsk University of Technology campus at 11/12 Gabriela Narutowicza Street. Staying near Gdańsk Wrzeszcz railway station is also a practical option, as the campus can be reached from Wrzeszcz by tram or by SKM train to Gdańsk Politechnika station.

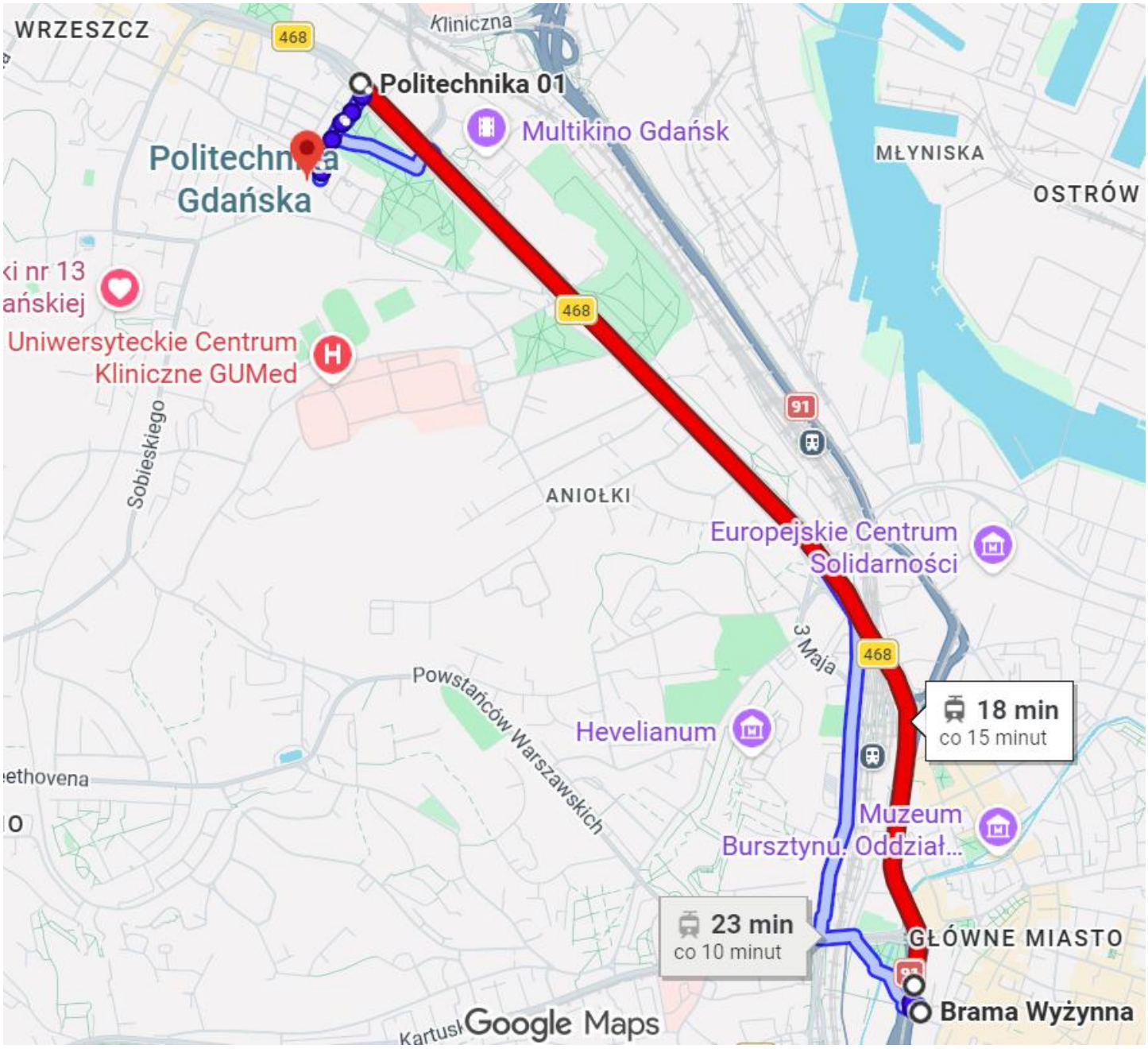
Participants looking for a hotel may consider, for example, Rooms and Apartments Collegia (ul. Sobieskiego 13, Wrzeszcz), Hotel Impresja (ul. Tuwima 12, Aniołki), Smart Hotel (ul. Słowackiego 3, Wrzeszcz), Focus Hotel Premium Gdańsk (ul. Nad Stawem 5, close to Gdańsk Wrzeszcz train station), Villa Eva (ul. Batorego 28B, Wrzeszcz), or Hotel Logos (ul. J. Uphagena 28, Wrzeszcz).

Private apartments are also a good option for guests who prefer more space, a kitchenette, or shared accommodation with colleagues. Apartments can be found throughout Gdańsk, especially in Wrzeszcz, Aniołki, and the city centre. The official Gdańsk tourism service notes that apartments are a popular accommodation choice in attractive locations across the city.

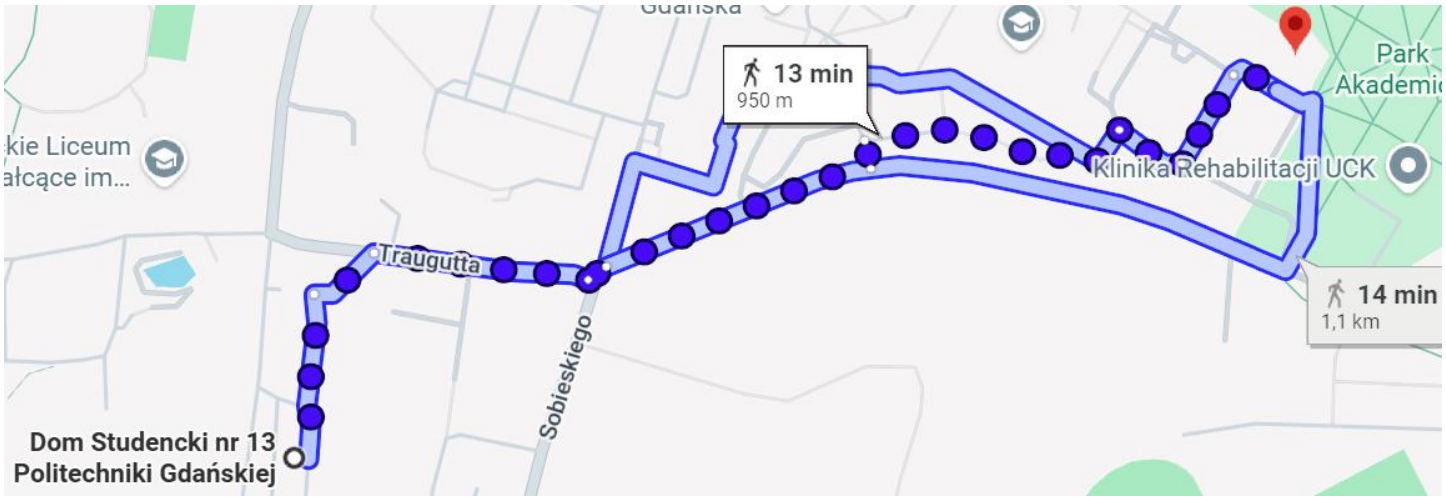
For guests who would like to combine the conference with sightseeing, accommodation in the city centre / Old Town is another convenient choice. Examples include Scandic Gdańsk, located opposite Gdańsk Główny railway station, Mercure Gdańsk Stare Miasto, near the main station and the Old Town, and Ibis Gdańsk Stare Miasto, just outside the Old Town.

Getting to Gdańsk University of Technology from the City Centre / Old Town

The easiest way to reach the Gdańsk University of Technology campus from the city centre / Old Town is by **tram**. The most convenient departure stops are **Brama Wyżynna** and **Dworzec Główny**, both located close to the central area of Gdańsk. From either stop, participants can take **tram lines 6 or 9** and get off at **Politechnika**. Another convenient option is tram line 8 to Politechnika SKM.The Gdańsk University of Technology campus is located at **Narutowicza 11/12** and is within a short walking distance of the nearest public transport stops. The closest tram stops are **Politechnika**, **Opera Bałtycka** and **Miszewskiego**.



For visitors staying in the Old Town area, the tram is usually the simplest and most convenient option.



Conference dinner

The conference dinner will take place in the **Daniel Gabriel Fahrenheit Courtyard**, located inside the **Main Building of Gdańsk University of Technology**. This historic courtyard, with its elegant architecture, glass-covered roof, and spacious interior, provides a distinguished setting for the evening gathering.

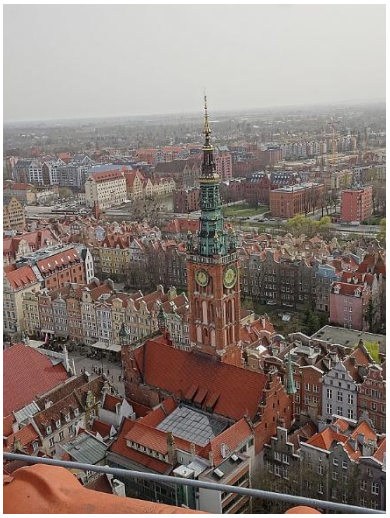
The dinner will offer participants an opportunity to relax after the scientific sessions, continue discussions in an informal atmosphere, and strengthen professional connections with researchers, invited speakers, and fellow attendees. The courtyard's unique character creates a warm and memorable environment for networking, conversation, and celebrating the conference together.

The venue is situated within the main campus area, making it easily accessible from the lecture halls and poster-session spaces. Further details regarding the dinner schedule and organisation will be provided during the conference.

Social Events

We are excited to share details of two planned social events below. Please note that we may need to modify these events due to circumstances beyond our control. We appreciate your understanding and look forward to creating memorable experiences together.

In the Footsteps of Gdańsk Scientists (60-minute guided walk)



Join a compact, walkable tour through Gdańsk's historic centre, dedicated to the city's scientific heritage in astronomy and physics. Along the way, we will meet four figures whose work helped shape early modern science: Jan Heweliusz and his rooftop observatory Stellaeburgum; Daniel Gralath and the rise of electrical experiments and learned societies; Daniel Gabriel Fahrenheit and the culture of precise measurement and thermometry; plus a brief note on Nathanael Matthaeus Wolf and the later tradition of systematic observations in the city.

The route is an easy walk (approximately 2–2.5 km) with brief stops for stories, historical context, and a few "science-in-the-street" moments. It is perfect for researchers looking for a local, inspiring break after long scientific sessions.

Motława River Cruise: Old Town–Westerplatte Round Trip (80 minutes)

Right after the "In the Footsteps of Gdańsk Scientists" walk, continue the experience on the water with a guided cruise along the Motława. This 80-minute round trip departs from the Old Town waterfront and heads outward through the port and shipyard areas, offering a striking contrast between the postcard skyline and the working maritime city—quays, cranes, harbour infrastructure, and the shipbuilding panorama of the Gdańsk Shipyard.

As you cruise farther downstream, you'll pass the historic Vistula River Mouth Fortress as you approach the port, continuing toward Westerplatte famous for being the site of the first shots fired in World War II in September 1939. Onboard, you'll enjoy a guide, live music during the return leg, and a buffet with drinks and snacks. This setting is perfect for informal conversations, taking photos, and enjoying a relaxing end to the evening.

Oliwa Organ Concert and Park Walk

Join us for an evening in one of Gdańsk's most remarkable districts. The social event will begin with a concert in the historic Oliwa Cathedral, famous for its magnificent organ and unique musical performances. Participants will have the opportunity to enjoy the exceptional acoustics and atmosphere of this landmark. After the concert, we will take a leisurely walk through the picturesque Oliwa Park, one of the city's most beautiful green spaces. The event offers an excellent opportunity to experience local culture, history, and nature while networking with fellow conference participants.

Committees

Conference Chairs:

- **Patryk Jasik**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

- **Dariusz Kędziera**

  Faculty of Chemistry, Nicolaus Copernicus University in Toruń

Members of the organizing committee:

- **Paweł Możejko**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

- **Justyna Dobrowińska-Seroka**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

- **Ewa Erdmann**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

- **Benjamin Ikuesan**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

- **Anna Kaczmarek-Kędziera**

  Faculty of Chemistry, Nicolaus Copernicus University in Toruń

- **Joanna Kozłowska**

  Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń

- **Marta Łabuda**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

- **Bartosz Majewski**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

- **Paweł Syty**

  Faculty of Applied Physics and Mathematics, Gdańsk University of Technology

Sponsors

RESEARCH UNIVERSITY
EXCELLENCE INITIATIVE

FACULTY OF APPLIED PHYSICS AND MATHEMATICS

NICOLAUS COPERNICUS UNIVERSITY IN TORUŃ
Faculty of Chemistry

World Scientific
Connecting Great Minds

Talks and posters – general info

For presentations

Speakers will be able to upload their presentations to the computer in the lecture room. Please upload your presentation during the coffee or lunch break immediately preceding your session, or earlier if possible.

The preferred file format is PDF, although PowerPoint presentations will also be accepted. We recommend bringing a backup copy of your presentation on a USB drive. Using your own laptop will be possible only as a last resort.

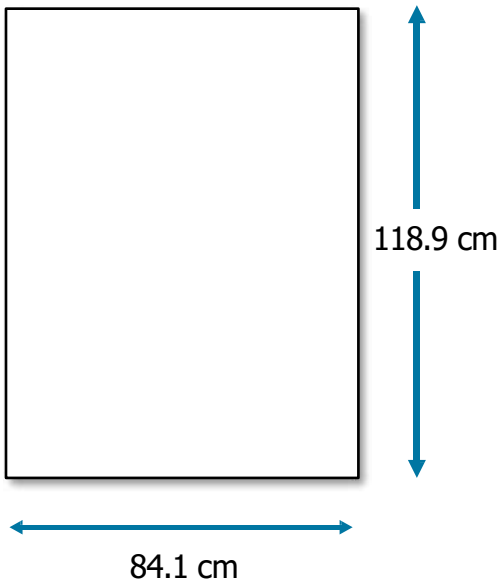
Please note that the presentation times shown in the conference programme include five minutes for questions and discussion. We therefore kindly ask all speakers to adjust the length of their talks accordingly:

- invited talks: maximum 25 minutes + 5 minutes discussion,
- contributed talks: maximum 15 minutes + 5 minutes discussion.

For poster session

The poster session will take place in the **main foyer of the Nanotechnology Centre A**.The preferred poster format is **A0**, with dimensions of **84.1 × 118.9 cm**. We kindly ask poster presenters to use this format whenever possible. Each poster should be displayed at the position corresponding to its number in the numbered list of posters (see page 21).

The Organising Committee will provide all necessary materials to securely attach the posters to the display stands.



Scientific Program – Detailed

Monday 22nd			Tuesday 23rd			Wednesday 24th			Thursday 25th			Friday 26th		
08:15-09:00	Registration													
09:00-09:10	Opening													
09:10-09:30	Sienkiewicz	Clary	09:10-09:30	Zanchet	Wester	09:00-09:30	Krylov	Henriksen	09:00-09:30	Peláez-Ruiz	Saalfrank	09:00-09:30	Curchod	Krylov
09:30-10:00		Carrington	09:30-10:00		Zuchowski	09:30-10:00		Sola	09:30-10:00		Rivero	09:30-10:00		Guillon
10:00-10:30		Bonnet	10:00-10:30		Yang	10:00-10:30		Curchod	10:00-10:30		Bacic	10:00-10:30		Cvitas
10:30-11:00		Babikov	10:30-11:00		Lezana	10:30-11:00		Slavicek	10:30-11:00		Hochlaf	10:30-11:00		Kanno
11:00-11:30	Coffee break		11:00-11:30	Coffee break		11:00-11:30	Coffee break		11:00-11:30	Coffee break		11:00-11:30	Coffee break	
11:30-12:00	Kanno	Roncero	11:30-12:00	Żuchowski	Stoecklin	11:30-12:00	Slavicek	Adhikari	11:30-12:00	Jasik	Colonna	11:30-12:00	Coletti	Esposito
12:00-12:30		Bulut	12:00-12:30		Zanchet	12:00-12:30		Gronowski	12:00-12:30		Coletti	12:00-12:30		Bossion
12:30-13:00		Takayanagi	12:30-13:00		Laricchiuta	12:30-13:00		Mukherjee	12:30-13:00		Możejko	12:30-13:00		Tonolo
13:00-14:30	Lunch		13:00-13:30		Demes	13:00-14:30	Lunch		13:00-13:20		Győri	13:00-13:20		Żółtowski
14:30-15:00	Roncero	Lendvay	13:30-13:45	Conference Photo		14:30-15:00	Lezana	Küpper	13:20-13:40		Szabó	13:20-13:40	Final conclusions	
15:00-15:30		Peláez-Ruiz	13:45-15:00	Lunch		15:00-15:30		Orr-Ewing	13:40-15:00	Lunch		13:40-15:30	Lunch	
15:30-16:00		Śmiałek-Telega	15:00-17:00	Free Time		15:30-16:00		García-Vela	15:00-16:00	Transfer to Oliwa Cathed.				
16:00-16:30	Coffee break					16:00-16:30	Coffee break		16:00-16:30	Oliwa Cathedral Organ				
16:30-17:00	Kędziera	Varandas				16:30-17:00	Bulut	Connor	16:30-17:30	Oliwa Park Walk				
17:00-17:30		Patkowski	17:00-18:45	In the Footsteps of Gdansk Scientists		17:00-17:30		Sokolovski	17:30-18:00	Transfer to Gdansk Tech.				
17:30-18:00		Skomorowski				17:30-18:00		Hele	18:00-20:00	Free Time				
						18:00-18:20		Olejnik						
						18:20-18:40		Yan						
18:00-19:30	Welcome reception		18:45-21:00	River Cruise		18:40-20:30	Poster Session		20:00-22:30	Conference dinner				

Scientific Program – Detailed

Monday 22

08:15–09:00	**Registration**
09:00–09:10	**Opening**
	Session chair: Józef E. Sienkiewicz (Gdansk University of Technology)
09:10–09:30	**WALTER KOHN AND HIS CONTRIBUTIONS TO QUANTUM SCATTERING THEORY** David Clary - *University of Oxford*
09:30–10:00	**MCTDH-LIKE DIFFERENTIAL EQUATIONS FOR DETERMINING SUM-OF-PRODUCT (SOP) WAVEFUNCTIONS** Tucker Carrington - *Queen's University*
10:00–10:30	**SEMICLASSICAL S-MATRIX IN THE INITIAL VALUE REPRESENTATION: COORDINATE CHOICE** Laurent Bonnet - *Bordeaux University*
10:30–11:00	**PHYSICAL INSIGHT FROM THE MIXED QUANTUM/CLASSICAL SIMULATIONS OF COLLISIONAL ENERGY TRANSFER** Dmitri Babikov - *Marquette University*
11:00–11:30	**Coffee break**
	Session chair: Manabu Kanno (Tohoku University)
11:30–12:00	**MULTISTATE COUPLED DIABATIC NEURAL NETWORK POTENTIAL FOR THE QUANTUM NON-ADIABATIC PHOTOFRAGMENTATION OF CH2+** Octavio Roncero - *Instituto de Física Fundamental (CSIC))*
12:00–12:30	**RADIATIVE ASSOCIATION OF C6H WITH METAL CATIONS: FORMATION MECHANISMS AND RATE CONSTANTS FOR MC6H+ ASTROCHEMICAL SPECIES** Niyazi Bulut - *Firat University, Gdańsk Tech*
12:30–13:00	**NUCLEAR QUANTUM EFFECTS IN COMPLEX CHEMICAL REACTIONS: A RING-POLYMER MOLECULAR DYNAMICS APPROACH** Toshiyuki Takayanagi - *Saitama University*
13:00–14:30	**Lunch**
	Session chair: Octavio Roncero (Instituto de Física Fundamental, CSIC)
14:30–15:00	**EXPLORATION OF THE FACTORS DETERMINING THE SHAPES OF POTENTIAL ENERGY SURFACES USING MAYER'S CHEMICAL ENERGY COMPONENT ANALYSIS** György Lendvay - *HUN-REN Research Centre for Natural Sciences*
15:00–15:30	**FUNCTIONAL ANALOGUES OF SEPARABLE TENSOR DECOMPOSITION ANSÄTZE AND APPLICATIONS** Daniel Peláez-Ruiz - *Paris-Saclay University, CNRS*
15:30–16:00	**QUANTUM-REACTIVE-SCATTERING PERSPECTIVES FROM DEA CLUB 2026: RESONANCES, ATTACHMENT AND FRAGMENTATION DYNAMICS** Małgorzata Śmiałek-Telega - *Gdańsk Tech*
16:00–16:30	**Coffee break**
	Session chair: Dariusz Kędziera (Nicolaus Copernicus University in Toruń)
16:30–17:00	**ENERGETICS AND DYNAMICS IN QUANTUM THEORY: A GREEN-THEORETICAL PERSPECTIVE** António Varandas - *University of Coimbra*
17:00–17:30	**INTERMOLECULAR INTERACTION ENERGIES: STRIVING FOR MAXIMUM ACCURACY AND INSIGHT** Konrad Patkowski - *Auburn University*
17:30–18:00	**MODELING THE STATE OF A FREE ELECTRON IN CHEMICAL REACTIONS** Wojciech Skomorowski - *University of Warsaw, Centre of New Technologies*

18:00–19:30	**Welcome reception**

Tuesday 23

	Session Chair: Alexandre Zanchet (CSIC)
09:00–09:30	**THE ROLE OF ROTATIONAL STATES IN ION-NEUTRAL REACTIONS** Roland Wester - *University of Innsbruck*
09:30–10:00	**ALL THE DETAILS MATTER: PREDICTING AND EXPLOITING SCATTERING RESONANCES IN HELIUM AND MOLECULAR HYDROGEN** Piotr Zuchowski - *Nicolaus Copernicus University*
10:00–10:30	**QUANTUM STATE-SELECTED REACTION DYNAMICS AT LOW TEMPERATURES** Tiangang Yang - *Southern University of Science and Technology (SUSTech)*
10:30–11:00	**ATOM-DIATOM REACTIONS OF INTEREST: THE DESTRUCTION OF CH+ AND HeH+ IN COLLISION WITH H** Tomas Gonzalez Lezana - *Instituto de Física Fundamental - CSIC*
11:00–11:30	**Coffee break**
	Session chair: Piotr Żuchowski (Nicolaus Copernicus University in Toruń)
11:30–12:00	**A COMPARATIVE QCT AND QUANTUM CLOSE COUPLING STUDY OF THE HeNa+, HeK+ AND H2 THREE BODY ASSOCIATION** Thierry Stoecklin - *CNRS*
12:00–12:30	**CHEMICAL PUMPING IN ATOM-DIATOM REACTIONS** Alexandre Zanchet (CSIC)
12:30–13:00	**TRANSPORT CROSS SECTIONS FOR CHARACTERIZATION OF PLANETARY ENTRY CONDITIONS** Annarita Laricchiuta - *CNR ISTP Bari section*
13:00–13:30	**INCREASING COMPLEXITY IN QUANTUM SCATTERING STUDIES OF POLYATOMIC INTERSTELLAR MOLECULES** Sándor Demes - *HUN-REN Institute for Nuclear Research*
13:30–13:45	**Conference Photo**
13:45–15:00	**Lunch**
15:00–17:00	**Free time**
17:00–18:45	**In the Footsteps of Gdańsk Scientists**
18:45–21:00	**Excursion / social event**

Wednesday 24

	Session chair: Anna Krylov (University of Southern California)
09:00–09:30	**POPULATION TRANSFER BETWEEN DEGENERATE CONTINUUM STATES VIA IMPULSIVE STIMULATED RAMAN SCATTERING: APPLICATION TO THE CONTROL OF HOD PHOTOFRAGMENTATION** Niels Engholm Henriksen - *Technical University of Denmark*
09:30–10:00	**INITIAL-STATE ENGINEERING AS AN ALTERNATIVE STRATEGY FOR QUANTUM CONTROL OF PHOTOCHEMICAL PROCESSES** Ignacio Sola - *Universidad Complutense de Madrid*
10:00–10:30	**ON THE DESCRIPTION OF PHOTOEXCITATION IN NONADIABATIC DYNAMICS** Basile Curchod - *University of Bristol*
10:30–11:00	**THE REAL BOTTLENECK IN PREDICTIVE NONADIABATIC DYNAMICS** Petr Slavicek - *University of Chemistry and Technology, Prague*
11:00–11:30	**Coffee break**
	Session chair: Petr Slavicek (University of Chemistry and Technology, Prague)

11:30–12:00	**SYMMETRY BREAKING IN REACTIVE SCATTERING PROCESSES: ELECTRON NUCLEAR COUPLING** Satrajit Adhikari - *School of Chemical Sciences, Indian Association for the Cultivation of Science*
12:00–12:30	**ULTRACOLD ATOM+MOLECULE SYSTEMS THROUGH THE LENS OF AB INITIO ELECTRONIC STRUCTURE THEORY** Marcin Gronowski - *Wydział Fizyki UW*
12:30–13:00	**RETHINKING SURFACE HOPPING: FROM NONADIABATIC COUPLINGS TO TIME-DERIVATIVE COUPLINGS** Saikat Mukherjee - *Faculty of Chemistry, Nicolaus Copernicus University in Torun, Poland*
13:00–14:30	**Lunch**
	Session chair: Tomas Gonzalez Lezana (Instituto de Física Fundamental - CSIC, Madrid)
14:30–15:00	**PROTON TRANSFER AND HYDRONIUM FORMATION IN IONIZED WATER** Jochen Küpper - *DESY, CFEL and Universität Hamburg*
15:00–15:30	**REACTIONS OF HYDROFLUOROOLEFINS WITH OZONE PRODUCE LONG-LIVED GREENHOUSE GASES** Andrew Orr-Ewing - *University of Bristol*
15:30–16:00	**QUANTUM CONTROL OF THE DYNAMICAL BEHAVIOR OF RESONANCE STATES IN SMALL POLYATOMIC MOLECULES WITH INTENSE FIELDS** Alberto García-Vela - *Consejo Superior de Investigaciones Científicas*
16:00–16:30	**Coffee break**
	Session chair: Niyazi Bulut (Firat University, Gdańsk Tech)
16:30–17:00	**TECHNIQUES FOR ANALYZING STRUCTURED ANGULAR SCATTERING IN THE PRODUCTS OF CHEMICAL REACTIONS** Jonathan Connor - *University of Manchester, UK*
17:00–17:30	**AN OLD QUESTION: ARE THERE RESONANCES IN THE F+H2 (v=0)→FH(v=3)+H REACTION?** Dmitri Sokolovski - *UPV/EHU*
17:30–18:00	**TOWARDS DERIVING NON-ADIABATIC QUANTUM DYNAMICS WITH QUANTUM BOLTZMANN CONSERVATION, RABI OSCILLATIONS AND CLASSICAL SCALING** Tim Hele - *University College London*
18:00–18:20	**QUANTUM SCATTERING STUDY OF COLLISIONAL EFFECTS IN ROTATIONAL SPECTRA OF O2-PERTURBED HYDROGEN HALIDES** Artur Olejnik - *Uniwersytet Mikołaja Kopernika w Toruniu*
18:20–18:40	**IMAGING COLD AND CONTROLLED REACTIVE COLLISIONS BETWEEN S(1D) AND D2** Dong Yan - *Radboud university*
18:40–20:30	**Poster session**

Thursday 25

	Session chair: Daniel Peláez-Ruiz (Paris-Saclay University, CNRS)
09:00–09:30	**MOLECULES COUPLED TO PHONONS AND PHOTONS** Peter Saalfrank - *Department of Chemistry, University of Potsdam*
09:30–10:00	**COMBINING AB INITIO MOLECULAR DYNAMICS WITH MACHINE LEARNING INTERATOMIC POTENTIALS TO STUDY GAS–SURFACE INTERACTIONS** Alejandro Rivero - *University of Lille*
10:00–10:30	**H2O AND D2O TRIMERS: RIGOROUS 12D QUANTUM CALCULATIONS OF THE INTERMOLECULAR VIBRATIONAL STATES, TUNNELING SPLITTINGS, AND LOW-FREQUENCY SPECTRA** Zlatko Bacic - *New York University*
10:30–11:00	**IONS IN THE ISM: SPECTROSCOPY AND UNIMOLECULAR DECOMPOSITION PROCESSES** Majdi Hochlaf - *Université Gustave Eiffel*
11:00–11:30	**Coffee break**
	Session chair: Patryk Jasik (Gdańsk University of Technology)

11:30–12:00	**MULTI-TEMPERATURE MODEL FROM STATE SPECIFIC DATA: APPLICATION TO ICE GIANTS** Gianpiero Colonna - *CNR-ISTP Bari section*
12:00–12:30	**STATE-RESOLVED VIBRATIONAL DYNAMICS FROM MIXED QUANTUM-CLASSICAL METHODS** Cecilia Coletti - *Università G. d'Annunzio Chieti-Pescara*
12:30–13:00	**ON THE SCATTERING OF ELECTRONS BY MOLECULES OF ASTROCHEMICAL AND TECHNOLOGICAL SIGNIFICANCE** Paweł Możejko - *Wydział Fizyki Technicznej i Matematyki Stosowanej, Politechnika Gdańska*
13:00–13:20	**AUTOMATED DEVELOPMENT OF POTENTIAL ENERGY SURFACES ACROSS THE ACCURACY GAMUT WITH ROBOSURFER** Tibor Győri - *University of Szeged*
13:20–13:40	**TWO SIDES OF WIGNER'S COIN: FROM R-MATRIX TO TRANSITION-STATE THEORY** Péter Szabó - *KU Leuven*
13:40–15:00	**Lunch**
15:00–16:00	**Bus transfer from Gdańsk Tech to Oliwa Cathedral**
16:00–16:30	**Oliwa Cathedral Organ Concert**
16:30–17:30	**Oliwa Park Walk**
17:30–18:00	**Bus transfer from Oliwa Park to Gdańsk Tech**
18:00–20:00	**Free time**
20:00–22:30	**Conference dinner**

Friday 26

	Session chair: Basile Curchod (University of Bristol)
09:00–09:30	**A FRESH LOOK AT SIGNATURES OF S-WAVE SCATTERING: SYMMETRY AND THE BREAKDOWN OF THE BORN–OPPENHEIMER APPROXIMATION** Anna Krylov - *University of Southern California*
09:30–10:00	**QUASI-EQUILIBRIUM O + O2 IGNITION OF OZONE FORMATION FROM O3* LIFETIME SPECTRUM: THE CASE OF 18O and 17O ISOTOPES** Gregoire Guillon (Universite Bourgogne Europe)
10:00–10:30	**TUNNELING DYNAMICS USING INSTANTON THEORY: ROVIBRATIONAL SPECTRA AND DECAY RATES IN MOLECULES** Marko Cvitas - *University of Zagreb Faculty of Science*
10:30–11:00	**STRUCTURE-BASED GAUSSIAN EXPANSION FOR EFFICIENT MULTIDIMENSIONAL WAVEPACKET CALCULATIONS: APPLICATIONS TO ISOLATED AND OPEN SYSTEMS** Manabu Kanno - *Tohoku University*
11:00–11:30	**Coffee break**
	Session chair: Cecilia Coletti (Università G. d'Annunzio Chieti-Pescara)
11:30–12:00	**MERGING SEMI- AND QUASI-CLASSICAL METHODS FOR THE ACCURATE CALCULATION OF VIBRATIONAL ENERGY EXCHANGE IN MOLECULAR COLLISIONS OF TECHNOLOGICAL INTEREST** Fabrizio Esposito - *Consiglio Nazionale delle Ricerche-Istituto per la Scienza e Tecnologia dei Plasmi*
12:00–12:30	**SM-NRPMD: A NON-ADIABATIC PATH INTEGRAL BASED METHOD TO STUDY QUANTUM DYNAMICS** Duncan Bossion - *Institut de Physique de Rennes-Université de Rennes*
12:30–13:00	**COLLISIONAL EXCITATION BY HEAVY PROJECTILES TO MODEL COMETARY AND PLANETARY ATMOSPHERES** Francesca Tonolo - *Institut de Physique de Rennes*

13:00–13:20	**COLLISIONAL STUDIES OF CH3CHO-He SYSTEM** Michał Żółtowski - *Nicolaus Copernicus University in Toruń*
13:20–13:40	**Final conclusions and the future**
13:40–15:30	**Lunch**

Scientific Program – Detailed

Poster Presentation Order

1. A. Pradhan, A. Ayasli, I. S. Vinklárek, H. Bromberger, S. Trippel, and J. Küpper

Direct observation of the metastable fragmentation of uracil cations

2. B. Majewski, M. Tatar and M. Łabuda

Prediction of Total Electron-Impact Ionization Cross Sections

3. B. A. Ikuesan, P. Jasik, N. Bulut and J. E. Sienkiewicz

Comprehensive Ab Initio Characterization of CO Electronic States for Quantum Dynamics and Reactive Scattering Applications

4. E. Erdmann, E. Olsson, V. D. Ideböhn, M. Wallner, R. J. Squibb, J. H. D. Eland and R. Feifel

Non-Ergodic Dissociative Valence Double Ionization of SF_6

5. L. Shirkov, H. Jóźwiak and P. Wcisło

Quantum Dynamics of $O_2(X^3\Sigma g^-)$ Complexes with Alkali and Alkaline-Earth Metal Atoms from Ab Initio Potentials

6. M. K. Sah, S. Adhikari, B. Smits, J. Meyer and M. F. Somers

Impact of Surface Modes on H_2/D_2 Scattering from Cu(111): A Time-Dependent Effective Hartree Approach

7. M. Welter, D. Dąbrowski, M. Przybytek and M. Tomza

Modelling Quantum Resonances in Cold Ion–Atom Collisions

8. P. Syty, M. Piłat and J. E. Sienkiewicz

From Noble Gases to Lanthanides: Low-Energy Electron Scattering with GRASP

9. P. Tóth and G. Czakó

Vibrational Mode-Specific Dynamics in the Cl + CH_3CN and O^- + CH_4/CD_4 Reactions

10. S. Akkari, W. Zrafi, M. Bejaoui, H. Ladjimi, J. Dhiflaoui, J. E. Sienkiewicz and H. Berriche

From Adiabatic to Diabatic Representation: An Ab Initio Investigation of the LiS Molecule

11. X. Huet, A. Aerts and N. Vaeck

Electron Transfer Reaction in H_2 + He^+ Collision at 3 eV

INVITED TALKS

XVIII QUANTUM REACTIVE SCATTERING WORKSHOP

A COMPARATIVE QCT AND QUANTUM CLOSE COUPLING STUDY OF THE $HeNa^+$, HeK^+ AND H_2 THREE BODY ASSOCIATION

R. M. García-Vázquez [(a)], P. Halvick [(a)], T. Stoecklin [(a),*]

[(a)] *Institut des Sciences Moléculaires, UMR5255-CNRS, Université de Bordeaux, 351 cours de la libération 33405 Talence cedex, France*

** Thierry.stoecklin@u-bordeaux.fr*

The termolecular reaction between three atoms, whereby a diatomic molecule is formed while the third atom remains free, is the process designated as three-body association (TBA). It has recently been the subject of renewed theoretical and experimental interest as it is engaged in research activities pertaining to a number of scientific disciplines, including cold and ultracold chemistry, astrophysics, plasma physics, atmospheric physics, and physical chemistry. From a technical standpoint, the enhanced capabilities of cryogenic ion traps were instrumental in driving recent advancements, enabling the measurement of three-body association in hydrogen and helium to cold ions [1]. The fundamental theory of TBA was established long ago while its application to real systems became possible only very recently because of the challenging complexity of the calculations. TBA can be described in two ways: either a simultaneous three-body collision or a two-step process by which two of the atoms collide first, yielding an excited diatomic molecule, that is further stabilized by collisions with the third body. The latter which is known as the Lindemann-Hinshelwood energy mechanism [2, 3] represents the primary source of quantum studies on the subject of three-body association and is used in the present study.

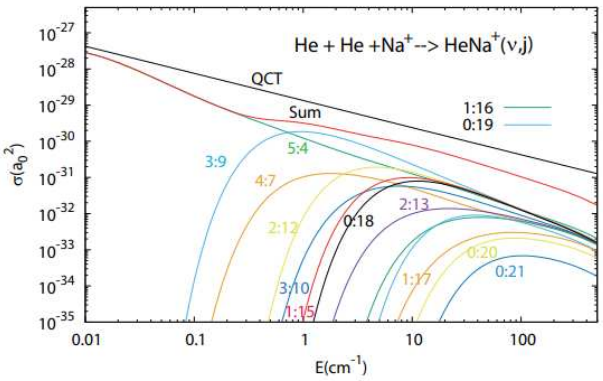


Figure 1: Comparison of state selected and global quantum and classical rates for the TBA of $HeNa^+$.

The Quasi Classical trajectory method is an interesting alternative approach which has recently been successfully applied to several systems. [4] In the present work we will compare the results of these two approaches for two ionic systems: $Na^+ + He + He \rightarrow HeNa^+ + He$; $K^+ + He + He \rightarrow HeK^+ + He$ [5] and one neutral collision: $H + H + He \rightarrow He + H_2$. In order to achieve this objective, two PES will be constructed for the two ionic systems and the bound and quasi-bound states of the resulting diatomic cations calculated. The same approach will be used for $H + H + He \rightarrow H_2 + He$ when comparing existing three bodies and two bodies PES. Subsequently, the collisional relaxation rates will be calculated, and the TBA rate obtained within the framework of the local thermodynamic equilibrium hypothesis. The comparison between the QCT and quantum approaches will ultimately allow us to gain complementary insight into the temperature dependence of TBA.

References

[1] R. Wild, M. Nötzold, C. Lochmann and R. Wester, J. Phys. Chem. A 125, 8581 (2021).
[2] F. A. Lindemann, S. Arrhenius, I. Langmuir, N. R. Dhar, J. Perrin, P. Lewis, Trans. Faraday Soc. 17 : 598 (1922).
[3] R. C. Forrey, Phys. Rev. A 88, 052709 (2013).
[4] J. Perez-Rios, S. Ragole, J. Wang and C. H. Greene, J. Chem. Phys. 140: 044307 (2014).
[5] R. M. García-Vázquez , T. Stoecklin , and P. Halvick, Phys. Rev. A 112: 062812 (2025)

Ions in the ISM: Spectroscopy and unimolecular decomposition processes

M. Hochlaf [1]

[1] Université Gustave Eiffel, COSYS/IMSE, 5 Bd Descartes 77454, Champs sur Marne, France.
E-mail: majdi.hochlaf@univ-eiffel.fr

I will present several examples of the use of high-level theoretical characterization of low-energy isomers of molecular species relevant in atmospheric, planetary and interstellar media. First, we explore their ground state potential energy surface using coupled cluster (CC) theory. Next, precise equilibrium structures and relative energies are determined using composite schemes based on CC theory and taking into account extrapolation to the complete basis set limit and core correlation effects. For all stable forms, rotational spectroscopy parameters as well as fundamental vibrational frequencies and infrared intensities are also determined. For illustration, I will treat the protonated isocyanic acid species. [1]

I will also consider the spectroscopy of ions formed by single photon ionization of their corresponding neutral molecules. These ions undergo later unimolecular decomposition processes via trivial bond breaking and/or intramolecular rearrangements before fragmentation(s). The latter processes lead to the formation of unexpected products. Several examples will be treated including $HNCS^+$ and $HCOOH^+$ ions and their reaction pathways leading to the formation of HS^+ and abiotic O_2, respectively. [2-5]

Acknowledgements

Part of the experiments were carried out at the PLEIADES beamline of the SOLEIL storage ring, proposal ID 20231852. We thank the SOLEIL staff for technical assistance and stable operation of the equipment and storage ring during the experiments.

References

1. M. Hochlaf, R. Linguerri, N. C. Kandi, S. Alessandrini, and C. Puzzarini. J. Phys. Chem. A 2026, 130, 3140−3150.
2. D. Schaffner, A. Bellili, M. Gerlach, E. Karaev, M. Mogren Al Mogren, J. Bozek, I. Fischer, and M. Hochlaf. J. Chem. Phys. 162, 164310 (2025).
3. E. Olsson, D. Schaffner, A. Bellili, M. Wallner, V. Daver Ideböhn, R. J. Squibb, M. Parriani, M. Gerlach, P. Hemberger, S. Lundberg, D. Cole, G. Nyman, M. Mogren Al Mogren, I. Fischer, J. H. D. Eland, R. Feifel, and M. Hochlaf. J. Chem. Phys. 163, 204303 (2025).
4. A. Gloriod, M. Mogren Al-Mogren, and M Hochlaf. Phys. Chem. Chem. Phys. 27, 25483-25497 (2025).
5. A. Gloriod, A. R. Milosavljević, A. Bellili, J. Palaudoux, F. Penent, R. Dupuy, and M. Hochlaf. J. Chem. Phys. 164, 174313 (2026).

Rethinking Surface Hopping: From Nonadiabatic Couplings to Time-Derivative Couplings

Saikat Mukherjee

Faculty of Chemistry, Nicolaus Copernicus University in Torun, Poland

saikat.mukherjee@umk.pl

Nonadiabaticity, which arises from the coupling between electronic and nuclear motion, plays a central role in a wide range of photophysical and photochemical processes. Modeling such dynamics is challenging because it requires describing transitions among multiple electronic states, often in regions of conical intersections or avoided crossings where the Born–Oppenheimer approximation breaks down. Among the various theoretical approaches for simulating nonadiabatic dynamics, ranging from full quantum dynamics to mixed quantum-classical and semiclassical methods, Tully's fewest-switches surface-hopping (FSSH) method has emerged as one of the most widely used and influential approaches. When combined with on-the-fly electronic-structure calculations, surface hopping provides a practical framework for exploring nonadiabatic processes at the full atomic level. However, the computational cost of such trajectory-based simulations can become prohibitive, since electronic energies, gradients, and coupling information must be evaluated repeatedly at each nuclear time step.

FSSH requires electronic energies, gradients, and nonadiabatic couplings between electronic states as inputs from quantum-chemical calculations. Explicit evaluation of nonadiabatic coupling vectors not only introduces additional computational expense but may also be unavailable, numerically unstable, or divergent near critical regions of the potential energy landscape. Recently, several strategies have been developed to approximate time-derivative couplings for use in the FSSH algorithm. In this talk, I will discuss selected strategies [1-3] for approximating time-derivative couplings and the associated hopping criteria. By reducing the need for explicit nonadiabatic coupling calculations, these approaches offer a promising route to extending nonadiabatic dynamics simulations to longer timescales while taming the formidable computational cost.

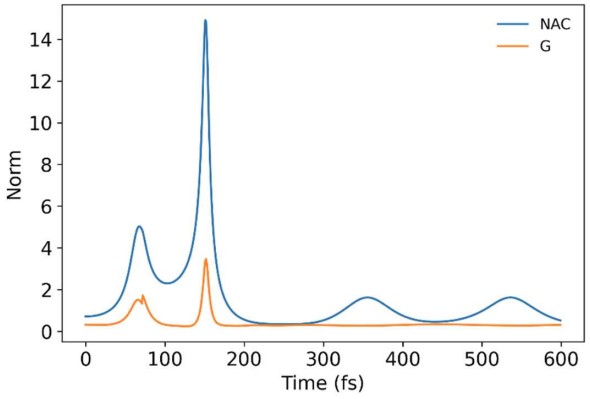


Figure 1: Comparison between the norm of the exact NAC vector and the effective NAC (norm G) obtained for a FSSH trajectory of the fulvene molecule.

References

[1] Y. Shu, L. Zhang, X. Chen, S. Sun, Y. Huang, D. G. Truhlar, *J. Chem. Theory Comput.* **18**, 1320-1328 (2022).

[2] J. M. Toldo, R. S. Mattos, M. Pinheiro Jr, S. Mukherjee, M. Barbatti, *J. Chem. Theory Comput.* **20**, 614-624 (2024).

[3] T. Jira, J. Janos, P. Slavicek, *J. Chem. Theory Comput.* **21**, 9784-9798 (2025).

All the details matter: predicting and exploiting scattering resonances in helium and molecular hydrogen

Piotr Żuchowski

Institute of Physics, Nicolaus Copernicus University in Torun Grudziądzka 5/7 87-100 Toruń
pzuch@fizyka.umk.pl

Groundbreaking work on merged molecular beams by Narevicius and co-workers, in which collision energies can be lowered into the sub-Kelvin regime, has made it possible to resolve quantum effects in scattering such as resonances. This enables a confrontation between theory and experiment at a level of detail previously unattainable. Because resonance positions are exquisitely sensitive to the details of the underlying potential energy surface, they allow theory and experiment to be compared far beyond the gold standard of quantum chemistry. I will present several examples of such confrontations: metastable helium with H2 and Rydberg helium (essentially: He ion) colliding with molecular hydrogen.

References

[1] A. B. Henson, S. Gersten, Y. Shagam, J. Narevicius, and E. Narevicius, Science **338**, 234–238 (2012).

[2] E. Lavert-Ofir, Y. Shagam, A. B. Henson, S. Gersten, J. Kłos, P. S. Żuchowski, J. Narevicius, and E. Narevicius, Nat. Chem. **6**, 332–335 (2014).

[3] A. Klein, Y. Shagam, W. Skomorowski, P. S. Żuchowski, M. Pawlak, L. M. C. Janssen, N. Moiseyev, S. Y. T. van de Meerakker, A. van der Avoird, C. P. Koch, and E. Narevicius, Nat. Phys. **13**, 35–38 (2017).

SM-NRPMD: A NON-ADIABATIC PATH INTEGRAL BASED METHOD TO STUDY QUANTUM DYNAMICS

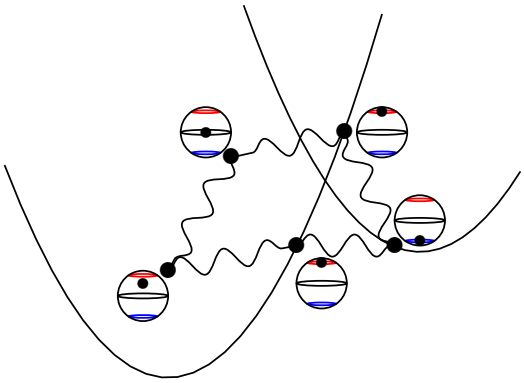
D. Bossion [a],*

[a] Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) - UMR 6251, F-35000 Rennes, France

* duncan.bossion@univ-rennes.fr

The study of complex systems with multiple degrees of freedom with quantum mechanical methodologies is very challenging and often impossible to deal with for molecules over few atoms. The best available methodologies for large systems are approximate quantum methods that can capture some quantum effects while retaining a numerical cost close to classical methodologies. Among those techniques are the path-integral based methods that take advantage of the quantum-classical isomorphism of the canonical partition function between a quantum system and a classical ring polymer of beads connected by harmonic springs. One of the methods base on this is the RPMD method (Ring Polymer Molecular Dynamics) [1]. Non-adiabatic versions of this RPMD method were developed to also capture non-adiabaticity with purely classical degrees of freedom.

I this talk, I will present the SM-NRPMD method [2,3] (for spin-mapping non-adiabatic RPMD), one of the most accurate of this class of methods, based on the spin-mapping formalism [4,5]. I will illustrates its performances with results of time-correlation functions of simple non-adiabatic models. I will also present the extension of this methodology to compute rate constants of reaction through flux-side correlation functions, and in particular electronic state-to-state reaction rates with preliminary results on a 1D model potential of the $F+H_2$ reaction.



References

[1] I. Craig and D. Manolopoulos, *J. Chem. Phys.* **121**, 3368–3373 (2004)

[2] D. Bossion, S. Chowdhury and P. Huo, *J. Chem. Phys.* **154**, 184106 (2021)

[3] D. Bossion, S. Chowdhury and P. Huo, *J. Chem. Phys.* **158**, 044123 (2023)

[4] D. Bossion et al., *J. Chem. Phys.* **157**, 084105 (2022)

[5] J. Runeson and J. Richardson, *J. Chem. Phys.* **152**, 084110 (2020)

THE ROLE OF ROTATIONAL STATES IN ION-NEUTRAL REACTIONS

Roland Wester*

Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck,
Technikerstraße 25, 6020 Innsbruck, Austria

* roland.wester@uibk.ac.at

Angle- and velocity-resolved differential scattering data provide important insight in the dynamics of ion-molecule reactions. We use crossed-beam scattering in combination with velocity map imaging to study ion-molecule reactions [1]. Recently, we have developed a new spectrometer that allows for higher reactant and product energy resolution [2]. With this setup, we have studied the charge transfer reaction of state-selected Ar^+ ions with N_2. We observed a profound change in reaction dynamics at near-thermal collision energies, where the coupling to vibrationally excited product ions is energetically closed [3]. In reactions of Ar^+ with rotationally cold H_2 at low collision energies we achieved product rotational state state resolution for both para- and ortho-H_2 [4]. The angle-differential cross section and the product rotational quantum state distribution agrees very well with ab initio quantum scattering calculations. The unexpected high rotational excitation of the H_2^+ products is attributed to the long-range attractive interaction in the reaction complex [4]. In experiments with rovibrational state-selected H_2^+ ions, we have studied the proton transfer reaction with Ne atoms and observed a collision energy-dependent back-scattering signal that may be indicative of a dynamical resonance [5].

References

[1] R. Wester, Phys. Chem. Chem. Phys. **16**, 396 (2014)
[2] D. Swaraj, T. Michaelsen, A. Khan, F. Zappa, R. Wild, R. Wester, Mol. Phys. **122**, e2194455 (2024)
[3] D. Swaraj, J. Judy, F. Zappa, V. C. Schmidt, R. Wester, J. Phys. Chem. **164**, 121101 (2026)
[4] D. Swaraj et al., in preparation
[5] J. Judy et al., in preparation

COMBINING AB INITIO MOLECULAR DYNAMICS WITH MACHINE LEARNING INTERATOMIC POTENTIALS TO STUDY GAS–SURFACE INTERACTIONS

A. Rivero Santamaría[(a),*], S. Del Fré[(a)], G. A. Alou Angulo[(a)], C. Toubin[(a)] and M. Monnerville[(a)]

[(a)]*Univ. Lille, CNRS, UMR 8523 – PhLAM – Physique des Lasers Atomes et Molécules, F-59000 Lille, France*
[*]alejandro.rivero@univ-lille.fr

Gas–surface interactions, including scattering and reactive processes, are central to many phenomena in atmospheric chemistry and heterogeneous catalysis. Here, we illustrate how the combination of Ab Initio Molecular Dynamics (AIMD) with Machine Learning-based Interatomic Potentials (MLIPs) advances our understanding of the fundamental processes governing gas-surface interactions. As representative systems, we examine nitric oxide (NO) interacting with graphite surfaces of increasing complexity, from scattering on pristine highly oriented pyrolytic graphite (HOPG) to oxidation on oxygen-functionalized HOPG (O-HOPG).

For NO scattering from HOPG, we will present results from a recent study [1] devoted to the development of a MLIP based on configurational sampling from AIMD calculations combined with an active learning strategy. NO scattering from graphite has long served as a benchmark system for studying gas-surface energy transfer, with molecular beam and laser-based experiments providing state-resolved angular, velocity, and rotational energy distributions over a wide range of surface temperatures. The availability of such detailed experimental data enables direct comparison with MLIP-based dynamical simulations, providing a stringent validation of the accuracy of the MLIP and deeper insight into the mechanisms governing gas-surface scattering.

For the more complex reactive system of NO on O-HOPG, we will present results from our recent AIMD study [2], together with ongoing work on the construction of a MLIP. AIMD trajectories identified accessible reaction channels and the role of surface oxygen groups in NO oxidation. The MLIP is then constructed, enabling extended simulations that provide robust statistics for reaction probabilities, energy transfer, and angular and energy distributions of the products, thereby revealing the microscopic mechanisms driving NO_2 formation and highlighting the catalytic role of oxygenated sites at the surface.

References

[1] S. Del Fré, G. A. Alou Angulo, M. Monnerville and A. Rivero Santamaría, arXiv:2603.18864 [physics.chem-ph] (2026)
[2] G. A. Alou Angulo, A. Rivero Santamaría, C. Toubin and M. Monnerville, J. Phys. Chem. C, **128**, 42, 17894–17904. (2024)

ON THE DESCRIPTION OF PHOTOEXCITATION IN NONADIABATIC MOLECULAR DYNAMICS

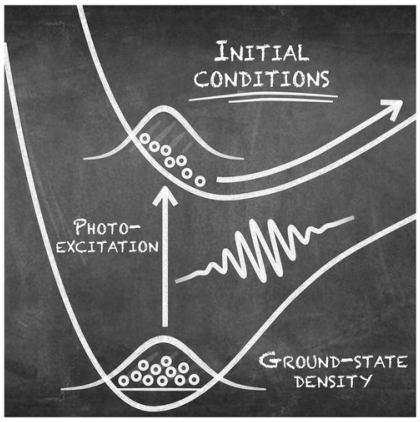
Basile F. E. Curchod [(a),*]

[(a)] School of Chemistry, University of Bristol, Bristol BS8 1TS, United Kingdom

A significant number of computational strategies have been developed over the past decades to simulate the excited-state dynamics of molecules beyond the Born-Oppenheimer approximation. When combined with advanced electronic-structure methods, these techniques – often based on coupled or uncoupled trajectories – have the potential to unravel the mechanistic details of photochemical reactions of direct interest to physical, atmospheric, and material chemists.

Despite all these extensive developments, the very first step of any photochemical reaction – photoexcitation – is dramatically approximated in most applications of nonadiabatic dynamics.[1] In an ideal world, the initial ground-state nuclear wavefunction, representing the molecule of interest, should be coupled, for example, to the time-dependent electromagnetic field of a laser pulse, leading to a transfer of nuclear amplitude to an excited electronic state based on the precise characteristics of the field. In practice, two strong approximations are made to simplify the photoexcitation process:[2] (1) A harmonic Wigner distribution is often used to represent the ground-state distribution of the molecule, from which initial nuclear positions and momenta can be sampled; (2) These pairs of nuclear positions-momenta are then promoted to a given excited electronic state and used to initiate the nonadiabatic molecular dynamics – a so-called sudden excitation approximation.

In this talk, I will discuss the limitations of these two approximations, supported by numerical simulations of realistic molecular systems. I will then present more rigorous strategies to describe the photoexcitation process: ab initio molecular dynamics with a quantum thermostat to sample pairs of nuclear positions-momenta in the ground electronic state[3] and the promoted nuclear density approach to incorporate the effect of a laser pulse at the level of the initial conditions at no cost.[4]



References

[1] J. Suchan, D. Hollas, B. F. E. Curchod, P. Slavíček, On the Importance of Initial Conditions for Excited-State Dynamics, Faraday Discuss., 212, 307 (2018).

[2] J. Janoš, P. Slavíček, B. F. E. Curchod, Selecting Initial Conditions for Trajectory-Based Nonadiabatic Simulations, Acc. Chem. Res., 58, 2, 261 (2025).

[3] A. Prlj, D. Hollas, B. F. E. Curchod, Deciphering the Influence of Ground-State Distributions on the Calculation of Photolysis Observables, J. Phys. Chem. A, 127, 7400 (2023).

[4] J. Janoš, P. Slavíček, B. F. E. Curchod, Including Photoexcitation Explicitly in Trajectory-Based Nonadiabatic Dynamics at No Cost, J. Phys. Chem. Lett., 15, 10614 (2024).

MULTISTATE COUPLED DIABATIC NEURAL NETWORK POTENTIAL FOR THE QUANTUM NON-ADIABATCI PHOTOFRAGMENTATION OF CH_2^+

O. Roncero [a,*], P. del Mazo-Sevillano [b], S. Gómez-Carrasco [b], A. Aguado [c]

[a] *Instituto de Física Fundamental, CSIC, Serrano 123, 28006 Madrid (Spain).*
[b] *Facultad de Químicas, University of Salamanca, 37008 Salamanca (Spain)*
[c] *Facultad de Ciencias M14, Universidad Autónoma de Madrid, 28049 Madrid (Spain)*
*octavio.roncero@csic.es

Tracking the complex non-adiabatic transitions in far-ultraviolet photodissociation demands highly accurate diabatic potential energy matrices (PEMs) across numerous excited states. To address this, we introduce a fully automated diabatization method that leverages artificial neural networks to fit PEMs [1]. Our approach divides the PEM into a physically grounded zeroth-order diagonal term, which is then corrected by a neural network matrix to capture electronic couplings. By enforcing symmetry constraints on off-diagonal elements and sharing degenerate diabatic states between the A' and A" irreducible representations, the fitting process becomes completely automatic. We validate this method using time-dependent wave packet calculations [2] to simulate the photodissociation of CH_2^+, incorporating relevant states up to approx. 13.6 eV. Finally, we compute partial cross-sections for all fragmentation channels (including total and partial fragmentation) yielding CH^+, CH, H_2, and H_2^+ diatoms, revealing a notably high cross-section for the formation of the CH radical.

References

[1] P. del Mazo-Sevillano, S. Gómez-Carrasco, A. Aguado, O. Roncero, *Submitted (2026)*
[2] O. Roncero and P. del Mazo-Sevillano, *Comput. Phys. Comm. 109471 (2025)*

ATOM-DIATOM REACTIONS OF INTEREST: THE DESTRUCTION OF CH^+ AND HEH^+ IN COLLISION WITH H

T. González-Lezana [(a)] *

[(a)] *Instituto de Física Fundamental (CSIC), Madrid, Spain.*

*t.gonzalez.lezana@csic.es

We have investigated the dynamics of two reactions of interest. On the one hand, rate constants for the $C^+ + H_2 \rightarrow CH^+ + H$, $CH^+ + H \rightarrow C^+ + H_2$ and $CH^+ + H \rightarrow CH^+ + H$ collisions [1] have been calculated for astrophysical applications. In particular, the produced data have been employed in the analysis of the multiple rotational and rovibrational transitions of the CH+ detected toward the planetary nebula NGC 7027 [2].

On the other hand, calculations on the $H + HeH^+ \rightarrow He + H_2^+$ [3, 4] reaction using a corrected potential energy surface with the right long-range behavior [4] have been extended to the case of ^{3}He and T instead ^{4}He and H, respectively in an attempt to quantify the possible relevance of the destruction of $^3HeT^+$, and ionic species formed during the single- decay of molecular tritium. Rate constants for a series of different rovibrational initial HeH^+ states have been calculated [5].

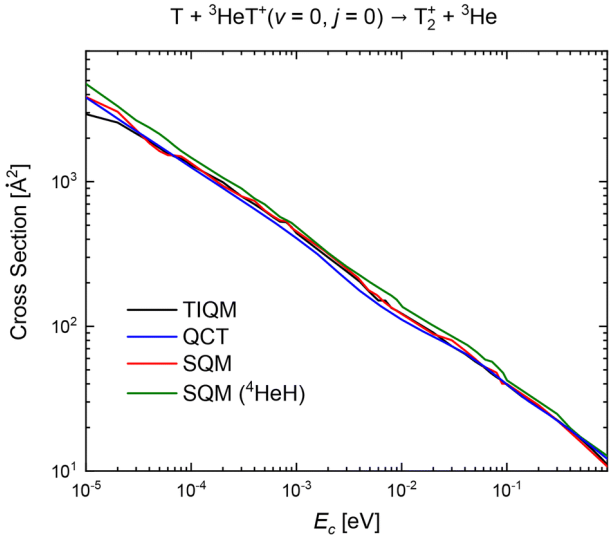


Figure 1: Integral cross sections for the $T + {}^3HeT^+ (v = 0, j = 0) \rightarrow {}^3He + T_2^+$ reaction obtained with exact time independent quantum mechanical, quasi-classical trajectory and statistical quantum methods.

References

[1] Tomás González-Lezana *et al.* Phys. Chem. Chem. Phys. **28**, 4065–4075 (2026).
[2] Milan Sil *et al.* A&A in press (2026).
[3] T. González-Lezana*et al.* J. Phys. Chem. A **123**, 10480-10489 (2019).
[4] J. Sahoo *et al.* J. Chem. Phys. **161**, 144312 (2024).
[5] J. Sahoo *et al.* Phys. Chem. Chem. Phys. **28**, 6323-6330 (2026).

REACTIONS OF HYDROFLUOROOLEFINS WITH OZONE PRODUCE LONG-LIVED GREENHOUSE GASES

A. J. Orr-Ewing,[(a), *] M. d.l.A. Garavagno,[(a)] K. M. Stanley,[(a)] D. E. Shallcross,[(a)] and K. T. Kuwata[(b)]

[(a)] *School of Chemistry, University of Bristol, Bristol, UK.*
[(b)] *Department of Chemistry, Macalester College, Saint Paul, Minnesota, USA.*
[*]a.orr-ewing@bristol.ac.uk

Hydrofluoroolefins (HFOs) and their partially chlorinated analogues (HCFOs, hydrochlorofluoroolefins) are increasingly replacing hydrofluorocarbons (HFCs) in refrigeration, air-conditioning, foam-blowing and other technological and industrial applications. As a consequence, atmospheric monitoring stations now report growing mixing ratios of these compounds in tropospheric air. The incorporation of an olefinic bond into the HFO molecular structure encourages reactive removal by OH radicals and O_3 in the lower atmosphere; hence, HFOs are considered to have much lower global warming potentials than HFCs, which are potent greenhouse gases. Our experimental laboratory and computational studies of HFO and HCFO oxidation reactions [1,2] reveal that under atmospheric conditions, the ozone-initiated degradation of these compounds can produce three long-lived greenhouse gases: trifluoromethane (HFC-23, CF_3H), perfluoromethane (PFC-14, CF_4), and trifluorochloromethane (CFC-13, CF_3Cl), the latter of which is also a stratospheric-ozone depleting substance. The persistent environmental pollutant trifluoroacetic acid (TFA) is also produced by this oxidation chemistry. This presentation will discuss the evidence for production of these environmentally harmful compounds, quantitative determinations of their yields, the mechanisms for the reactions (see figure 1), and the climate implications of widespread use of HFOs and HCFOs.

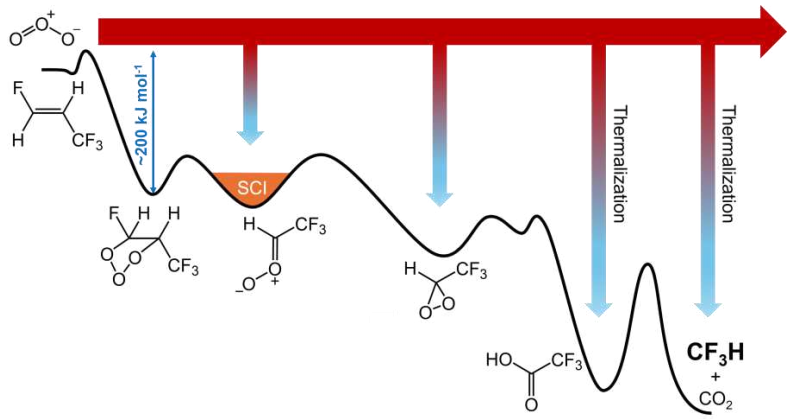


Figure 1: Ozone oxidation of HFOs and HCFOs is an unexpected source of atmospheric PFC-14, HFC-23 and CFC-13, in competition with production of trifluoroacetic acid and stabilized Criegee intermediates (SCI).

References

[1] M.R. McGillen, Z.T. Fried, M.A.H. Khan, K.T. Kuwata, C.M. Martin, S. O'Doherty, F. Pecere, D.E. Shallcross, K.M. Stanley, K. Zhang. *Proc. Natl. Acad. Sci. USA* **120,** e2312714120 (2023).

[2] M.d.l.A. Garavagno, A. Wenger, R. Holland, B.R. Fena, S.D. Goldstein, D.E. Hicks, F. Liu, J.B. Madell, S.J. Solomon K.T. Kuwata, M. McGillen, M.A.H. Khan, D.E. Shallcross, K.M. Stanley and A.J. Orr-Ewing, Environ. Sci. Technol. **59**, 26031–26040 (2025).

NUCLEAR QUANTUM EFFECTS IN COMPLEX CHEMICAL REACTIONS: A RING-POLYMER MOLECULAR DYNAMICS APPROACH

Toshiyuki. Takayanagi[a]

[a] *Department of Chemistry, Saitama University, Japan.*
*tako@mail.saitama-u.ac.jp

Understanding nuclear quantum effects in complex chemical reactions occurring in aqueous solutions and on ice surfaces remains both important and challenging in the field of theoretical chemistry. In recent years, our group has been investigating such reaction systems using the real-time ring-polymer molecular dynamics (RPMD) method, which can approximately account for nuclear quantum effects, including zero-point vibrational motion and quantum tunneling.

In this talk, I will present two recent studies. The first concerns an organic reaction that exhibits post-transition-state bifurcation (PTSB) behavior, in which the reaction pathway via a single transition state subsequently bifurcates into two (or more) distinct product channels due to the presence of a valley-ridge transition region on a high-dimensional potential energy surface. We applied RPMD simulations to a PTSB reaction between 2-aminoacrolein and 1,3-butadiene using a size-selected water-cluster model. This reaction yields either a (4 + 3) seven-membered-ring product or a (4 + 2) Diels-Alder six-membered-ring product. In addition, both intramolecular and water-mediated proton-transfer processes can occur in the (4 + 3) product region. Our results show that nuclear quantum effects play an important role in determining the product branching ratios as well as the proton-transfer dynamics in the product region [1, 2].

The second system we studied involves the collision dynamics of HCl with ice clusters composed of 48 or 49 water molecules showing crystalline and amorphous structures, respectively. We investigated HCl solvation, subsequent acid dissociation, and proton-transfer processes within the hydrogen-bond network. By systematically comparing the RPMD results with classical molecular dynamics simulation results, we found that inclusion of nuclear quantum effects significantly enhances both the initial acid dissociation and proton mobility along the hydrogen-bond network [3, 4].

References

[1] H. Matsubuchi, D. Hayashi, D. Okamoto, A. Noguchi, S. Nakagawa, T. Takayanagi, T. Murakami, Solvent Effects on the Selectivity of Ambimodal Dipolar/Diels-Alder Cycloadditions: A Study Using Explicit Solvation Models. ChemPhysChem, **26**, e202500494 (2025).

[2] S. Nakagawa, H. Matsubuchi, H. Ota, T. Takayanagi, T. Murakami, Nuclear Quantum Effects on the Organic Bifurcation Reaction in Aqueous Solution: Ring-Polymer Molecular Dynamics Calculations Using an Explicit Solvation Model. Submitted for publication.

[3] T. Murakami, H. Ueno, Y. Kikuma T. Takayanagi, Nuclear Quantum Effects in the Ionic Dissociation Dynamics of HCl on the Water Ice Cluster, Molecules **30**, 442 (2025).

[4] Y. Sasaki, H. Ueno, K. Okada, T. Toshiyuki, T. Murakami, Nuclear Quantum Effects in the Ionic Dissociation Dynamics of HCl on Amorphous and Crystalline Ice at 100 K. To be published.

RADIATIVE ASSOCIATION OF C_6H WITH METAL CATIONS: FORMATION MECHANISMS AND RATE CONSTANTS FOR MC_6H^+ ASTROCHEMICAL SPECIES

Niyazi Bulut[1,4], Octavio Roncero[2], Marıa Mallo[2], Germán Molpeceres[2], Maysa Yusef-Buey[2], Marcelino Agúndez[2], José Cernicharo[2], Carlos Cabezas[2], and Piotr Zuchowski [3]

[1]*Faculty of Applied Physics and Mathematics, Gdansk University of Technology, Poland.*
[2]*Instituto de Física Fundamental (IFF-CSIC), Serrano, 123, 28006 Madrid, Spain*
[3]*Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, 87-100 Torun, Poland*
[4]*Faculty of Science Physics Department, Firat University, Elazig, Türkiye.*
nbulut@firat.edu.tr

Metal-bearing molecules are important tracers of the chemical processing of refractory elements in space, particularly in carbon-rich circumstellar envelopes where metal atoms and cations can remain in the gas phase. Recent astronomical detections of Mg-bearing carbon-chain cations have highlighted radiative association as a possible formation mechanism for larger metal-containing molecules. In this work, we investigate the formation of MC_6H^+ adducts, where M = Na, Mg, and Al, through the reaction of C_6H with metal cations.

The electronic structure of the $M^+ + C_6H$ systems was examined using multireference configuration interaction calculations based on state-averaged CASSCF wave functions. The potential energy curves reveal strong attractive interactions in the entrance channel, mainly governed by the ion-dipole interaction. For Mg^+ and Al^+, electronic crossings associated with charge-transfer character, while Na^+ shows a different behavior because of its much higher second ionization energy. To assess the structural stability of the products, the isomeric landscapes of MC_6H^+ were explored using automatic reaction discovery calculations. The results show that the linear structures are the most stable isomers for all three metal cations, lying significantly below the competing cyclic and bent configurations.

Radiative association rate constants were then evaluated using statistical methods that include capture, radiative emission, and back-dissociation processes. Quasi-classical trajectory calculations were used to refine the capture rates, and the influence of low-frequency vibrational modes on the stabilization probability was analyzed.

We found that radiative association is an efficient pathway for the formation of MgC_6H^+ and may also contribute to the production of other metal-bearing carbon-chain cations in astrophysical environments. The present results provide molecular data and rate constants that can be incorporated into astrochemical models of carbon-rich circumstellar envelopes such as IRC+10216.

Keywords: astrochemistry; radiative association; metal-bearing molecules; interstellar chemistry.

Energetics and Dynamics in Quantum Theory: A Green-Theoretical Perspective

A.J.C. Varandas
Department of Physics, Qufu Normal University, China
Department of Physics, Universidade Federal do Espírito Santo, 29075-910 Vitória, Brazil
Coimbra Chemistry Centre, University of Coimbra, 3004-535 Coimbra, Portugal
Email: varandas@uc.pt

No problem has an exact solution in Physics and Chemistry: while highly error-resilient, the experiments are themselves error-affected. One then wonders whether calculations designed to deliver accurate solutions at a high cost can be the best way to proceed? Even if such a view prevails for small systems, can it challenge the curses of physical-size and basis-set size? In this talk, a green-theoretical perspective is advocated: extrapolation of cost-effective first-principles results with asymptotic theories. For the energetics, a divide-to-conquer approach is also employed while the use of the correspondence principle is well suited for the dynamics, by using quantum theory for low angular momenta and classical mechanics for their extrapolation. Examples are given, while others are pinpointed.

MERGING SEMI- AND QUASI-CLASSICAL METHODS FOR THE ACCURATE CALCULATION OF VIBRATIONAL ENERGY EXCHANGE IN MOLECULAR COLLISIONS OF TECHNOLOGICAL INTEREST

F.Esposito[(a), *], N. Bulut [(b,c)], P. S. Żuchowski [(d)], G. C. McBane [(e)]

[(a)] *Istituto per la Scienza e Tecnologia dei Plasmi, Consiglio Nazionale delle Ricerche, Sede Territoriale di Bari, Bari, Italy*
[(b)] *Department of Physics, Faculty of Science, Firat University, Elazig, Turkey*
[(c)] *Faculty of Applied Physics and Mathematics, Gdansk University of Technology, Poland*
[(d)] *Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland*
[(e)] *Department of Chemistry, Grand Valley State University, Allendale, MI, USA*

[*]fabrizio.esposito@cnr.it

The accurate treatment of large ranges of total energy for vibrational energy exchange processes in molecular collisions is needed [1] for quantitative simulations of non-equilibrium plasmas of great technological interest, like those used for CO_2 destruction and nitrogen fixation. Simulations are in turn key for formulating the best recipe for achieving high energy efficiency, crucial for industrial applications. An effort [2] to merge semiclassical and quasiclassical methods is presented, with the aim of exploiting the best of each approach in the variety of conditions met in non-equilibrium plasmas simulations. The two approaches are ideally merged at the level of trajectories, using a metric recently introduced [3], based on the observations of Ian W.M. Smith in the seventies. The results are definitely encouraging, getting very good comparisons as in Figure 1 with highly accurate but also extremely challenging time-dependent and time-independent quantum-mechanical calculations. The metric is particularly useful for better understanding and discriminating the physics of the collision in vibrational energy exchange processes of potentially reactive collisional systems.

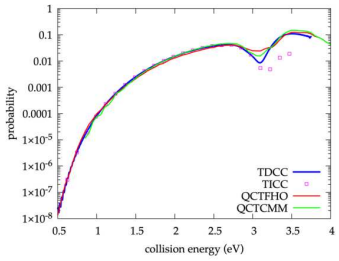


Figure 1: Comparison of different dynamical approaches for the calculation of vibrational energy exchange probability for $O+N_2(v=0, j=0) \rightarrow O+N_2(v=1, j' \leq 10)$.

References

[1] Esposito, F.: On the relevance of accurate input data for vibrational kinetics in air cold plasmas: the case of nitrogen fixation. Plasma Sources Sci. Technol. 31, 094010 (2022). https://doi.org/10.1088/1361-6595/ac9082
[2] Esposito, F., Bulut, N., Żuchowski, P.S., McBane, G.C.: Towards a hybrid semi-quasi-classical trajectory method for the accurate calculation of vibrationally inelastic probabilities in atom–diatom collisions. Phys. Chem. Chem. Phys. 28, 2631–2651 (2026). https://doi.org/10.1039/D5CP03853G
[3] Esposito, F., Armenise, I.: Reactive, Inelastic, and Dissociation Processes in Collisions of Atomic Nitrogen with Molecular Oxygen. J. Phys. Chem. A. 125, 3953−3964 (2021). https://doi.org/10.1021/acs.jpca.0c09999

Ultracold Atom+Molecule Systems through the Lens of *Ab Initio* Electronic Structure Theory

Marcin Gronowski [(a),*]

[(a)] Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland

[*] m.gronowski3@uw.edu.pl

Experiments with ultracold atoms have achieved an unprecedented level of control. Similarly, co-trapping molecular ions with laser-cooled atomic ions enables single-molecule spectroscopy in fundamentally new ways [1]. In contrast, complex quantum dynamics governs ultracold collisions between neutral molecules and atoms, where attractive van der Waals interactions promote the formation of long-lived collision complexes with a high density of states.

In this talk, I focus on ultracold collisions between alkali-metal dimers and alkali-metal atoms to illustrate the complexity arising from the rich internal structure of the collision complexes, including their vibrational, rotational, and hyperfine degrees of freedom. In the NaLi($a^3\Sigma^+$) + Na(^2S) system [2, 3], nonadditive three-body interactions significantly reshape the highly anisotropic potential energy surface. This anisotropy, in combination with spin-spin and spin-rotation interactions, strongly influences the collision dynamics. In the KRb ($X^1\Sigma^+$) + Rb(^2S) system [4], we identify an energetically accessible conical intersection between the ground and first excited electronic states. Such a conical intersection significantly alters the hyperfine interactions within the complex, for example through enhanced spin-rotation coupling, and may contribute to the experimentally observed hyperfine-to-rotational energy transfer.

References

[1] Z. Wu, T. Duka, M. Isaza-Monsalve, M. Kautzky, V. Švarc, A. Turci, R. Nardi, M. Gronowski, M. Tomza, B. J. Furey, and P. Schindler, Infrared absorption spectroscopy of a single polyatomic molecular ion, submitted to Nature (2025).

[2] J. J. Park, H. Son, Y.-K. Lu, T. Karman, M. Gronowski, M. Tomza, A. O. Jamison, and W. Ketterle, Physical Review X **13**, 031018 (2023).

[3] T. Karman, M. Gronowski, M. Tomza, J. J. Park, H. Son, Y.-K. Lu, A. O. Jamison, and W. Ketterle, Physical Review A **108**, 023309 (2023).

[4] Y.-X. Liu, L. Zhu, J. Luke, M. C. Babin, M. Gronowski, H. Ladjimi, M. Tomza, J. L. Bohn, T. V. Tscherbul, and K.-K. Ni, Nature Chemistry **17**, 688 (2025).

CHEMICAL PUMPING IN ATOM-DIATOM REACTIONS

A. Zanchet [(a), *]

[(a)] *Instituto de Física Fundamental, CSIC, Madrid, Spain.*
[*]alexandre.zanchet@csic.es

In the last decade, we entered the golden age of "Astrochemistry", where the number of detected new molecules in the Interstellar Medium (ISM) is now increasing exponentially. In order to rationalize their observations, astronomers have to rely on the knowledge of the physico-chemical properties of the observed molecules and their spectroscopy in order to infer the physical conditions of the source they are observing. However, in some environments, the Local Thermodynamical Equilibrium (LTE) is not achieved, and the assumption of LTE conditions cannot be applied. In such cases, to achieve a correct interpretation of the observations, astronomers need to rely on the molecular excitation processes at individual scales.

Among those excitation processes, in this presentation we will focus on the "chemical pumping", which corresponds to the quantum states distribution of the products after a chemical reaction, and in particular in the case of atom-diatom reactive collisions. The reaction mechanism of this kind of processes and the distribution of products are governed by the Potential Energy Surface (PES) of the system and the physical conditions of the reactants. If those are known, it is possible to estimate theoretically the resulting chemical pumping of products. Fundamentally, the chemical pumping is connected to the state-to-state chemistry, and more specifically on how the quantum states distribution of products is directly related to the quantum states of the reactants. Taking advantage of this property, we will see how it is possible to disentangled and understand the IR emission of OH radical in UV irradiated protoplanetary disks[1].

References

[1] Zannese, *et al.* OH as a probe of the warm-water cycle in planet-forming disks. *Nat Astron* **8**, 577–586 (2024).

Proton transfer and hydronium formation in ionized water

Jochen Küpper

Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
Department of Physics, Universität Hamburg, Germany
Department of Chemistry, Universität Hamburg, Germany
Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

Radiation chemistry in aqueous systems, induced by ionizing radiation, primarily leads to the ultrafast dynamics of water molecules. The initial response of the aqueous system to ionizing radiation involves the formation of hydrated electrons and ultrafast proton transfer, which was recently probed in the ionized water dimer [1]. However, so far the subsequent fragmentation pathways into highly reactant intermediates were only explored by molecular dynamics simulations. We utilized purified molecular beams of water dimer and strong-field ionization at 800 nm to investigate the early phase of the dynamics following ionization of the aqueous environment. Using velocity map imaging, we revealed that water dimer can either stabilize or undergo fragmentation along more than ten distinct reaction pathways [2].

To address the ultrafast dynamics of these ion-reaction pathways, we set up a disruptive-probing [3] pump-probe experiment that enabled us to track the formation and energies of all ionic-species products simultaneously, directly yielding a reaction network and branching pathways as well as effective reaction-rate constants and their energy dependence [4]. These findings provide crucial insights into the post-ionization processes in aqueous environments, with implications for both atmospheric chemistry and radiation therapy.

References

[1] K. Schnorr, M. Belina, et int (7 authors), P. Slavíček, and R. Moshammer, *Sci. Adv.* **9**, eadg7864 (2023)

[2] I.S. Vinklárek, H. Bromberger, N. Vadassery, W. Jin, J. Küpper, and S. Trippel, *J. Phys. Chem* A **128**, 1593 (2024); arXiv:2308.08006 [physics]

[3] B. Jochim, L. DeJesus, and M. Dantus, *Rev. Sci. Instrum.* **93**, 033003 (2022)

[4] I.S. Vinklárek, S. Trippel, M. Belina, L. Blum, H. Bromberger, P. Slavíček, J. Küpper, *under review*; arXiv:2602.17505 [physics]

Quantum State-Selected Reaction dynamics at Low Temperatures

Tiangang Yang*

Department of Chemistry, and Center for Advanced Light Source, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China.

**Email: yangtg@sustech.edu.cn*

Understanding chemical reactions at the quantum level requires precise control over molecular quantum states and collision energies, especially at low temperatures where quantum effects dominate. We present recent progress in developing integrated platforms for quantum-state-resolved studies of ion–molecule reaction dynamics. Our system combines a laser-cooled ion trap with high-resolution TOF-MS and fluorescence imaging, enabling sub-kelvin cooling of Be^+ and C^+ ions with accurate micromotion compensation [1-2].

To prepare quantum-state-selected neutral reactants, we employ a stimulated Raman pumping (SRP) system with a fast chopper for H_2 (v = 1) [3] and N_2 (v = 2) [4], and a cavity-enhanced IR excitation scheme that achieves >30% population in the CO (v = 3) overtone state [5]. These tools enable us to investigate how vibrational excitation, orientation, and isotope effects influence reactivity under cold conditions. Together, these capabilities provide a robust platform for studying state-to-state dynamics in cold collisions and for benchmarking theoretical models of interaction potentials and non-adiabatic couplings. Current work explores the roles of vibrational excitation, orientation, and isotope substitution in systems like $BeD^+ + O_2$ [6] and $C^+ + H_2$(v=1). Recent results and future directions for quantum-controlled reactivity will be discussed.

References

[1] Xiao, Y.; Peng, Y.; Chen, L.; et al., Commun. Phys. **7**: 423 (2024).
[2] Xiao, Y.; Wen, L.; Xie, Y.; et al., Rev. Sci. Instrum. **96** (8), 085205-1-9 (2025).
[3] Xie, Y.; Han, J.; Wen, L.; et al., J. Phys. Chem. Lett. **14**: 11603 (2023).
[4] Xiao Y.; Wen L.; Li, Z.; et al, J. Phys. Chem. Lett. **15** (46), 11767 (2024).
[5] Liu Q.; Zhang, H.; Wen, L.; et al, J. Phys. Chem. Lett. **15** (39), 9926-9931 (2024).
[6] Peng, Y.; Li, J.; Song, Z.; et al., JACS Au **5** (9), 4260-4267 (2025).

STATE-RESOLVED VIBRATIONAL DYNAMICS FROM MIXED QUANTUM-CLASSICAL METHODS

C. Coletti *

[a] *Dipartimento di Farmacia, Università G. d'Annunzio Chieti-Pescara, Italy.*
*cecilia.coletti@unich.it

Mixed quantum-classical (MQC) methods [1] provide an effective framework for the study of molecular collisions in regimes where a fully quantum treatment becomes computationally impractical, yet a purely classical description fails to capture the relevant vibrational dynamics. Their central idea is to retain a quantum treatment of the vibrational motion while describing translational and rotational degrees of freedom classically, thus preserving the state-resolved character of vibrational transitions at an affordable computational cost.

Here we discuss two complementary MQC formulations for the calculation of vibrational excitation and relaxation observables in atom-diatom and diatom-diatom collisions. The first one [2,3,4] is designed for non-reactive inelastic scattering and combines classical trajectory propagation with a close-coupled treatment of the vibrational dynamics. This formulation is particularly efficient for the generation of extensive sets of state-to-state cross sections and rate coefficients and can also be extended to quantities relevant for transport collision integrals [3]. The second formulation [5] is based on wavefunction propagation on a grid and is more flexible in regimes involving highly excited vibrational states, near-dissociation dynamics, or bond rearrangement. Together, the two methods provide a versatile computational strategy for tackling a broad class of collisional problems.

The complementarity of the two MQC formulations is discussed in connection with their range of applicability, computational cost, and ability to describe different dynamical regimes. The generation of complete datasets can be further supported by machine-learning tools. Gaussian-process regression or Neural Network techniques [6] can be employed to predict the observables obtained from the mixed quantum-classical calculations and provide coverage extension across all accessible vibrational states, collision energies and temperatures [7].

References

[1] G.D. Billing The Quantum Classical Theory, Oxford University Press (2003).
[2] G. D. Billing, Comp. Phys. Comm. **32,** 45–62 (1984)
[3] Q. Hong, L. Storchi, Q. Sun, M. Bartolomei, F. Pirani, and C. Coletti, J. Chem. Theory and Comput. **19,** 8557–8571 (2023).
[4] M. Pezzella, F. Pirani, M. Bartolomei, Q. Hong, F. Lique, L. Storchi, C. Coletti, Phys Chem Chem Phys **28**, 29202931 (2026)
[5] C. Coletti, G. D. Billing, J. Chem. Phys. **113** 11101–11108 (2000)
[6] Q. Hong, L. Storchi, M. Bartolomei, F. Pirani, Q. Sun, and C. Coletti, Eur. Phys. J. D **77** (2023) 128.
[7] Q. Hong, M. Bartolomei, F. Pirani, Q. Sun, and C. Coletti, J. Chem. Phys. **162** (2025) 114308

TOWARDS DERIVING NON-ADIABATIC QUANTUM DYNAMICS WITH QUANTUM BOLTZMANN CONSERVATION, RABI OSCILLATIONS AND CLASSICAL SCALING

Lauren E. Cook[(a)], James R. Rampton[(a)] and Timothy J. H. Hele[(a)*]

[(a)] *Department of Chemistry, University College London, UK.*
[*]t.hele@ucl.ac.uk

Non-adiabatic quantum dynamics is vital for understanding reactions involving more than one Born-Oppenheimer potential energy surface. However, the exact equations are too complex to apply to large systems and therefore there have been a plethora of approximate methods developed. Ideally such an approximate method should conserve the quantum Boltzmann distribution, reproduce Rabi oscillations between electronic states, scale classically with system size and have a derivation from exact quantum dynamics. To the best of our knowledge, no such method yet exists which satisfies all of these criteria simultaneously and exactly for a general system, and in this presentation I will discuss efforts in our group to examine this challenging problem. For single-surface (adiabatic) systems, Matsubara dynamics [1] can be derived by truncating in the higher normal modes of the imaginary-time path integral. From Matsubara dynamics, single surface RPMD, CMD and TRPMD can be obtained [2,3], which scale classically and also conserve the quantum Boltzmann distribution. This motivates extending Matsubara dynamics to non-adiabatic systems, and building on previous attempts [4,5] I will discuss our investigations of truncating in the electronic degrees of freedom for the Meyer-Miller-Stock-Thoss [6] and Spin-Mapping representations [7] of non-adiabatic dynamics, as well our research developing symplectic propagation algorithms for the corresponding Hamiltonians [8-10]. We find (perhaps surprisingly) that for electronic-only systems truncating in the MMST path-integral normal modes does not lead to accurate dynamics or distribution conservation at the level of a single trajectory [6] but truncating in all but the lowest normal mode in the spin-mapping representation leads to exact dynamics and distribution conservation [7]. We hope this will motivate future research to derive accurate and scalable non-adiabatic quantum dynamics.

References

[1] T. J. H. Hele, M. J. Willatt, A. Muolo and S. C. Althorpe, J. Chem. Phys 142 (2015) 134103.
[2] T. J. H. Hele, M. J. Willatt, A. Muolo and S. C. Althorpe, J. Chem. Phys 142 (2015) 191101
[3] T. J. H. Hele, *Mol. Phys.* **114** *9* (2016) 1461-1471
[4] S. N. Chowdhury and P. Huo, J. Chem. Phys. 154, 124124 (2021)
[5] D.L. Bossion, S.N. Chowdhury, P. Huo. J. Chem. Phys. 158, 044123 (2023)
[6] LE Cook, TJH Hele, J. Chem. Phys. 163 (17) 174113 (2025)
[7] LE Cook, JR Rampton and TJH Hele *in preparation*
[8] MS Church, TJH Hele, GS Ezra, N Ananth, J. Chem. Phys. 148 (10)
[9] LE Cook, JE Runeson, JO Richardson, TJH Hele, J. Chem. Theor. Comp. 19 (18), 6109-6125
[10] LE Cook, JR Rampton, TJH Hele, J Chem Phys 164 (14)

QUANTUM CONTROL OF THE DYNAMICAL BEHAVIOR OF RESONANCE STATES IN SMALL POLYATOMIC MOLECULES WITH INTENSE FIELDS

A. García-Vela [(a), *]

[(a)] *Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Spain.*
garciavela@ff.csic.es

A variety of molecular reaction processes are governed or mediated by resonance states. Some examples are the photodissociation of intermediate molecular species in chemical cycles, and the resonance-mediated reactive collisions of such intermediate species with other reagents. When these resonance-mediated processes compete, control over the resonance behavior (essentially the resonance lifetime and the product fragment distributions) can be crucial in order to steer the molecular reaction process in a desired direction. In previous works, control schemes using weak laser fields were applied to induce quantum interference in order to modify the lifetime [1,2] and the product fragment distributions [3,4] of resonance-mediated molecular photodissociation. Later on, moderately intense (of the order of 10^{11}-10^{12} W/cm^2) laser fields were applied to change (either reduce or increase) the resonance lifetime of a photodissociation process [5]. In the work presented here, relatively intense fields (of the order of 10^{13}-10^{14} W/cm^2) are applied to modify the product fragment distribution of the photodissociation of the CH_3 radical [6]. The control scheme suggested applies an intense control pulse that produces a light-induced conical intersection (LICI) between the ground and the excited electronic states, that reshapes the natural diabatic potentials of the radical, generating new adiabatic light-induced potentials (LIPs). The new LIPs lead to different photodissociation dynamics, opening new pathways for population transfer between the electronic states, and then producing different fragment distributions compared to the weak-field regime. Varying the position of the LICI (which is determined by the frequency of the intense laser pulse) makes possible to vary the shape of the LIPs created, which allows a large degree of control. It is found that in addition to the product distribution, the resonance lifetime can also be modified (reduced in this case). The scheme appears to be of universal application to resonance-mediated molecular photodissociation.

References

[1] A. García-Vela, J. Chem. Phys. **136**, 134304 (2012).
[2] A. García-Vela, J. Phys. Chem. Lett. **3**, 1941-1945 (2012).
[3] A. García-Vela and Niels E. Hemriksen, J. Phys. Chem. Lett. **6**, 824-829 (2015).
[4] A. García-Vela, Phys. Rev. Lett. **121**, 153204 (2018).
[5] A. García-Vela, J. Chem. Theory Comput. **21**, 1547-1560 (2025).
[6] A. García-Vela, Small Struct. **7**, e202500541 (2026). https://doi.org/10.1002/sstr.202500541.

Population transfer between degenerate continuum states via impulsive stimulated Raman scattering: application to the control of HOD photofragmentation

Niels E. Henriksen

Department of Chemistry, Technical University of Denmark, Denmark
neh@kemi.dtu.dk

A key feature of reactive bimolecular collisions is the underlying degenerate continuum scattering states at fixed energies. Descriptions can be either energy-resolved or time-resolved. This distinction is also reflected experimentally: velocity-selected crossed molecular beam setups versus pump-probe femtochemistry.

Unimolecular photofragmentation has also been denoted as “half-collisions” and can be described in terms of a “half-scattering” operator. The time-resolved description has formed the foundation of femtochemistry, but a few bimolecular collisions have also been studied starting from weakly bound van der Waals complexes, i.e., the femtochemistry of pseudo-bimolecular reactions.

The possible control of such collisions beyond the selection of energy is an intriguing question. For photofragmentation this can, e.g., involve the creation of vibrational wave packets in the electronic ground state prior to short-pulse phase-coherent excitation to excited electronic states. Modulation of the phases associated with the different frequency components translates into the control of quantum interferences. Alternatively, one could create a wave packet in an excited electronic state and subsequently modulate this wave packet with a second laser pulse.

In the present work, we explore such a scheme, inspired by previous experimental and theoretical work where a vibrational wave packet in an electronically excited bound state of I_2 was modulated with a non-resonant femtosecond laser pulse in the near-infrared (NIR) [1]. In a proof-of-principle study for scattering states, we consider the control of bond-selective photofragmentation of HOD in its first electronically excited state. Once the molecule is electronically excited to this state, it dissociates within 20–30 fs into two possible products: OD + H or OH + D. An ultrashort non-resonant NIR laser pulse is applied to the system right after the electronic excitation has taken place. Population transfer and interference between the continuum eigenstates are thus generated and scrutinized with respect to the control of the branching ratio between the two product channels [2].

References

[1] H. Goto, H. Katsuki, H. Ibrahim, H. Chiba, and K. Ohmori, Nat. Phys. **7**, 383–385 (2011).
[2] P. Dal Cin and N.E. Henriksen, Phys.Chem.Chem.Phys. **26**, 29846-29852 (2024).

An old question: are there resonances in the $F + H_2(v = 0) \rightarrow FH(v = 3) + H$ reaction?

D. Sokolovski [a,d],*, D. De Fazio [b], E. Akmatskaya [c,d]

[a] Department of Physical Chemistry, University of the Basque Country, Leioa, Bizkaia, 48940, Spain,
[b] Istituto di Struttura della Materia-Consiglio Nazionale delle Ricerche, 00016 Roma, Italy
[c] Basque Center for Applied Mathematics (BCAM), Alameda de Mazarredo 14, 48009 Bilbao, Bizkaia, Spain,
[d] IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 5, 48009, Bilbao, Bizkaia, Spain
* dgsokol15@gmail.com

The answer is yes. There is one dominant resonance in the 62.09-100 meV energy range. The problem is that one cannot see its signature in the integral cross sections (ICS), since the life time τ is too small for that. The resonance is, however, visible in the angular distributions, where one cannot discard the possibility of a resonance effects simply because τ is deemed to be "too short". What matters is the angle by which the metastable complex rotates before breaking up, i.e., the product of τ and the angular velocity ω. This angular life can be significant for light rapidly spinning systems, in which case characteristic oscillations will be produced in the differential cross sections (DCS) [1,2]. Recently we developed computer codes to analyse the ICS [3], and to deal with the "scattering interferometry" peculiar to the DCS [4]. Our conclusions are confirmed by analysing both integral and differential cross sections obtained for two different potential surfaces, FXZ [5] and CSZ [6]. We use numerical scattering data recently provided by Prof. D. De Fazio [7].

References

[1] C. Xiahou, J. N. L. Connor, D. De Fazio and D. Sokolovski, *Phys. Chem. Chem. Phys.*, **6**, 3647 (2024).
[2] D. Sokolovski, D. De Fazio, and E. Akhmatskaya, *ACS Phys. Chem Au* , **5**, 219?226 (2025).
[3] E. Akhmatskaya and D. Sokolovski, and C. Echeverr.a-Arrondo, *Comp. Phys. Comm.*, **185**, 2127 (2014).
[4] E. Akhmatskaya and D. Sokolovski, *Comp. Phys. Comm.*, **277**, 108370 (2022).
[5] C. Xiahou, J. N. L. Connor, D. De Fazio and D. Sokolovski, *Phys. Chem. Chem. Phys.*, **26**, 3647 (2024).
[6] B. Fu, X. Xu, and D. H. J. Zhang, *Chem. Phys.* , **129**, No. 011103 (2008).
[7] D. De Fazio (private communication).

STRUCTURE-BASED GAUSSIAN EXPANSION FOR EFFICIENT MULTIDIMENSIONAL WAVEPACKET CALCULATIONS: APPLICATIONS TO ISOLATED AND OPEN SYSTEMS

M. Kanno *, T. Koshiba, F. Misaizu, H. Kono

Department of Chemistry, Graduate School of Science, Tohoku University, Japan.
*manabu.kanno.d2@tohoku.ac.jp

The theoretical treatment of molecular wavepackets remains computationally demanding and becomes increasingly impractical for complex systems with a large number of atoms. To tackle this problem, we have developed the structure-based Gaussian (SBG) expansion method [1]. In the SBG expansion of wavepackets, space-fixed Gaussian basis functions with widths determined by the local potential Hessian matrix are densely placed around reaction pathways connecting equilibrium structures and transition states. Furthermore, to make our method more efficient and versatile, we have recently introduced two machine learning techniques [2]: principal component analysis for the systematic construction of the SBG basis set and Gaussian process regression for the interpolation of potential energy surfaces. As a benchmark, we constructed full-dimensional nuclear wave functions for the umbrella-inversion tunneling in H_3O^+ [2]. The expansion using 33 SBGs successfully reproduced the experimental vibrational energies up to overtone excited states with only 19 quantum chemical calculations.

Proton transfer reactions in biological molecules are influenced not only by the quantum nature of hydrogen nuclei but also by the surrounding environment such as solvents. Here, we describe the density matrix of the target system using the SBG expansion, while environment-induced dissipation is treated within the Lindblad formalism [3]. We apply this approach to the double proton transfer in the guanine–cytosine (G–C) base pair consisting of 29 atoms. The double proton transfer in G–C generates an unstable tautomer G^*–C^*, which can lead to spontaneous mutations in DNA. The calculated lifetime of G^*–C^* is approximately 250 fs, indicating that tunneling effects strongly enhance the double proton transfer.

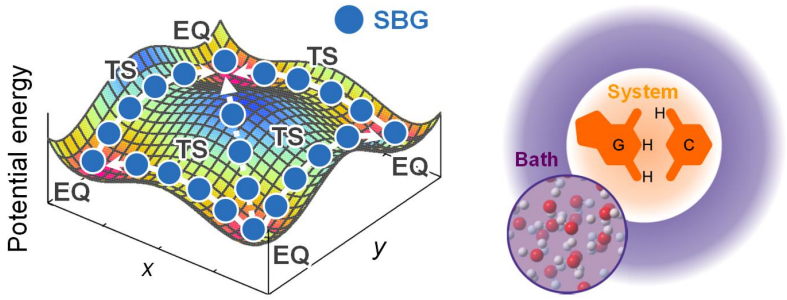


Figure 1: Schematic of the SBG expansion. (Left) Gaussian basis functions (blue circles) placed along reaction pathways connecting equilibrium structures (EQs) via transition states (TSs). (Right) The G–C base pair modeled as a quantum open system interacting with the surrounding environment as a heat bath.

References

[1] Kazuma Suzuki, Manabu Kanno, Shiro Koseki, and Hirohiko Kono, J. Phys. Chem. A **127**, 4152–4165 (2023).
[2] Takumi Koshiba, Manabu Kanno, Fuminori Misaizu, and Hirohiko Kono, J. Phys. Chem. Lett. **16**, 5986–5992 (2025).
[3] Heinz-Peter Breuer and Francesco Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, 2002).

INITIAL-STATE ENGINEERING AS AN ALTERNATIVE STRATEGY FOR QUANTUM CONTROL OF PHOTOCHEMICAL PROCESSES

I. R. Sola [(a), *], A. García-Vela [(b)]

[(a)] *Departamento de Química Física, Universidad Complutense de Madrid, Spain*
[(b)] *Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Madrid, Spain.*
[*]isolarei@ucm.es

Quantum interference plays a fundamental role in coherent control schemes and is essential for applications spanning quantum-state engineering, quantum information technologies, and the control of chemical reactions [1]. A key challenge in reactive scattering is steering photochemical processes toward desired fragmentation channels. Motivated by pump–probe femtochemistry, quantum optical control and general quantum optimal control theory have been extensively used to manipulate molecular wave packets as they evolve through transition states in photodissociation reactions [2].

Here, we propose an alternative control paradigm based on geometrical optimization [3], in which reaction selectivity is governed by engineering the molecular initial state, rather than enacting complex interactions on the dynamics after excitation. In practice, this approach inverts the conventional sequence by introducing the control pulse prior to photoexcitation. We show that coherences encoded in the prepared initial wave function can effectively predetermine the outcome of a wide range of processes, from asymmetric ionization and state-selective absorption to selective fragmentation in complex photodissociation reactions. In this work, we illustrate the potential of this technique through several representative examples.

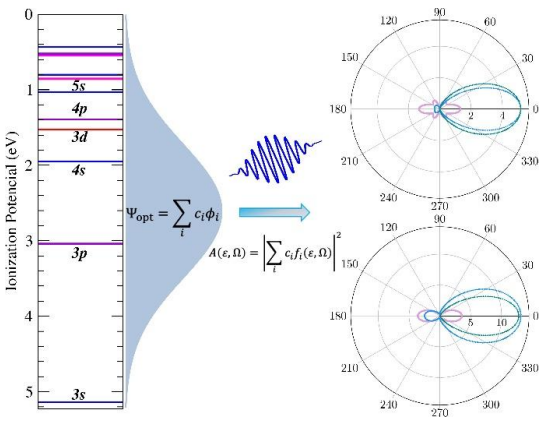


Figure 1: Photoangular distributions that maximize the anisotropy using 1 fs and 5 fs pulses, obtained through initial state optimization

References

[1] Sola, I. R.; Chang, B.; Malinovskaya, S.; Malinovsky, V. Adv. At. Mol. Opt. Phys. 67, 151-256 (2018).
[2] Judson, R. S.; Rabitz, H. Phys. Rev. Lett. 68, 1500 (1992).
[3] Sola, I. R.; García-Vela, A. Chem. Sci. 15, 15255 (2024).

PHYSICAL INSIGHT FROM THE MIXED QUANTUM/CLASSICAL SIMULATIONS OF COLLISIONAL ENERGY TRANSFER

V. Vijay, J. Sahoo, C. Joy, D. Bostan and D. Babikov*

Department of Chemistry, Marquette University, Milwaukee, Wisconsin, USA.
*dmitri.babikov@marquette.edu

Collisional energy transfer processes play critical roles in the interstellar medium, cometary comae, exoplanetary atmospheres and atmospheres of icy planets. However, full quantum mechanical treatments of inelastic molecular collisions become computationally expensive and even unaffordable for molecule + molecule collisions, particularly in cases when the projectile is heavy (which multiplies the number of rotational states of the system) and at higher collision energies (when the number of partial waves required for the description of scattering increases substantially). This presentation highlights recent developments in the Mixed Quantum/Classical Theory (MQCT), which combines quantum mechanical treatment of internal ro-vibrational motion with classical descriptions of scattering, providing an optimal balance between accuracy and computational efficiency. Our implementation employs time-dependent Schrödinger equation for the internal molecular states while using mean-field trajectories for translational motion. This approach preserves essential quantum phenomena including state quantization, zero-point energy, selection rules, and quantum interference — while achieving significant computational speedup compared to fully quantum methods. Recent algorithmic improvements and massive parallelization [1] have permitted us to extend MQCT to previously inaccessible complex systems. In this talk we will present new applications of MQCT to several interesting systems that include an open-shell diatom + atom system NO + Ar [2,3], molecule + molecule systems $H_2O + H_2$ and $HDO + H_2$ [4], and a polyatomic ethanimine molecule CH_3CHNH collided with He and H_2 [5]. Comparison with available benchmark quantum calculations demonstrate that MQCT provides reliable predictions across broad energy range, while offering unique time-dependent insights into collision dynamics. The infusion of artificial intelligence (AI) [6] and quantum computing (QC) [7] into MQCT methodology will also be presented.

References

[1] D. Bostan, C. Joy, V. Vijay and D. Babikov "MQCT 2026: A Program for Calculations of Inelastic Scattering of Two Molecules" Comput. Phys. Commun. 324, 110153, 2026.

[2] J. Sahoo, B. K. Kendrick, and D. Babikov, "Mixed Quantum/Classical Theory for Fine-Structure Inelastic Transitions in the Scattering of $^2\Pi$ Molecule with Structureless Target", to be submitted, 2026.

[3] K. Imanzi, D. Bostan, M. McCrea, M. Brouard, and D. Babikov, "Symmetry Breaking – A Classic Example of Quantum Interference Captured by Mixed Quantum/Classical Theory", J. Phys. Chem. Lett. 14, pp. 10617–10623, 2023.

[4] C. Joy, I. Gaidai, A. Faure and D. Babikov, "Mixed quantum/classical theory (MQCT) for Rotational Excitation of HDO in Collisions with H_2: Symmetry Breaking Effects and Time-Dependent Dynamics" J. Chem. Theor. Comp. 21, pp. 10669–10678, 2025.

[5] V. Vijay, F. Tonolo, E. Quintas-Sánchez, C. Joy, R. Dawes, F. Lique and D. Babikov, "Collisional energy transfer in ethanimine + He system" Phys. Chem. Chem. Phys., submitted, 2026.

[6] C. Joy, G. Occhiogrosso, B. Mandal, and D. Babikov "A Machine Learning Approach for Computationally Efficient Prediction of State-to-State Transition Cross Sections for Molecular Collision Processes", J. Phys. Chem. Lett., submitted, 2026.

[7] J. Andrade-Plascencia, T. Kuanysheva, D. Bostan, B. Kendrick and D. Babikov "Mixed Quantum/Classical Theory Approach to Rotationally Inelastic Molecular Collisions Implemented on a Quantum Computer", J. Chem. Theor. Comp. 21, pp. 6305–6314, 2025.

WALTER KOHN AND HIS CONTRIBUTIONS TO QUANTUM SCATTERING THEORY

David C. Clary,

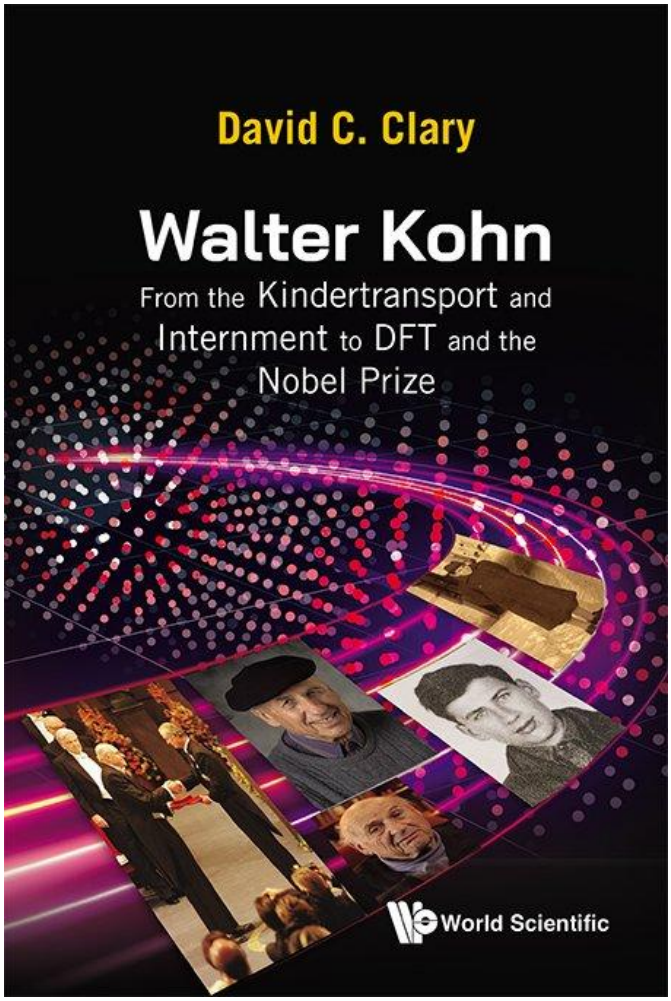
Department of Physical and Theoretical Chemistry
University of Oxford
Oxford OX1 3QZ
UK

david.clary@chem.ox.ac.uk

This talk will describe the life and career of Walter Kohn with particular emphasis on his contributions to quantum scattering theory. Reference will be made to recent books by the speaker [1-2].

[1] D. C. Clary, *Walter Kohn: From the Kindertransport and Internment to DFT and the Nobel Prize* (World Scientific Publishing, 2025).

[2] D. C. Clary, *Schrödinger in Oxford* (World Scientific Publishing, 2022).



MULTI-TEMPERATURE MODEL FROM STATE SPECIFIC DATA: APPLICATION TO ICE GIANTS

G. Colonna [a],*, D. Ninni [b], F. Bonelli [b], G. Pascazio [b], L. Walpot [c], L.D. Pietanza [a],*, A. Laricchiuta [a],*

[a] CNR-ISTP Bari, Italy
[b] DMMM, Politecnico di Bari, Italy
[c] ESA-ESTEC, Noordwijk, The Netherland
* gianpiero.colonna@cnr.it

In recent years, it has been shown that State-to-State (StS) kinetics gives very good agreement with experimental results when modeling the strong non-equilibrium conditions observed in the shock layer of a body entering the Earth [1] and Giant [2] atmospheres. The use of GPU's makes feasible to implement StS kinetics also in 2D configurations [1]. However, for faster calculations multi-temperature (mT) models are preferred for hypersonic flow simulations but available models are based on heuristic kinetic data obtained from density measurements. The point here is to construct a mT model coherently derived from the StS kinetics. This result has been be obtained calculating the mean rate coefficients weighting the StS data, that depend on the gas temperature and on the vibrational level, with the vibrational Boltzmann distribution at a given temperature T_v. This approach allows also to determine the rate of loss/production of vibrational energy due to internal transitions and chemical processes, the latter not available in traditional mT. This has been applied to the H_2/He mixture (Gas Giants) including ionization kinetics [3]. The result is encouraging, as can be observed in the Fig 1, where the electron density profile measured in a shock tube are compared with results obtained by the mT model. While for H_2/He mixture a detailed kinetic scheme is available, when contaminant are present StS data are very scanty, needing the use of approximate expressions, such as the Fridman-Macheret scaling low. The same problem exists for vibrational relaxation rates and simplified approaches, such as FHO can be used.

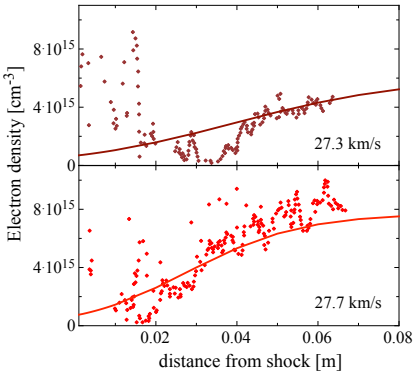


Figure 1: Comparison of calculated (line) and measured (dots) electron density for two entry velocities.

References

[1] G. Colonna et al., *Physical Review Fluids* **4** 033404 (2019)

[2] G Colonna et al., *International Journal of Heat and Mass Transfer* **156** 119916 (2020)

[3] G Colonna et al., *International Journal of Heat and Mass Transfer* **259** 128376 (2026)

Transport cross sections for characterization of planetary entry conditions

A. Laricchiuta [(a),*], F. Pirani [(b)], G. Colonna [(a)]

[(a)] CNR ISTP, Bari section, Bari, Italy
[(b)] Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, Italy
* annarita.laricchiuta@cnr.it

The novel impulse to the solar system exploration, with the NASA Dragonfly mission to Titan, the largest Saturn's moon, and the ESA Martian Moons eXploration - MMX, commits the research to new challenges. The reliable fluid dynamic modelling of hypersonic entry of bodies in the atmosphere of planets needs information relevant to the transport properties of the plasma formed in the shock. The chemistry of major atmosphere-components is affected by the presence of minority chemical species, e.g. CH_4, H_2O, NH_3 ..., and further complicated, in the vicinity of the vehicle surface, by the presence of carbon/oxygen contaminants from the TPS tiles. The transport properties relevant to planetary atmospheres are calculated, in the frame of the Chapman-Enskog theory, by exploiting the features of the tool EquilTheTA (EQUILibrium for plasma THErmodynamics and Transport Applications) [1] designed and implemented within the cooperation between the CNR ISTP Bari and University of Basilicata. The tool, accurate, stable and reliable in wide temperature and pressure ranges, derives transport coefficients from a core database of collision integrals for binary interactions. For heavy-particle interactions, namely neutral-neutral and neutral-charged species collision-pairs, a hybrid procedure is adopted that combines the traditional *multi-potential* with the *phenomenological* approach . The phenomenological approach [2-5], that allows the derivation of complete and consistent datasets of collision integrals for virtually any pair, models the average interaction by the Improved Lennard Jones (ILJ) potential whose features (depth and position of the well) are derived by correlation formulas given in terms of fundamental physical properties of interacting partners (dipole polarizability, charge, number of electrons effective in polarization). The hybrid approach together with the asymptotic approach for the estimation of the resonant charge-exchange contribution to odd-order collision integrals, and the calculation of electron-neutral transport cross sections from quantum elastic differential cross sections, provide the theoretical framework for the construction of an accurate and complete database of collision integrals.

References

[1] G. Colonna, A. D'Angola and A. Laricchiuta, in the IoP book *Plasma Modeling: Methods and applications* Eds. G. Colonna and A. D'Angola (Second Edition) Chapter 21 (2022)
[2] M. Capitelli, D. Cappelletti, G. Colonna, C. Gorse, A. Laricchiuta, G. Liuti, S. Longo, F. Pirani, *Chem. Phys.* **338**, 62–68 (2007).
[3] A. Laricchiuta, G. Colonna, D. Bruno, R. Celiberto, C. Gorse, F. Pirani, M. Capitelli, *Chem. Phys. Letters* **445** 133–139 (2007)
[4] F. Pirani, S. Falcinelli, F. Vecchiocattivi, V. Aquilanti, A. Laricchiuta, G. Colonna, M. Capitelli, *Rendiconti Lincei. Scienze Fisiche e Naturali* **34**, 983–995 (2023)
[5] F. Pirani, M. Bartolomei, G. Colonna and A. Laricchiuta, *Entropy* **28**, 325 (2026).

Increasing complexity in quantum scattering studies of polyatomic interstellar molecules

S. Demes [a],* and F. Lique [b]

[a] HUN-REN Institute for Nuclear Research (ATOMKI), Debrecen, Hungary
[b] Univ Rennes, IPR (Institut de Physique de Rennes), Rennes, France
* demes.sandor@atomki.hu

Recently, more and more complex molecular species are found throughout interstellar clouds, and these star-forming regions are particularly important for understanding how the early Universe evolved. Recent high-sensitivity observations are offering new and detailed views of the chemical diversity and physical structure of interstellar matter. At the same time, these observations rely heavily on complementary experimental and theoretical molecular data, which mimic the extreme conditions in space. In such environments, molecular level are populated due to the competition between collisional and radiative processes, as local thermodynamic equilibrium conditions are generally not satisfied. While the radiative properties of the observed polyatomic species are well known, their collisional properties are often poorly characterized or entirely missing. Nevertheless, collisional rate coefficients are essential ingredients for reliable astrophysical modelling of these molecules. This, in turn, allows for a correct interpretation of observed molecular emission lines and the derivation of molecular abundances, shedding light on the physico-chemical conditions of the emitting regions.

In my talk, I will provide an overview of the standard methodologies and the most significant challenges in quantum scattering studies of interstellar polyatomic species. I will demonstrate this using our recent results obtained for molecules with increasing complexity, ranging from H_3O^+ and NH_3 to H_2Cl^+ and C_5H_6 [1]. I will also provide insights into our current project, which aims to develop a quasi-classical scattering model that is suitable for the collision of polyatomic species, with the resolution of the rotational and vibrational states of both colliders.

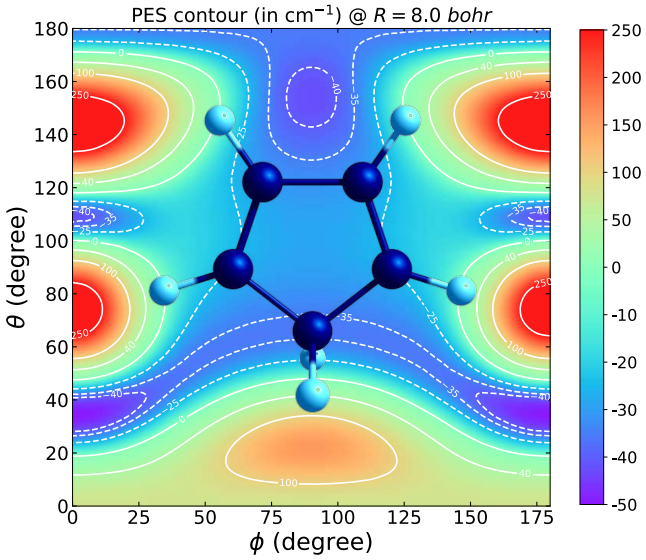


Figure 1: Contour plot of the C_5H_6 – He interaction potential at fixed intermolecular distance

References

[1] S. Demes, C. T. Bop, M. B. Khalifa, and F. Lique, *Phys. Chem. Chem. Phys.* **26**, 16829–16837 (2024).

THE REAL BOTTLENECK IN PREDICTIVE NONADIABATIC DYNAMICS

P. Slavíček [(a)] *

[(a)] *Department of Physical Chemistry, University of Checmistry and Technology,Prague, Czech Republic*
*petr.slavicek@vscht.cz

Nonadiabatic molecular dynamics is now considered to be a mature tool, yet its predictive power remains questionable. The recent blind challenge on cyclobutanone showed that technically sound simulations, based on different electronic structures and dynamics protocols, provides quite diverse photochemical pictures [1]. It turns out that the non-adiabatic techniques are generally forgiving [2] and improved sampling of initial conditions and photoexcitation can substantially refine the simulated ensemble [3].

The remaining and major bottleneck is the electronic-structure layer. The choice of electronic-structure method dominantly controls lifetimes, branching ratios, and even the qualitative mechanism more strongly than the choice of nonadiabatic algorithm [4]. Does this make dynamics developers passive users of better *ab initio* potentials? Because nonadiabatic trajectories are sensitive probes of potential-energy surfaces and electron-nuclear couplings, they can define what "good enough" means for photochemistry. I will discuss three complementary directions: systematic sensitivity analysis, where small chemically motivated perturbations expose fragile predictions [5]; diabatic formulations, which make chemical character explicit and provide smoother targets for machine learning [6]; and careful calibration of new electronic-structure ideas and diagnostics before they become black-box tools [7].

Predictive nonadiabatic dynamics will therefore require not a single best algorithm, but uncertainty-aware protocols, chemical representations and a closer dialogue between dynamics and electronic structure.

References

[1] J. Janoš et al., arXiv:2604.12749 (2026).
[2] T. Jíra, J. Janoš, P. Slavíček, J. Chem. Theory Comput. 21, 9784–9798 (2025).
[3] J. Janoš, P. Slavíček, B. F. E. Curchod, Acc. Chem. Res. 58, 261–270 (2025).
[4] J. Janoš, P. Slavíček, J. Chem. Theory Comput. 19, 8273–8284 (2023).
[5] T. Jíra, J. Janoš, P. Slavíček, J. Chem. Theory Comput. 20, 10972–10985 (2024).
[6] Š. Sršeň, O. A. von Lilienfeld, P. Slavíček, Phys. Chem. Chem. Phys. 26, 4306–4319 (2024).
[7] J. Janoš, A. J. Orr-Ewing, B. F. E. Curchod, P. Slavíček, arXiv:2604.09230 (2026).

SYMMETRY BREAKING IN REACTIVE SCATTERING PROCESSES: ELECTRON NUCLEAR COUPLING

Satrajit Adhikari[(a)*]

[(a)]*School of Chemical Sciences, Indian Association for the Cultivation of Science, Kolkata-700032, West Bengal, India*
*Email: pcsa@iacs.res.in

The *ab initio* calculated adiabatic potential energy surfaces (PESs) and nonadiabatic coupling terms (NACTs) are employed to construct highly accurate Beyond Born-Oppenheimer (BBO) [1-3] based diabatic Hamiltonians [4-7] for triatomic reactive scattering processes. Jahn-Teller (JT) and Renner-Teller (RT) types of conical intersections (CIs)/seam(s) along with Pseudo Jahn-Teller (PJT) interactions are investigated for specific scattering systems [4-7]. The role of nonadiabatic coupling is depicted in the reaction attributes of $D^+ + H_2$, $He + H_2^+$, $F + H_2$ and $H + H_2/D_2$ collisions through fully close coupled (FCC) quantum dynamical calualtions employing diabatic PESs of H_3^+, HeH_2^+, $F + H_2$ and H_3 species, respectively, which exhibit good accord with the experimentally measured ones. [7-10] The role of rotational symmetry breaking in ortho-to-para conversion in the $H^+ + H_2$ collision is investigated using accurate quantum dynamics on the ground adiabatic PES of H_3^+, which has been substantiated by the peak for the ortho–para ratio around 140 K.[11]

References

[1] B. Mukherjee, K. Naskar, S. Mukherjee, S. Ghosh, T. Sahoo and S. Adhikari, Int. Rev. Phys. Chem. **38**, 287 (2019).
[2] K. Naskar, S. Mukherjee, B. Mukherjee, S. Ravi, S. Mukherjee, S. Sardar and S. Adhikari, J. Chem. Theory Comput. **16**, 1666-1680 (2020).
[3] J. Dutta, S. Mukherjee, K. Naskar, S. Ghosh, B. Mukherjee, S. Ravi and S. Adhikari, Phys. Chem. Chem. Phys. (Perspective) **22**, 27496-27524 (2020).
[4] S. Mukherjee, D. Mukhopadhyay and S. Adhikari, J. Chem. Phys. **141,** 204306 (2014)
[5] B. Mukherjee, K. Naskar, S. Mukherjee, S. Ravi, K. R. Shamasundar, D. Mukhopadhyay and S. Adhikari, J. Chem. Phys. **153** (17) 174301 (2020).
[6] K. Naskar, S. Ravi, S. Adhikari, M. Baer and N. Sathyamurthy, J. Phys. Chem. A **127,** 3832 (2023)
[7] A Ghosh, A Roy, A Kumar, K Naskar, S Ravi and S Adhikari, J. Phys. Chem. A **129**, 6315−6332 (2025)
[8] S. Ghosh, S. Mukherjee, B. Mukherjee, S. Mandal, R. Sharma, P. Chaudhury and S. Adhikari, J. Chem. Phys. **147,** 074105 (2017).
[9] K. Naskar, S. Mukherjee, S. Ghosh and S. Adhikari, J. Phys. Chem. A **128**, 1438 (2024).
[10] K. Naskar, S. Ghosh, S. Adhikari, M. Baer and N. Sathyamurthy, J. Chem. Phys. **159**, 034302 (2023).
[11] S. Hazra, K. Naskar, S. Ravi, S. Adhikari and A. J. C. Varandas, J. Phys. Chem. A **128**, 41, 8833-8844 (2024).
[12] S. Mukherjee, S. Saha, S. Ghosh, S. Adhikari, N. Sathyamurthy and M. Baer, J. Phys. Chem. A **128**, 36, 7691−7702 (2025).

TUNNELING DYNAMICS USING INSTANTON THEORY: ROVIBRATIONAL SPECTRA AND DECAY RATES IN MOLECULES

M. T. Cvitaš [(a), *], N. Tokić [(a)]

[(a)] *University of Zagreb Faculty of Science, Zagreb, Croatia..*
[*]mcvitas.phy@pmf.hr

In molecules with multiple equivalent symmetry-related minima, separated by potential barriers, splittings of rotational and vibrational energy levels arise from molecular rearrangements that occur at zero temperature via tunneling. Another manifestation of tunneling at zero temperature is the decay of a metastable state that is temporarily trapped behind a potential barrier. We show that a multidimensional instanton theory [1-4] can provide semiclassical estimates of tunneling splittings and decay rates in such systems, including molecules whose size makes them intractable for accurate variational methods. The method is formulated in Cartesian coordinates and requires only a modest number of electronic-structure potential and gradient evaluations, typically on the order of ~1000. It is therefore broadly applicable to medium-sized molecules and can be combined with accurate electronic-structure methods.

We apply the method to calculate tunneling splittings of the ground and vibrationally excited states in formic acid dimer. We also use it to identify possible rearrangement pathways responsible for the formation of the ground-state tunneling splitting pattern in the water hexamer book isomer [5]. We present a new approach to calculating tunneling splittings in rotationally excited states and apply it to water dimer. A stable and efficient method for calculating decay rates of metastable molecules is also developed. We discuss the relation of the present Jacobi-field-based approach to ring-polymer instanton method, the WKB method and Heller's imaginary-time wavepackets, and outline possible future directions.

Acknowledgements: This work was supported by Croatian Science Foundation Grant IP-2020-02-9932 and IP- 2022-4648 and QuantiXLie Centre of Excellence Grant PK.1.1.02.

References

[1] M. Eraković, C.L. Vaillant, M.T. Cvitaš, J. Chem. Phys. **152**, 084111 (2020).
[2] M. Eraković, M.T. Cvitaš, J. Chem. Phys. **153**, 134106 (2020).
[3] M. Eraković, M.T. Cvitaš, J. Chem. Phys. **160**, 154112 (2024).
[4] M. Eraković, M.T. Cvitaš, J. Chem. Theory Comput. **18**, 2785-2802 (2022).
[5] N. Tokić, M. Eraković, M.T. Cvitaš, Phys. Chem. Chem. Phys. **27**, 6938-6957 (2025).

EXPLORATION OF THE FACTORS DETERMINING THE SHAPES OF POTENTIAL ENERGY SURFACES USING MAYER'S CHEMICAL ENERGY COMPONENT ANALYSIS

G. Lendvay

Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Budapest, Hungary
lendvay.gyorgy@ttk.hu

Energy partitioning is a way to decompose the energy calculated using numerical quantum chemistry into components corresponding to atoms and atom pairs, providing chemically interpretable information. We applied two schemes developed by István Mayer, the Chemical Energy Component Analysis, CECA, and the scheme named E2 to reveal how the interactions between atoms change during chemical reactions, expressed in terms of energy components. The test reactions are hydrogen-atom abstractions from simple prototype molecules by a methyl radical, CH_3 + H'R → CH_3H' + R, with R=H, CH_3, $C(CH_3)_3$ and OH. The CECA diatomic energy component associated with the forming bond is zero in the reactant limit and gradually becomes attractive when one moves along the minimum energy path (MEP) toward the product limit; that of the breaking bond simultaneously changes from attractive to zero. Their sum displays a maximum which appears to be a contributor to the potential barrier (Fig. 1). The dominant term in the increase/decrease of the diatomic energy components is associated with exchange, which characterizes the strength of covalent interactions. Its change indicates that the build-up of one covalent interaction does not completely cover the energy needed to break the other. Another major contributor to the formation of the potential barrier is the repulsion involving overlap densities of the atoms from/to which the H-atom is transferred. Overlap repulsion is also responsible for the steric repulsion involving the spectator atoms. Energy component analysis performed on wave functions calculated with different basis sets yields the same semiquantitative information. The diatomic energy components derived with the E2 scheme are close in magnitude to bond dissociation energies and change smoothly with molecular geometry, but they cannot be decomposed to contributions like overlap and exchange.

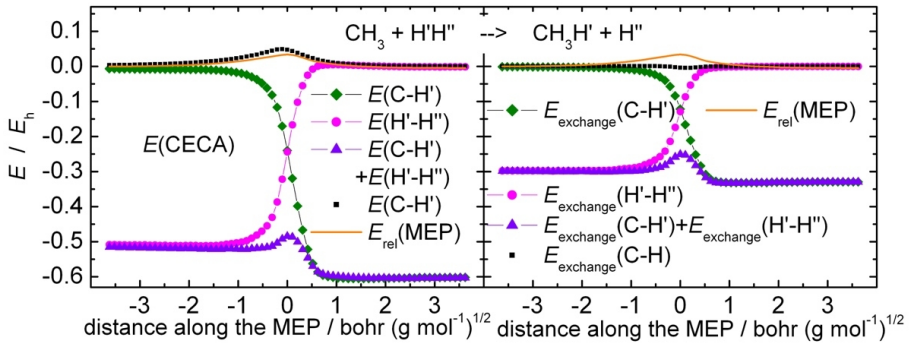


Figure 1: CECA diatomic energy components along the MEP of the CH_3 + H'H" → CH_3H' + H" reaction from the HF/6-31G** wave function

References

[1] György Lendvay, Phys. Chem. Chem. Phys. **28**, 11690–11702 (2026).
[2] István Mayer, J. Comput. Chem. **28**, 204–221 (2007).

Molecules coupled to phonons and photons

Peter Saalfrank [a],*, Eric Fischer [b], Foudhil Bouakline [a]

[a] University of Potsdam, Chemistry Department, Karl-Liebknecht-Strasse 14-15, D-14476 Potsdam, Germany

[b] Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Straße 2, D-12489 Berlin, Germany

* peter.saalfrank@uni-potsdam.de

Molecules in contact with surface phonons and with photons share some common features, and can be treated with similar theoretical models and methods to solve the underlying time-dependent, (possibly multi-dimensional) Schrödinger equation. In this talk we will first present recent work of our group to treat the vibrational relaxation of adsorbates near surfaces due to vibration-phonon coupling, emphasizing the following aspects: (i) The "reduction" of multi-oscillator bath models by a hierarchical effective mode (HEM) approach [1,2], and (ii) the quantification of non-Markovian effects in multi-dimensional system-bath problems [1,2]. In a second part, the strong coupling of photons in a cavity to molecular vibrations will be considered, with special attention given to: (i) The formation of vibro-polaritons and their signatures in vibrational spectra [3], and (ii) the influence of vibrational strong coupling (VSC) on rates and yields of chemical reactions [4-7].

References

1 Eric W. Fischer, Michael Werther, Foudhil Bouakline, Peter Saalfrank, A hierarchical effective mode approach to phonon-driven multilevel vibrational relaxation dynamics at surfaces. J. Chem. Phys. **153**, 064704 (2020).

2 Eric W. Fischer, Michael Werther, Foudhil Bouakline, Frank Grossmann, Peter Saalfrank, Non- Markovian vibrational relaxation dynamics at surfaces. J. Chem. Phys. **156**, 214702 (2022).

3 Eric W. Fischer, Jan A. Syska, P. Saalfrank, A Quantum Chemistry Approach to Linear Vibro-Polaritonic IR Spectra with Perturbative Electron-Photon Correlation, J. Phys. Chem. Lett. **15**, 2262 (2024).

4 Eric W. Fischer, Janet Anders, Peter Saalfrank, Cavity-altered thermal isomerization rates and dynamical resonant localization in vibro-polaritonic chemistry. J. Chem. Phys. **156**, 154305 (2022).

5 Eric W. Fischer, Peter Saalfrank, Cavity-catalyzed Hydrogen Transfer Dynamics in an Entangled Molecular Ensemble under Vibrational Strong Coupling. Phys. Chem. Chem. Phys. **25**, 11771 (2023)

6 A.R. Ramos Ramos, E.W. Fischer, P. Saalfrank, and O. Kühn, Shaping the Laser Control Landscape of a Hydrogen Transfer Reaction by Vibrational Strong Coupling. A Direct Optimal Control Approach, J. Chem. Phys. **160**, 074101 (2024).

7 R. Gundermann, P. Saalfrank, Rates for cavity-altered H-transfer reactions in dissipative environments, to be published (2026).

QUANTUM-REACTIVE-SCATTERING PERSPECTIVES FROM DEA CLUB 2026: RESONANCES, ATTACHMENT AND FRAGMENTATION DYNAMICS

M. Śmiałek-Telega [(a),*]

(a) Institute of Shipbuilding, Faculty of Mechanical Engineering and Ship Technology, Gdańsk University of Technology, Poland.

*smialek@pg.edu.pl

Dissociative electron attachment (DEA) offers a molecularly specific route to quantum reactive scattering: a low-energy electron is captured into a transient negative-ion state and the ensuing competition between autodetachment, vibrational energy redistribution and bond cleavage determines the observed product channels. This contribution summarizes the scientific perspective emerging from the DEA Club Meeting 2026, held in Sopot, Poland, which brought together experimental and theoretical work on low-energy electron interactions, resonant scattering, total and differential cross sections, cluster and surface processes, radiation chemistry, astrochemical media, biomolecular damage and applications in focused electron-beam technologies [1].

Across the programme, a common theme was the need to connect resonance parameters with reaction observables. Velocity-map imaging, electron energy-loss spectroscopy, crossed-beam mass spectrometry, total cross-section measurements and ab initio resonance calculations were discussed as complementary probes of attachment and fragmentation dynamics. The contributions showed that DEA is not only a fragmentation mechanism, but also a sensitive test of nonadiabatic nuclear dynamics on temporary anion potential-energy surfaces. Particularly strong links to quantum reactive scattering arise in the treatment of vibronic coupling, virtual and dipole-supported states, microhydration effects, competing decay channels and threshold behaviour.

The synthesis highlights three directions relevant to the QRS community: benchmark-quality data for electron-driven reactions, quantum-dynamical models that include resonance formation and decay on equal footing, and closer integration between gas-phase, cluster and condensed-phase measurements. DEA therefore provides a compact but demanding platform for testing reactive-scattering theory in systems where electronic metastability, nuclear motion and chemical rearrangement are inseparable.

References

[1] DEA Club Meeting 2026, *Book of Abstracts*, Sopot, Poland, 13-15 April 2026.

MODELING THE STATE OF A FREE ELECTRON IN CHEMICAL REACTIONS

W. Skomorowski [(a),*], S. Roy [(a)], D. Mahato [(a)]

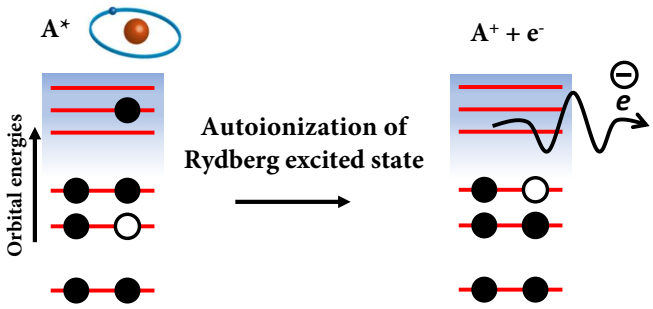
[(a)] Centre for New Technologies, University of Warsaw, Poland

[*] w.skomorowski@cent.uw.edu.pl

Many chemical and physical processes involve formation or interaction with unbound electrons. These include phenomena such as photoionization, electron-impact scattering, or Auger decay of core-ionized states. Accurate theoretical description of such processes requires a proper treatment of continuum electrons interacting with atomic or molecular targets. This remains highly challenging for conventional quantum-chemistry methods, which are primarily designed for bound states and rely on basis sets and boundary conditions inappropriate for continuum problems.

Here we present an approach in which continuum electron is represented in a discrete basis of standard Gaussian-type orbitals (GTOs). The scattering orbital is obtained by solving the Lippmann–Schwinger equation with proper outgoing-wave boundary conditions using an analytic representation of the Green's function in the GTO basis[1]. This formulation enables an accurate and systematically improvable description of continuum electronic states within a framework fully compatible with conventional quantum-chemical methods.

The method is benchmarked against new experimental data for the energies and lifetimes of selected autoionizing Rydberg states in Ne and CO_2, showing excellent agreement. As a main application, we present *ab initio* calculations of complex-valued potential-energy surfaces for Penning ionization reactions in simple systems such as metastable He* atom colliding with Ar atom or H_2 molecule. We show that the GTO-based continuum representation naturally captures different ionization mechanisms, either via electron transfer or energy transfer, which are particularly evident in the long-range behavior of the Penning ionization rates.



References

[1] D. Mahato and W. Skomorowski, arXiv:2605.18564.

FUNCTIONAL ANALOGUES OF SEPARABLE TENSOR DECOMPOSITION ANSÄTZE AND APPLICATIONS

D. Peláez

Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405, Orsay, France.
daniel.pelaez-ruiz@universite-paris-saclay.fr

Tensors are multidimensional collections of ordered data that naturally emerge when physical properties are mapped onto a grid representing a discretization of a physical or configuration space. In the context of molecular science, tensors and their associated algebra are utilized to represent and operate grid-based objects such as wave functions or potential energy surfaces (PES). Tensor representations face significant challenges, the volume of data grows exponentially with dimensionality while the relevant information simultaneously becomes sparser. These drawbacks have motivated the sustained development of grid-based tensor decomposition methods, which have recently gained momentum through integration with Deep Learning techniques. Some of those methods lead to data compression and separability of the contribution of the different degrees of freedom, a feature of utmost relevance in frameworks like MCTDH quantum dynamics. Despite these advantages, tensor-decomposed ansätze are typically bound to a fixed grid definition and cannot be readily interpolated. This limitation becomes problematic when a simulation grid must be redefined in terms of shape or density, a common requirement when benchmarking new systems, modifying physical conditions (such as the total simulation energy), or when generating new tensor values is computationally expensive.

In this contribution, we present an overview of our semi-automated approaches for generating analytical and separable tensor-decomposed ansätze, including Tucker, Canonical Polyadic, and Tree-Tensor Network expressions. By virtue of their functional nature, these approaches circumvent the aforementioned grid-dependency issues while maintaining both compactness and separability. In addition to this, they can be expressed symbolically as MCTDH operators. We illustrate these methods within the context of full quantum simulations for bound molecular systems, as well as for unbound systems ranging from non-adiabatic dynamics [1] to pre-Born-Oppenheimer molecular dynamics [2].

References

[1] Z. Qiu, F. Magoulès, D. Peláez, J. Chem. Theo. Comp. (*accepted*) (2026).

[2] S. K. Das, A. Bande, D. Peláez, J. Chem. Theo. Comp. (*accepted*) (2026).

INTERMOLECULAR INTERACTION ENERGIES: STRIVING FOR MAXIMUM ACCURACY AND INSIGHT

Konrad Patkowski [a],*

[a] Department of Chemistry and Biochemistry, Auburn University, United States

* patkowsk@auburn.edu

Accurate calculations of potential energy surfaces have been indispensable for interpreting experimental data and guiding future measurements. However, spectroscopic (1 cm^{-1}) accuracy is quite hard to attain in interaction energy calculations. First, it requires a precise leading-order electron correlation contribution, preferably from the "gold-standard" coupled-cluster singles, doubles, and perturbative triples [CCSD(T)] complete basis set (CBS) limit. Even more importantly, one also needs a reliable account of subtle corrections beyond the CCSD(T) level, such as the correlation of core electrons, coupled-cluster excitations beyond CCSD(T), relativistic effects, and the post-Born-Oppenheimer corrections. For the former term, significant benchmarking efforts have led to the recommendations for computing the most precise and cost-effective CCSD(T)/CBS limit values, often including specialized approaches such as explicit correlation (F12) and basis functions on the intermolecular bond [1,2]. For the higher-order coupled-cluster corrections, CCSDT(Q) calculations in basis sets of at least aug-cc-pVDZ quality are needed to obtain a reliable estimate. However, some complexes, notably those with triple bonds such as CO–CO and N_2–N_2, exhibit a particularly slow convergence of high-order coupled-cluster excitations [3,4].

Notably, supermolecular calculations such as CCSD(T) produce just one number per a geometry of the complex. This total interaction energy value says little about the underlying physics of the interaction, and an *energy decomposition* is needed to understand noncovalent forces in meaningful quantitative terms. Symmetry-adapted perturbation theory (SAPT) [5] is one of the most successful approaches to provide insights through interaction energy decomposition. After providing a brief overview of SAPT for interaction energies, I will showcase its very recent extension to interaction-induced properties such as dipole moments and densities [6].

References

[1] Lori A. Burns, Michael S. Marshall, and C. David Sherrill, *J. Chem. Phys.* **141**, 234111 (2014).

[2] Narendra Nath Dutta and Konrad Patkowski, *J. Chem. Theory Comput.* **14**, 3053-3070 (2018).

[3] Monika Kodrycka and Konrad Patkowski, *J. Chem. Phys.* **151**, 070901 (2019).

[4] Roland Tóbiás, Csaba Fábri, Marlene Bosquez, Monika Kodrycka, Konrad Patkowski, and Attila G. Császár, *Communications Chemistry* **8**, 339 (2025).

[5] Konrad Patkowski, *WIREs Comput. Mol. Sci.* **10**, e1452 (2020).

[6] Bartosz Tyrcha, Tarun Gupta, Konrad Patkowski, and Piotr S. Żuchowski, *J. Chem. Theory Comput.* **21**, 4562-4578 (2025).

Collisional excitation by heavy projectiles to model cometary and planetary atmospheres

F. Tonolo [a]

[a] Institut de Physique de Rennes (IPR) – Université de Rennes– France

The advent of the new generation of telescopes has shed light on scarcely explored astrophysical environments, such as cometary, planetary atmospheres, and exoplanets. Here, the strong deviations from thermodynamic equilibrium highlight the need for accurate datasets of collisional rate and pressure-induced coefficients to guide astrophysical modeling[1]. In many of these environments, the dominant collisional partners are heavy species such as CO, CO_2, H_2O, and N_2. Their high density of ro-vibrational states poses a major methodological challenge, as it dramatically increases the computational cost and makes full quantum mechanical approaches impractical in most cases. Since these molecular datasets are extremely difficult to obtain experimentally, a current frontier in molecular astrophysics is the development and validation of new theoretical methodologies capable of providing the best compromise between accuracy and computational efficiency. Among these, the Statistical Adiabatic Channel Model (SACM) is particularly noteworthy[2,3]. While remaining affordable from a computational point of view, the SACM has demonstrated excellent performance at low temperatures, successfully capturing prominent quantum effects[4]. At higher temperatures, the Open Channel Method has also shown promising results in predicting pressure-induced coefficients[5]. In this work, the main advances achieved along this direction will be presented, with particular emphasis on novel strategies to generate accurate collisional datasets for the modeling of cometary and planetary atmospheres.

References

[1] F. Tonolo *Front. Astron. Space Sci.* **12**, 1713849 (2025). [2] M. Quack and J. Troe *Ber. Bunsenges. Phys. Chem.* **79**, 170–183 (1975). [3] J. Loreau, F. Lique, and A. Faure *Astrophys. J. Lett.* **853**, L5 (2018). [4] F. Tonolo, E. Quintas-Sánchez, A. Batista-Planas, R. Dawes, and François Lique *J. Chem. Phys. Comm.*, **164**, 201101 (2026). [5] F. Tonolo, H. J. Jóźwiak, L. Bizzocchi, M. Melosso, P. Wcisło, F. Lique and C. Puzzarini *J. Quant. Spectrosc. Radiat. Transfer* **345**, 109521 (2025).

SEMICLASSICAL S-MATRIX IN THE INITIAL VALUE REPRESENTATION: COORDINATE CHOICE

L. Bonnet

Univ. Bordeaux, CNRS, Bordeaux INP, ISM, UMR 5255, F-33400 Talence, France.
Claude-laurent.bonnet@u-bordeaux.fr

We show that the values of semiclassical S-matrix elements computed within the initial value representation depend on the choice of coordinates, with some coordinate systems yielding more accurate results than others [1]. For clarity, we focus primarily on a simple model of light-induced rotational transitions for which the dynamics can be described analytically. As a byproduct of this analysis, we also propose a straightforward method for improving the preparation of vibrational states of polyatomic molecules in quasi-classical trajectory (QCT) calculations [2].

References

[1] L. Bonnet, J. Chem. Phys. 153 (2020) 174102; 155 (2021) 059901; 155 (2021) 174103; 158 (2023) 114112; Chem. Phys. Lett. 851 (2024) 141459.
[2] M. Braunstein and L. Bonnet, Phys. Chem. Chem. Phys. 2024, 26, 26084.

ON THE SCATTERING OF ELECTRONS BY MOLECULES OF ASTROCHEMICAL AND TECHNOLOGICAL SIGNIFICANCE

P. Możejko [(a), *]

[(a)] *Faculty of Applied Physics and Mathematics, Gdansk University of Technology, Poland.*
[*]paw@pg.edu.pl

A thorough understanding of the interaction of electrons, including those with low and medium energies, with molecules is essential for explaining and understanding many significant processes in astrochemistry and modern technologies such as focused electron beam-induced deposition (FEBID). The quantity, that can be most accurately determined experimentally, describing electron molecule collisions is the total cross section (TCS). TCS provides comprehensive information on the scattering efficiency across all open channels at a given scattering energy. Due to its summary nature, however, the total cross section is only a measure of the probability that electron–target molecule interaction of any type occurs, with no information on the contribution of specific scattering events. Nevertheless, the total cross section can be used to normalize results obtained on a relative scale and to verify scattering theories.

The current state of research on the measurement of total electron scattering cross sections for electron scattering on simple molecules of astrochemical and technological significance will be discussed. In particular, in this context, recent results obtained for the scattering of low-energy electrons on tetramethylsilane [2], tetramethylgermane [2], methyl formate [3], and acetic acid [4] molecules will be presented and discussed.

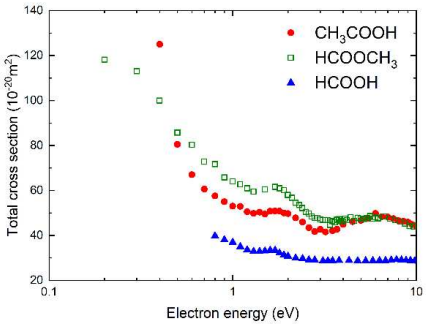


Figure 1: Comparison of TCS for electron scattering on formic acid, methyl formate and acetic acid molecules [4].

References

[1] Czesław Szmytkowski and Paweł Możejko, Eur. Phys. J. D **74**, 90 (2020).
[2] Sylwia Stefanowska-Tur, Paweł Możejko, Elżbieta Ptasińska-Denga and Czesław Szmytkowski, J. Chem. Phys. **150**, 094303 (2019).
[3] Natalia Tańska, Edvaldo Bandeira, Alessandra S. Barbosa, Kuba Wójcik, Sylwia Dylnicka, Elżbieta Ptasińska-Denga, Czesław Szmytkowski, Marcio H.F. Bettega and Paweł Możejko, J. Phys. Chem. A **127**, 7594-7604 (2023).
[4] Natalia Tańska, Kuba Wójcik, Thiago C. Freitas, Marcio H.F. Bettega, Czesław Szmytkowski and Paweł Możejko, J. Phys. Chem. A **129**, 270-281 (2025).

QUASI-EQUILIBRIUM O + O_2 IGNITION OF OZONE FORMATION FROM O_3^* LIFETIME SPECTRUM: THE CASE OF ^{18}O and ^{17}O ISOTOPES

G. Guillon [(a),*] and P. Honvault [(a)]

[(a)] Lab. ICB, Université Bourgogne Europe, France

[*] gregoire.guillon@ube.fr

The origin of the anomalous isotopic enrichment of ozone [1], first observed in the stratosphere [2], is now accepted to come from the associative recombination reaction [3]: $O + O_2 + M \longrightarrow O_3 + M$, M being a stabilizer. In this talk, I will present, from a theoretical perspective, the first of the two steps involved in the Lindemann mechanism approach of this global reaction of ozone formation: the fast quasi-equilibrium process $O + O_2 \rightleftharpoons O_3^*$, where O_3^* is metastable (ro-vibrationally excited) ozone. I will discuss the behavior of the quasi-equilibrium constant [4,5,6] with temperature, obtained from a full quantum dynamical approach based on the lifetime [7] spectrum of O_3^* [8]. I will describe in particular the effect of isotopes ^{17}O [9] and ^{18}O [10], with the hope that these results might help understand this isotope anomaly from a theoretical viewpoint.

References

[1] M. H. Thiemens and J. E. Heidenreich III *Science* **219** 1073–1075 (1983). [2] K. Mauersberger *Geophys. Res. Lett.* **8** 935–937 (1981). [3] C. Janssen, J. Guenther, K. Mauersberger and D. Krankowsky *Phys. Chem. Chem. Phys.* **3** 4718–4721 (2001). [4] Y. Q. Gao and R. A. Marcus *Science* **293** 259–263 (2001). [5] J. M. Bowman *J. Chem. Phys.* **90** 3492–3495 (1986). [6] D. Charlo and D. C. Clary *J. Chem. Phys.* **117** 1660–1772 (2002). [7] F. T. Smith *Phys. Rev.* **118** 349–356 (1960). [8] E. Privat, G. Guillon and P. Honvault *J. Chem. Phys.* **154** 104303-1–9 (2021). [9] G. Guillon and P. Honvault *J. Chem. Phys.* **162** 144307-1–8 (2025). [10] G. Guillon and P. Honvault *Phys. Rev. Research* **6** 043181 (2024).

A FRESH LOOK AT SIGNATURES OF S-WAVE SCATTERING: SYMMETRY AND THE BREAKDOWN OF THE BORN–OPPENHEIMER APPROXIMATION

A. Krylov [(a)]

[(a)] *Department of Chemistry, University of Southern California, Los Angeles, CA 90089, USA*
[*] krylov@usc.edu

The peculiar behavior of sigma-type anionic states is analyzed in terms of the interaction between bound and continuum states. Within a simple Landau–Zener model, strong diabatic coupling leads to a broad avoided crossing and strongly mixed adiabatic states, whereas weak diabatic coupling leads to a narrow avoided crossing and an abrupt change in the character of the adiabatic states. By using symmetry analysis and numeric calculations, I will show that sigma-type anionic states such as those in HCl, methyl chloride, and pyrrole interact much stronger with the continuum than pi-type anionic states such as the N_2 resonance. Strong interaction leads to the breakdown of the Born–Oppenheimer approximation, which results in a finite probability to decay into the detachment continuum even in the regions where the anionic state is energetically below the neutral state. We show that calculations with a complex absorbing potential capture this special character of sigma-type anions through removal of the detachment continuum, affording diabatization of the anionic state, while describing the decay into the continuum via imaginary energy Gamma.

Rethinking Surface Hopping: From Nonadiabatic Couplings to Time-Derivative Couplings

Saikat Mukherjee

Faculty of Chemistry, Nicolaus Copernicus University in Torun, Poland

saikat.mukherjee@umk.pl

Nonadiabaticity, which arises from the coupling between electronic and nuclear motion, plays a central role in a wide range of photophysical and photochemical processes. Modeling such dynamics is challenging because it requires describing transitions among multiple electronic states, often in regions of conical intersections or avoided crossings where the Born–Oppenheimer approximation breaks down. Among the various theoretical approaches for simulating nonadiabatic dynamics, ranging from full quantum dynamics to mixed quantum-classical and semiclassical methods, Tully's fewest-switches surface-hopping (FSSH) method has emerged as one of the most widely used and influential approaches. When combined with on-the-fly electronic-structure calculations, surface hopping provides a practical framework for exploring nonadiabatic processes at the full atomic level. However, the computational cost of such trajectory-based simulations can become prohibitive, since electronic energies, gradients, and coupling information must be evaluated repeatedly at each nuclear time step.

FSSH requires electronic energies, gradients, and nonadiabatic couplings between electronic states as inputs from quantum-chemical calculations. Explicit evaluation of nonadiabatic coupling vectors not only introduces additional computational expense but may also be unavailable, numerically unstable, or divergent near critical regions of the potential energy landscape. Recently, several strategies have been developed to approximate time-derivative couplings for use in the FSSH algorithm. In this talk, I will discuss selected strategies [1-3] for approximating time-derivative couplings and the associated hopping criteria. By reducing the need for explicit nonadiabatic coupling calculations, these approaches offer a promising route to extending nonadiabatic dynamics simulations to longer timescales while taming the formidable computational cost.

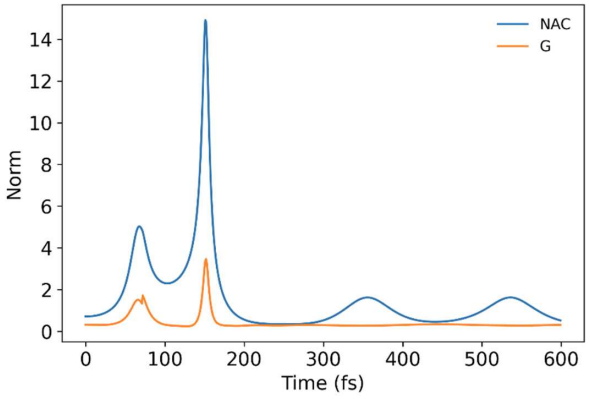


Figure 1: Comparison between the norm of the exact NAC vector and the effective NAC (norm G) obtained for a FSSH trajectory of the fulvene molecule.

References

[1] Y. Shu, L. Zhang, X. Chen, S. Sun, Y. Huang, D. G. Truhlar, *J. Chem. Theory Comput.* **18**, 1320-1328 (2022).

[2] J. M. Toldo, R. S. Mattos, M. Pinheiro Jr, S. Mukherjee, M. Barbatti, *J. Chem. Theory Comput.* **20**, 614-624 (2024).

[3] T. Jira, J. Janos, P. Slavicek, *J. Chem. Theory Comput.* **21**, 9784-9798 (2025).

H_2O AND D_2O TRIMERS: RIGOROUS 12D QUANTUM CALCULATIONS OF THE INTERMOLECULAR VIBRATIONAL STATES , TUNNELING SPLITTINGS, AND LOW-FREQUENCY SPECTRA

Z. Bačić [(a),*], I. Simkó [(a)], P. M. Felker [(b)]

[(a)] Department of Chemistry, New York University, New York, New York 10003, USA
[(b)] Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095-1569, USA
* qrs2026@pg.edu.pl

Water trimer is of fundamental importance as the smallest water cluster in which the nonadditive three-body interactions arise. They play a key role in shaping the structural, dynamical, and spectroscopic properties of liquid and solid phases of water and aqueous solutions. I will present our newly developed methodology which has allowed for the first time rigorous rigid-monomer quantum calculations of the 9D bending [1] and the 12D intermolecular vibrational states and tunneling splittings of $(H_2O)_3$ [2] and $(D_2O)_3$ [3], with the monomers treated as rigid. The absorption spectra of the low-frequency vibrations of $(H_2O)_3$ simulated using these 9D [1] and 12D eigenstates [2] agree remarkably well with the FIR spectrum of the trimer in helium nanodroplets measured by Havenith, Bowman, and co-workers [4], over the entire frequency range of the measurements from 70 to 620 cm^{-1}, as evident from Fig. 1. Moreover, for both $(H_2O)_3$ [1,2] and $(D_2O)_3$ [3], the calculated 9D and 12D ground-state torsional tunneling splittings are in excellent agreement with the spectroscopic data. The calculations also show that the nonadditive three-body interactions strongly affect both the intermolecular vibrational energies and the FIR spectrum of the trimer [3].

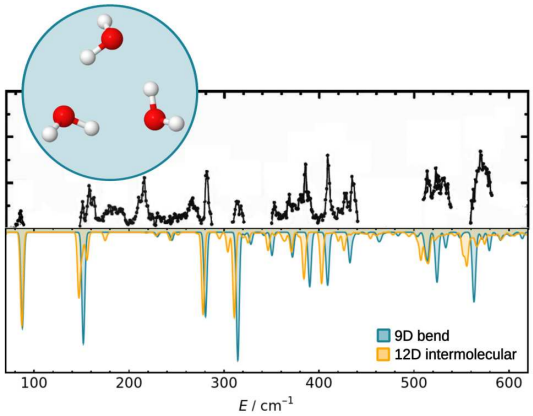


Figure 1: Top: measured FIR spectrum of $(H_2O)_3$ [4]. Bottom: Spectra calculated using the intermolecular eigenstates from the quantum 9D bend [1] and 12D rigid-monomer [2] calculations for $(H_2O)_3$.

References

[1] Peter M. Felker, Irén Simkó, and Zlatko Bačić, *J. Phys. Chem A* **128**, 8170 (2024)
[2] Irén Simkó, Peter M. Felker, and Zlatko Bačić, *J. Chem. Phys.* **162**, 034301 (2025).
[3] Irén Simkó, Peter M. Felker, and Zlatko Bačić, *J. Chem. Phys.* **163**, 184304 (2025).
[4] Raffael Schwan, Chen Qu, Devendra Mani, Nitish Pal, Gerhard Schwaab, Joel M. Bowman, Gregory S. Tschumper, and Martina Havenith, *Angew. Chem. Int. Ed.* **59**, 11399 (2020).

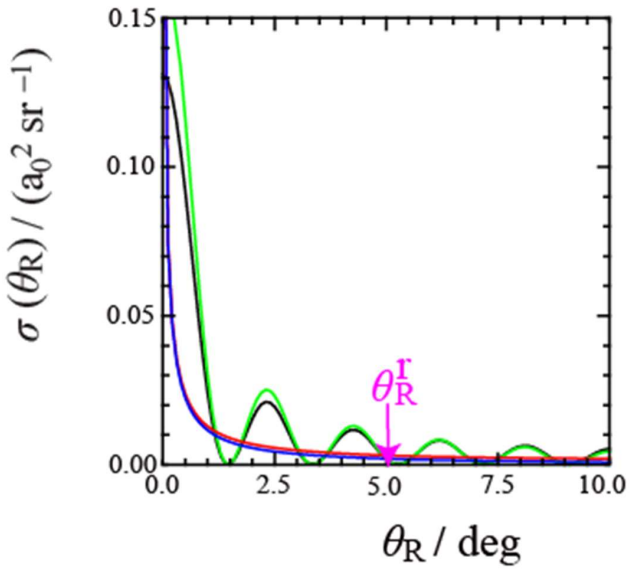
TECHNIQUES FOR ANALYZING STRUCTURED ANGULAR SCATTERING IN THE PRODUCTS OF CHEMICAL REACTIONS

J. N. L. Connor [(a)] and Chengkui Xiahou [(b)]

(a) Department of Chemistry, University of Manchester, Manchester M13 9PL, UK.
(b) School of Pharmacy, Qilu Medical University, Zibo City, 255300, Shandong, PRC.

The differential cross section (DCS) for a state-to-state reactive collision contains important information on the dynamics and mechanism of the reaction. The DCSs can exhibit intricate interference patterns and understanding and analyzing these patterns is an important and difficult problem. The following techniques will be discussed with chemical examples:

- Nearside-Farside (NF) decomposition (including resummations) of the partial wave series (PWS) representation of the scattering amplitude.
- Local Angular Momentum (LAM) analysis, including resummations.
- CoroGlo test to distinguish glory from corona scattering.
- Complex Angular Momentum (CAM) theory, including the extraction of Regge poles.
- Backward scattering: The semiclassical (SC) optical model of Herschbach (1965).
- Forward glory scattering: Six SC theories are available.
- Rainbow scattering at sideward angles, both nearside and farside.
- Forward glory scattering in the shadow of a nearside rainbow (NEW RESULT). The following diagram compares PWS (black), Nearside (red), Farside (blue) and a Laplace asymptotic approximation (green).



Recent Reference: C. Xiahou, J.N.L. Connor, D. De Fazio, D. Sokolovski, *Phys. Chem. Chem. Phys.,*2024, **26**, 3647-3666.

MCTDH-LIKE DIFFERENTIAL EQUATIONS FOR DETERMINING SUM-OF-PRODUCT (SOP) WAVEFUNCTIONS

R.Wodraszka [(a)], T.Carrington [(a)]

[(a)] *Queen's University, Kingston, Canada*

To solve the Schrödinger equation to study the motion of nuclei in a molecule or a reacting system, it is common to use a direct product basis. A direct product basis includes all products of functions in 1-D bases. The popular Multiconfiguration time-dependent Hartree (MCTDH) method uses a direct-product basis and optimized 1-D basis sets. An optimized direct product representation is called a Tucker format representation by mathematicians. Direct product structure facilitates the evaluation of matrix-vector products, but the size of a direct product basis scales as n^D, where n is a representative number of basis functions for a single coordinate and D is the number of dimensions (coordinates). Well established tricks such as mode combination, multi-layer trees, and pruning reduce the cost of MCTDH calculations. In this talk, I present a new idea to reduce the cost. It is called CPTDH. In CPTDH, wavefunctions are not represented in a direct product basis but as sums of products (SOP) of 1-D functions. In contrast to a direct product representation, each 1-D function appears in only one term in the SOP. Mathematicians call this CP format. We use MCTDH-like ideas to derive differentaial equations for optimized 1-D functions. We propose new ideas for dealing with problems posed by the need to choose a "guage" and encounter numerical problems when implementing them. We test the ideas by computing the vibrational spectrum of CH_2NH.

CONTRIBUTED TALKS

XVIII QUANTUM REACTIVE SCATTERING WORKSHOP

TWO SIDES OF WIGNER'S COIN: FROM R-MATRIX TO TRANSITION STATE THEORY

P. Szabó [a,b] *

[a] *Department of Chemistry, KU Leuven, Belgium,*
[b] *Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Brussels, Belgium*
*peter88szabo@gmail.com

Wigner introduced two central ideas in reaction dynamics: the R-matrix formulation of quantum scattering [1] and the dividing-surface picture of transition-state theory (TST) [2]. Despite their common origin, these frameworks are usually treated as conceptually distinct, representing exact dynamical and statistical descriptions, respectively. In this work, we show that they can be connected directly within a unified boundary perspective.

We demonstrate that the R-matrix formulation naturally gives rise to a net-flux description of reactivity at the dividing surface, from which a systematic pathway toward TST emerges. In parallel, we introduce a boundary spectral viewpoint in which the dividing surface supports its own reduced quantum dynamics, providing a complementary route from exact scattering theory to statistical rate descriptions. These two formulations reveal that the dividing surface is not an external construct, but an intrinsic element of the exact quantum description.

Together, these results establish two exact boundary routes linking quantum reactive scattering and transition-state theory, thereby reconnecting Wigner's R-matrix and dividing-surface concepts within a common framework. This perspective provides a unified way to understand how statistical rate theories emerge from underlying quantum dynamics.

References

[1] Wigner, E. P., & Eisenbud, L. (1947). Higher angular momenta and long range interaction in resonance reactions. Physical Review, 72, 29–41.
[2] Wigner, E. (1938). The transition state method. Transactions of the Faraday Society, 34, 29–41

COLLISIONAL STUDIES OF CH_3CHO-HE SYSTEM

M. Żółtowski [(a),*], D. Kędziera [(a)],

[(a)] *Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Poland.*
[*]mzoltowski@umk.pl

Acetaldehyde CH_3CHO is one of the most commonly detected complex organic molecules in the interstellar medium and is of considerable astrochemical interest because of its role in chemical networks related to prebiotic chemistry [1,2]. A reliable interpretation of its observed spectra requires non-local thermodynamic equilibrium modelling and, consequently, accurate collisional data. However, no such data are currently available for the CH_3CHO–He system.

In this contribution, We present ongoing work aimed at providing the first collisional dataset for CH_3CHO–He. The study is based on the construction of a new potential energy surface using SAPT(DFT) and the autoPES package [3], followed by its preparation for scattering calculations. We will discuss the main features of the potential, the treatment of the rotational structure of acetaldehyde [4], and the computational strategy adopted for the collisional calculations.

The long-term goal of this work is to derive rate coefficients that can be used in the modelling of astrophysical spectra of acetaldehyde in cold environments, including sources such as L1521E [5]. Such data are expected to improve the interpretation of current and future observations of complex organic molecules in the interstellar medium.

References

[1] Molpeceres, G., et al. (2025). Astronomy & Astrophysics, 694, A299.
[2] Marks, J. H., et al. (2023). Chem, 9, 3286-3303.
[3] Metz, M. P., Piszczatowski, K., and Szalewicz, K. (2016). Automatic Generation of Intermolecular Potential Energy Surfaces. Journal of Chemical Theory and Computation, 12, 5895-5919.
[4] Herzberg, G. (1966). Electronic Spectra and Electronic Structure of Polyatomic Molecules. New York: Van Nostrand.
[5] Scibelli, S., et al. (2021). Monthly Notices of the Royal Astronomical Society, 504, 5754-5767.

AUTOMATED DEVELOPMENT OF POTENTIAL ENERGY SURFACES ACROSS THE ACCURACY GAMUT WITH ROBOSURFER

T. Győri [(a), *], N. Szabadszállási [(a)], G. Czakó [(a)]

[(a)] *MTA-SZTE Lendület "Momentum" Computational Reaction Dynamics Research Group, Interdisciplinary Excellence Centre and Department of Physical Chemistry and Materials Science, University of Szeged, Hungary.*

[*] tibor.gyori@chem.u-szeged.hu

The development of model potentials for molecules is just about as old as modern chemical theory. What started with the harmonic approximation and the Morse potential for the spectroscopy of diatomics, then progressed to triatomic reactions with the London–Eyring–Polanyi–Sato potential energy surface (LEPS PES), has since blossomed into the fitting of full-dimensional PESs for systems of 12 atoms and beyond using accurate *ab initio* energies. An essential part of developing such PESs is the efficient sparse sampling of the $3N-6$ dimensional configuration space of an N-atomic system, which becomes difficult for systems that are large or have rich chemical reactivity. We tame this problem by continuing to develop ROBOSURFER [1], a suite of programs that automates the iterative sampling of chemically relevant regions, and here we present three recent PESs that have been developed with its latest improvements.

Two of the PESs span the gamut of local accuracy vs. global coverage tradeoffs: from the single-minimum PES of CH_3OH that achieved a weighted RMS fitting error of 17.3 cm^{-1} and enabled a variational vibrational computation to match all experimentally determined frequencies within 5 cm^{-1} [2], to the rapidly developed PES for the $CH_3F + PH_2^-$ system which describes both S_N2 and post-S_N2 proton-transfer reactions accurately and is suitable for quasi-classical trajectories up to a collision energy of 40 kcal/mol. Lastly, a new $CH_3Cl + F^-$ PES was developed *ex nihilo*, starting only from reactant geometries. Despite no initial stationary-point information, all notable stationary points spontaneously emerged during PES development, demonstrating that with the latest improvements to ROBOSURFER, PES development can begin before the stationary points are mapped.

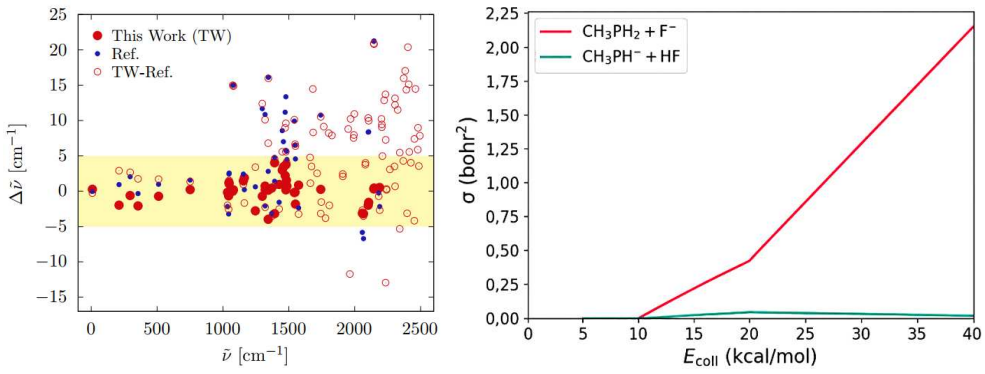


Figure 1: Successful applications of ROBOSURFER: the error of CH_3OH vibrational band origins is reduced below ± 5 cm^{-1}on a new PES, and the $CH_3F + PH_2^-$ PES produces both the S_N2 and the post-S_N2 proton-transfer products.

References

[1] Tibor Győri and Gábor Czakó, J. Chem. Theory Comput. **16**, 51–66 (2020).

[2] Ayaki Sunaga, Tibor Győri, Gábor Czakó and Edit Mátyus, J. Chem. Phys. **163**, 064101 (2025).

Imaging cold and controlled reactive collisions between S(^{1}D) and D_2

D. Yan, A. Tsoukala, N. Janssen, J. Schrijer, S. Bruil, S. Pieters, X.-D. Wang, S.Y.T. van de Meerakker, and J. Onvlee

Radboud University, Institute for Molecules and Materials (IMM)

Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

*dong.yan@ru.nl

What exactly happens during a chemical reaction? We experimentally investigate fundamental chemical reactions and their underlying dynamics at the full quantum level by letting individual atoms and molecules collide and react in a crossed molecular beam machine. Specifically, we focus on the prototypical insertion reaction between electronically excited sulfur atoms (S) and deuterium molecules (D_2), which serves as a sensitive benchmark for potential energy surfaces and scattering calculations.[1-3] This reaction is of particular astrophysical relevance, since mercapto radicals (SH/SD) play important roles in interstellar chemistry, and their absorption spectra serve as valuable probes of the diffuse interstellar medium.[4] Although the formation of SH/SD via S(^{1}D) + H_2/D_2/HD has been widely studied, important aspects of its dynamics remain unexplored. In this work, we combine a multistage Zeeman decelerator [5,6] with velocity map imaging (VMI) and resonance enhanced multiphoton ionization (REMPI) to perform state-resolved measurements of SD products across a broad collision energy range (1300–0.7 cm^{-1}). Our aim is to provide a sensitive test for potential energy surfaces and scattering calculations used to describe the molecular reaction dynamics in this system. This will enable us to deepen our understanding of the intricate dynamics underlying a chemical reaction.

References:

(1) Lara, M. et. al., *J. Chem. Phys.* **158**, 184303(2023).
(2) Lee, S. et. al., *J. Phys. Chem. A*, **102**, 8637–8640(1998).
(3) Li, Y. et. al., *J. Phys. Chem. A* **128**, 10234–10239(2024).
(4) Zhou, J. et. al., *Nat. Commun.* **11**, 15472020(2020).
(5) Cremers, T. et. al., *Rev. Sci. Instrum.* **90**, 013104(2019).
(6) Alexandra, T. et .al, Phys. Rev. A . **112**, 053113(2025).

QUANTUM SCATTERING STUDY OF COLLISIONAL EFFECTS IN ROTATIONAL SPECTRA OF O_2-PERTURBED HYDROGEN HALIDES

A. Olejnik [a],*, H. Jóźwiak [a], M. Rachko [a], M. Gancewski [a], E. Quintas-Sánchez [b], R. Dawes [b], P. Wcisło [a],

[a] Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Poland
[b] Department of Chemistry, Missouri University of Science and Technology, Rolla, Missouri, USA
* artur.olejnik@doktorant.umk.pl

Molecular collisions modify observed spectral line profiles, making molecular spectra sensitive probes of intermolecular interactions and collision dynamics. A quantitative description of these effects can be obtained directly from scattering calculations based on accurate intermolecular Potential Energy Surfaces (PESs).

Hydrogen halides are well suited for such studies because of their permanent dipole moments and anisotropic interactions with dominant atmospheric bath gases, such as N_2 and O_2. As a result, their spectra are particularly sensitive to collisional effects. They are important atmospheric species relevant for terrestrial, astrophysical, and industrial applications [1].

In this work, we present the first fully quantum scattering calculations of collision-induced line-shape parameters for rotational transitions of HCl and HF perturbed by O_2. The calculations are performed using BIGOS, a computational package developed in our group, and are based on newly developed, highly accurate PESs for the HCl- and HF-O_2 systems. By solving close-coupling equations, we obtain scattering matrices (S-matrices), from which generalized spectroscopic cross sections are determined. The calculated cross sections are used to obtain temperature-dependent line-shape parameters, including pressure broadening and pressure shift coefficients together with their speed dependence.

Our previous results for a single rotational transition of O_2-perturbed HCl showed very good agreement with the available experimental measurements [2]. We are currently extending the methodology to multiple pure rotational and rovibrational transitions relevant for atmospheric spectroscopy and spectroscopic databases.

References

[1] G. Li et al., *JQSRT* **130**, 284 (2013)
[2] A. Olejnik et al., *J. Chem. Phys.* **159**, 134301 (2023).

POSTERS

XVIII QUANTUM REACTIVE SCATTERING WORKSHOP

Non-ergodic dissociative valence double ionization of SF_6

E. Erdmann [a],*, E. Olsson [b], V. Daver Ideböhn [b] M. Wallner [b], R. J. Squibb [b] J. H. D. Eland [c], R. Feifel [b]

[a] Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland

[b] University of Gothenburg, Department of Physics, Origovägen 6B, 412 58 Gothenburg, Sweden

[c] Oxford University, Department of Chemistry, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, United Kingdom

* ewa.erdmann@pg.edu.pl

Sulphur hexafluoride, SF_6, is a highly symmetric octahedral molecule of broad scientific and technological relevance. Its role as an etchant in semiconductor plasma processing, as a potent long-lived greenhouse gas, and as a benchmark system in studies of molecular ionization and electron scattering has motivated extensive investigation of its spectroscopy and fragmentation dynamics across multiple charge states. The present work addresses dissociative valence double ionization of SF_6 in the ionization energy range from threshold up to 48.4 eV, with a particular focus on characterizing the fragmentation dynamics of nascent SF_6^{2+} and rigorously assessing the validity of statistical descriptions for doubly charged molecular ions.

The experimental fragmentation patterns obtained via multi-electron–multi-ion coincidence spectroscopy are interpreted through a three-pronged theoretical framework. Molecular dynamics simulations on a ground-state potential energy surface are used to identify dominant reaction pathways and likely product geometries. Exploration of the SF_6^{2+} potential energy surface at the B3LYP/6-311+G(d) level of theory yields key stationary points, including reactants, intermediates, transition states, and products. Branching ratios are then predicted using the M_3C statistical model [1], in which entropy maximization governs the partitioning among fragmentation channels.

While molecular dynamics simulations reproduce many observed features of the dissociation, a purely statistical treatment substantially underestimates the population of charge-retaining product channels (e.g. $SF_4^{2+} + F_2$). This failure indicates that intramolecular vibrational energy redistribution and/or electronic energy degradation are insufficiently rapid or complete to establish a microcanonical ensemble prior to bond rupture in SF_6^{2+}. The dissociation thus occupies an intermediate regime between fully statistical and fully dynamical behavior. We conclude that the onset of ergodicity in doubly and multiply charged ions is shifted toward larger molecular sizes relative to neutral and singly charged species. Such conclusion indicates broader implications for the applicability of statistical mass spectrometric models to multiply charged molecular ions.

References

[1] N. Aguirre *et al.* 2017 J. Chem. Theory Comput. **13** 992–100

Direct observation of the metastable fragmentation of uracil cations

Aditi Pradhan, Atilay Ayasli, Ivo S. Vinklárek, Hubertus Bromberger, Sebastian Trippel, and Jochen Küpper

Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
Department of Physics, Universität Hamburg, Germany
Department of Chemistry, Universität Hamburg, Germany
Center for Ultrafast Imaging (CUI), Universität Hamburg, Germany

Nucleobases are photostable biomolecules with complex relaxation dynamics at picosecond timescales [1], rendering them a useful, practical test bed to explore atomic-scale ultrafast fragmentation dynamics. We employ the versatile transportable endstation for controlled molecules (eCOMO) [2] to study isolated uracil molecules as well as hydrated clusters in a size-selected fashion [3]. Our photodissociation experiment in the strong-field regime reveals a metastable fragmentation pathway of the uracil(-water) cation, where multi-mass velocity-map-imaging (VMI) data serve as the key enabler for our findings. Our observations are supported by lifetime estimates and accompanied by preliminary theoretical results.

References

[1] Nachtigallová, et int. (4 authors), Lischka, *J. Phys. Chem.* A, **115** (2011)

[2] Jin, et int. (8 authors), Küpper, submitted (2024), arXiv:2406.16491 [physics]

[3] Chang, Horke, Trippel, Küpper, Int. Rev. Phys. Chem., **34**, 1077838 (2015) arXiv:1505.05632 [physics]

IMPACT OF SURFACE MODES ON H_2/D_2 SCATTERING FROM CU(111): A TIME-DEPENDENT EFFECTIVE HARTREE APPROACH

Mantu K. Sah[(a)] *, Satrajit Adhikari[(a)], Bauke Smits[(b)], Jörg Meyer[(b)], Mark F. Somers[(b)]
[(a)]*School of Chemical Sciences, IACS Kolkata, India*
[(b)]*Leiden Institute of Chemistry, Leiden University, The Netherlands.*
*scsmks2537@iacs.res.in

We have carried out six-dimensional (6D) quantum wavepacket dynamics calculations for H_2/D_2 (v=0, j=0, 2) scattering and reacting on a Cu(111) surface. In this investigation, a time- and temperature-dependent effective Hartree potential (EHP) is employed incorporating finite temperature effects originating from the combined treatment of thermally expanded PESs and surface vibrational modes. [1] The EHP captures interactions between molecular degrees of freedom and surface vibrational modes within a mean field and linear coupling approximation. Surface modes/phonons are modelled through cluster-based, slab-derived and EAM quasi-harmonic approaches, where their states are distributed using either Bose-Einstein (BE) or Maxwell-Boltzmann (MB) statistics at non-zero surface temperature. The BE- based EHPs show closer agreement with experimental [2, 3] chemisorption thresholds and depict substantial broadening for 925 K phonons, 0 K phonons and cluster modes, whereas MB-based results display little sensitivity on temperature. [4]

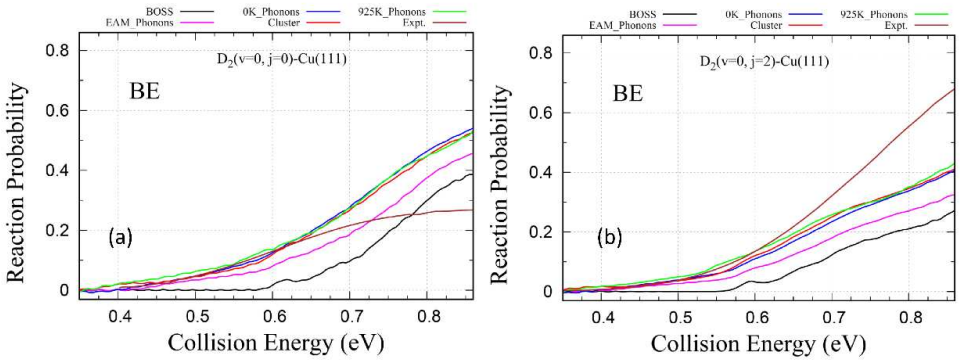


Figure 1: The effects of BE (quantum) state distributions on reaction probability of D_2 on Cu(111) at 925 K for different approaches.

References

[1] M. K. Sah, K. Naskar, S. Adhikari, B. Smits, J. Meyer and M. F. Somers, J. Chem. Phys. **161**, 014306 (2024)
[2] C. T. Rettner, H. A Michelsen and D. J. Auerbach, Faraday Discuss. **96**, 17 (1993).
[3] S. Kaufmann, Q. Shuai, D. J. Auerbach, D. Schwarzer and A. M. Wodtke, J. Chem. Phys. **148**, 194703 (2018).
[4] M. K. Sah, S. Adhikari, B. Smits, J. Meyer and M. F. Somers, J. Phys. Chem. C (submitted, 2026).

VIBRATIONAL MODE-SPECIFIC DYNAMICS IN THE Cl + CH_3CN AND O^- + CH_4/CD_4 REACTIONS

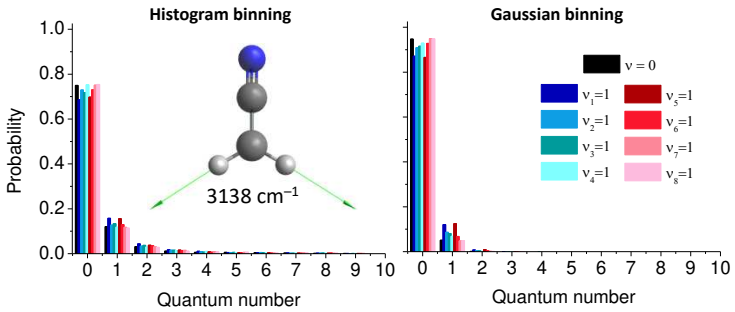
P. Tóth [(a), *] and G. Czakó [(a)]

[(a)] *MTA-SZTE Lendület "Momentum" Computational Reaction Dynamics Research Group, Interdisciplinary Excellence Centre and Department of Physical Chemistry and Materials Science, Institute of Chemistry, University of Szeged, Rerrich Béla tér 1, Szeged H-6720, Hungary*
[*]toth.petra.294@gmail.com

We present a theoretical investigation of vibrational mode-specific effects in the Cl + CH_3CN and O^- + CH_4/CD_4 reactions. After characterizing the stationary points,[1,2] full-dimensional analytical potential energy surfaces (PESs) were developed using high-level ab initio calculations and permutationally invariant polynomial fitting within the ROBOSURFER framework.[3] Extensive quasi-classical trajectory (QCT) simulations were performed for both ground-state and selectively vibrationally excited reactants over broad collision-energy and impact-parameter ranges.[4] Particular emphasis was placed on mode-specific product-state analysis and energy redistribution mechanisms. Product vibrational-state populations were analyzed using both histogram binning (HB) and Gaussian binning (GB) methods, enabling direct comparison of the two approaches in describing vibrational product-state distributions. The simulations also provide detailed information on integral cross sections, scattering-angle distributions, attack-angle preferences, and translational, rotational, and vibrational energy partitioning.

For the Cl + CH_3CN reaction, all eight normal modes of CH_3CN were selectively excited across multiple collision energies, resulting in more than 4.5 million trajectories.[4] The calculations reveal substantial differences among vibrational modes in promoting hydrogen abstraction and steering product energy flow, along with a strong preference for methyl-end attack and collision-energy-dependent reaction mechanisms.

For the O^- + CH_4/CD_4 reactions, mode-specific simulations were carried out for four vibrational modes of both isotopologues, comprising over 5.2 million trajectories. The results show clear vibrational enhancement effects and isotope-dependent dynamical behavior. Simulated scattering-angle and internal-energy distributions are in good agreement with available experimental measurements.



References

[1] P. Tóth, T. Szűcs, and G. Czakó, J. Phys. Chem. A **126**, 2802 (2022).
[2] A. Ayasli, P. Tóth, T. Michaelsen, T. Gstir, F. Zappa, D. Papp, G. Czakó, and R. Wester, J. Phys. Chem. A **128**, 3078 (2024).
[3] P. Tóth, T. Szűcs, T. Győri, and G. Czakó, J. Chem. Phys. **161**, 084304 (2024).
[4] P. Tóth and G. Czakó, J. Chem. Phys. **163**, 064306 (2025).

FROM NOBLE GASES TO LANTHANIDES: LOW-ENERGY ELECTRON SCATTERING WITH GRASPC

P. Syty [(a), *], M. Piłat [(a)], J.E. Sienkiewicz [(a)]

[(a)] *Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland.*
[*]pawel.syty@pg.edu.pl

Low-energy electron–atom scattering is essential for understanding electron–matter interactions in fields such as plasma physics, spectroscopy, and ultracold collisions. In the near-threshold regime, the process is governed by a few partial waves and can be characterized by scattering lengths and low-energy elastic cross sections.

We present calculations performed with a newly developed computational tool, GRASPC [1], which extends the GRASP atomic structure package [2] to describe continuum orbitals of scattered electrons. The method is based on the multiconfiguration Dirac–Hartree–Fock (MCDHF) framework, treating the system as an N+1-electron problem. Scattering parameters are extracted from phase shifts obtained via the asymptotic behavior of relativistic continuum wave functions.

Benchmark calculations were carried out for noble gases (Ar, Kr, Xe, Rn, Og) [3]. Results for Ar, Kr, and Xe show good agreement with available data, while predictions are provided for heavier systems. The method was further applied to electron–strontium scattering, yielding phase shifts, scattering length [4], and elastic cross sections (0.001–15 eV) [5], with generally good consistency with experiment and previous theory.

Preliminary calculations for lanthanides (La–Lu) indicate negative scattering lengths, increasing monotonically with atomic number, suggesting attractive interactions insufficient to form stable negative ions.

These results demonstrate that GRASPC is an efficient and versatile relativistic framework for computing low-energy electron–atom scattering parameters across a wide range of atomic systems.

References

[1] P. Syty, M.P. Piłat, J.E. Sienkiewicz, GRASPC – GRASP package adapted for the generation of continuum orbitals wave functions. Comput. Phys. Commun. 315, 109691 (2025)

[2] C.F. Fischer, G. Gaigalas, P. Jönsson, J. Bieroń, GRASP2018 – A Fortran 95 version of the General Relativistic Atomic Structure Package. Comput. Phys. Commun. 237, 184–187 (2019)

[3] P. Syty, M.P. Piłat, J.E. Sienkiewicz, Calculation of electron scattering lengths on Ar, Kr, Xe, Rn and Og atoms. J. Phys. B: At. Mol. Opt. Phys. 57, 175202 (2024)

[4] P. Syty, M.P. Piłat, J.E. Sienkiewicz, Low-energy phase shifts and scattering length of strontium from Dirac-Coulomb and polarization potential modeling. At. Data Nucl. Data Tables 168, 101783 (2026)

[5] P. Syty, M.P. Piłat, Moein Sahraei, J.E. Sienkiewicz, Total, momentum-transfer, differential and spin-polarization cross sections for elastic electron-strontium scattering at low energies. Atoms 14(6), 44 (2026)

PREDICTION OF TOTAL ELECTRON-IMPACT IONIZATION CROSS SECTIONS

B.Majewski [(a),*], M.Tatar [(a)], M.Łabuda [(a,b)]

[(a)] *Department of Theoretical Physics and Quantum Information, Gdańsk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland*

[(b)] *BioTechMed Center, Gdańsk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland*

[*] bartosz.majewski@pg.edu.pl

Accurate prediction of molecular cross sections across a range of collision energies is a challenging regression task due to the multi-point energy dependence of each molecule and the limited chemical diversity available in quantum chemistry datasets. We present preliminary results for a study concerned with the prediction of total electron-impact ionization cross sections for molecules of astrochemical interest through machine learning (ML) methods. The study provides thorough benchmark of few well known ML models: Light Gradient Boosting Machine (LGBM), CatBoost, Multilayer Perceptron (MLP) and a Graph Neural Network (GNN) on a dataset of 212 unique molecules with cross section values computed across a shared energy grid [1-3].

The GNN model represents each molecule as an atomic graph with chemically-informed node and edge features, incorporating collision energy as an additional input to the readout layer. Gradient boosted tree models and MLP operate on precomputed molecular descriptors selected via Boruta and correlation-based feature selection. All models are evaluated under a grouped cross-validation scheme that prevents data leakage across molecules, with a held-out test set of 42 molecules used for final performance assessment.

Model performance is assessed using root mean squared error, mean absolute error, and Spearman rank correlation, supplemented by bootstrap confidence intervals and per-molecule error decomposition. Additionally learning curves are evaluated across different training set fractions to investigate performance of the models in low data availability conditions.

References

[1] Brandt A. L. Gaches, Tommaso Grassi, Stefan Vogt-Geisse, Giulia M. Bovolenta, Claire Vallance, David Heathcote, Marco Padovani, Stefano Bovino, and Prasanta Gorai, arXiv e-prints, arXiv:2310.10739 (2023)

[2] David Heathcote and Claire Vallance, J. Phys. B: At. Mol. Opt. Phys. **51**, 195203 (2018)

[3] Weiwei Zhou, Lorna Wilkinson, Jason W. L. Lee, David Heathcote, and Claire Vallance, Mol. Phys. **117**, 3066–3075 (2019)

Modelling Quantum Resonances in Cold Ion-Atom Collisions

Marcin Welter [(a),*], Dawid Dąbrowski [(a)], Michał Przybytek [(b)], Michał Tomza [(a)]

[(a)] Faculty of Physics, University of Warsaw, Pasteura 5, 02-093, Warsaw, Poland.
[(b)] Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093, Warsaw, Poland.
[*] m.welter@student.uw.edu.pl

Charge transfer reactions play a fundamental role across chemistry, biology, and physics, occurring in environments ranging from condensed matter and liquid solutions to interstellar space and plasmas [1]. Electron transfer has attracted considerable attention because charge transfer is fundamentally governed by quantum-mechanical effects. The phenomenon arises from non-adiabatic coupling between different Born–Oppenheimer potential energy surfaces. However, a rigorous test of the first-principles theory has not yet been performed due to the demanding experimental conditions required to reach sufficiently low energies where quantum effects enable quantitative comparison with theory. Only limited evidence of quantum effects have been observed, most notably an observation of Feshbach-type resonances in laser-cooled ion–atom collisions [2]. We present theoretical results for electron charge transfer between cold helium ions and atoms, in agreement with recent experimental findings in which Rydberg atoms are used as "shielded" ions to access the cold quantum collision regime for species that are not amenable to laser cooling [3]. The resonances in the reaction rate observed in the experiment are explained and confirmed by our calculations to be quantum shape resonances arising from tunneling through the centrifugal barrier, making it the first direct observation of shape resonances in the ion-atom system.

References

[1] Rudolph A Marcus and Norman Sutin. Electron transfers in chemistry and biology. *Biochimica et Biophysica Acta (BBA)-Reviews on Bioenergetics*, 811(3):265–322, 1985.

[2] Pascal Weckesser, Fabian Thielemann, Dariusz Wiater, Agata Wojciechowska, Leon Karpa, Krzysztof Jachymski, Michał Tomza, Thomas Walker, and Tobias Schaetz. Observation of feshbach resonances between a single ion and ultracold atoms. *Nature*, 600(7889):429–433, 2021.

[3] Arijit Das, Yufeng Wang, Marcin Welter, Karl Horn, Dawid Dąbrowski, Michał Przybytek, Julia Narevicius, Michał Tomza, and Edvardas Narevicius. Observation of quantum resonances in cold ion-atom collisions.

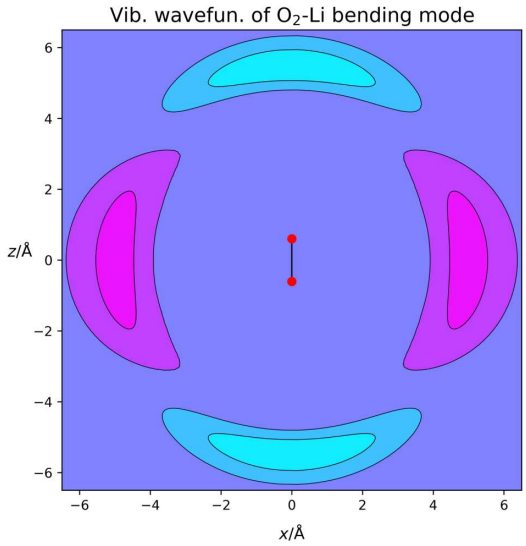
Quantum dynamics of $O_2(X^3\Sigma_g^-)$ complexes with alkali and alkaline-earth metal atoms from *ab initio* potentials

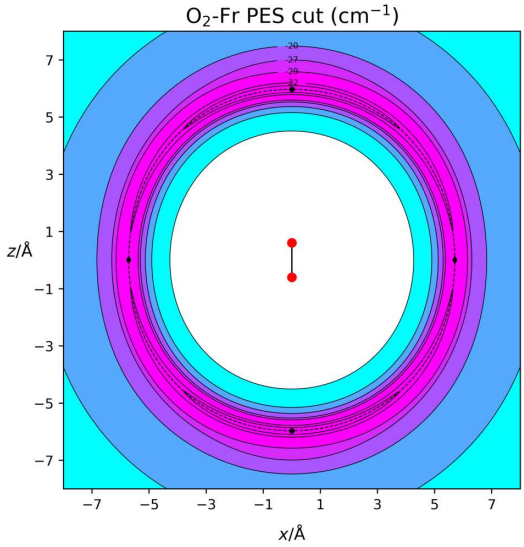
Leonid Shirkov, Hubert Jóźwiak, Piotr Wcisło

Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziądzka 5/7, 87-100 Toruń, Poland

leonid.shirkov@umk.pl

Understanding quantum scattering calculations, including collisional cross sections and the control of scattering lengths, is essential in the context of ultracold experiments [1]. We present a theoretical study of the interaction between O_2 in its ground electronic state, $O_2(X^3\Sigma_g^-)$, and alkali (Li–Fr, $^2S_{1/2}$, high-spin complexes) as well as alkaline-earth (Be–Ra, $^1S_0$) metal atoms. The interaction potentials were calculated using spin-restricted open-shell CCSD(T), with HF reference stabilized by CASSCF. Two-dimensional analytical potentials were constructed using the Legendre expansion $V(R,\theta) = \sum_\lambda V_\lambda(R)\, P_\lambda(\cos\theta)$ and applied to study the structure and quantum dynamics of the complexes. Rovibrational bound states, scattering lengths, and cross sections as functions of potential scaling were analyzed using our in-house suite of codes [2]. This study provides a foundation for future investigations of the quantum scattering dynamics of these complexes in magnetic fields, including spin-orbit and hyperfine couplings.





References

[1] N. Akerman, M. Karpov, Y. Segev, N. Bibelnik, J. Narevicius, and E. Narevicius, Phys. Rev. Lett. **119**, 073204 (2017).

[2] H. Jóźwiak, T. V. Tscherbul, and P. Wcisło, J. Chem. Phys. **160**, 094304 (2024).

Electron transfer reaction in H_2 + He^+ collision at 3 eV

Huet X.[a], Aerts A.[a], Vaeck N.[a]

[a]Spectroscopy, Quantum Chemistry and Atmospheric Remote Sensing (SQUARES), Université libre de Bruxelles, Brussels, B-1050, Belgium

Electron-transfer reactions induced by collisions between a neutral diatomic molecule and an atomic cation are important in a variety of environments, including astrophysical media [1] and plasma- containment devices [2]. In the Earth's upper atmosphere, neutral diatomic molecule can collide with incoming proton (H^+) and helium cation (He^+) fluxes originating from the solar corona and transported by the solar wind; such collisions contribute to the ion–neutral chemistry that governs ionospheric composition [3]. This study investigates the electron-transfer reaction between H_2 and He^+, a process widely regarded as a benchmark system. We aim to deliver an integrated description combining high-level electronic-structure calculations with time-dependent dynamical simulations.

At a collision energy of 3 eV, two product channels are energetically accessible, yielding different electronic states of the molecular ion:

$$H_2(X\,^1\Sigma_g^+) + He^+(1\,s) \longrightarrow H_2{}^+(^2\Sigma_g^+) + He(1\,s^2), \quad (1)$$

$$\longrightarrow H_2{}^+(^2\Sigma_u^+) + He(1\,s^2). \quad (2)$$

To characterize the electronic structure relevant to the reaction, we computed the multi-dimensional adiabatic potential energy surfaces (PESs) of the six lowest A' electronic states at the MRCI/AVTZ level of theory, chosen to provide a balanced description of both the ground and excited states. Non-adiabatic coupling terms (NACs) between these states were evaluated by finite-difference from the MRCI wavefunctions.

Constructing a reliable diabatic representation for the lowest-lying states is commonly challenging, notably because of the limited-size of the adiabatic basis. We therefore introduced a hybrid diabatization procedure that combines NAC-based diabatization with quasi-diabatization [4]. This hybrid approach mitigates artifacts associated with an incomplete adiabatic basis and produces a smooth, physically meaningful diabatic potential energy surfaces suitable for nuclear dynamics computation.

Reaction cross sections for channels (1) and (2) were obtained using time-dependent wavepacket propagation on the diabatic representation. The propagation yields state-resolved reaction probabilities $P_{i\to f}(E)$ from which energy-dependent cross sections $\sigma_{i\to f}(E)$ are computed.

These results contribute to the understanding of atomic ion–diatomic neutral electron-transfer processes relevant to upper-atmosphere and astrophysical chemistry. Furthermore, it provides a transferable computational framework for other diatomic–cation collision systems.

References

[1] Brekke A. *SSBM* Physics of the upper polar atmosphere. (2012)

[2] Janev, R. K. *Contrib. Plasma Phys* **38** 307-318 (1998)

[3] Michel, F. C. *Rev. Geophys.* **9**(2) 427–435 (1971)

[4] Simah D., Hartke B. and Werner H.-J. *J. Chem. Phys.* **111** 4523–4534 (1999)

From adiabatic to diabatic representation: an *ab initio* investigation of the LiS molecule

Sana Akkari[1], Wissem Zrafi[1], Mohamed Bejaoui[1], Hela Ladjimi[1], Jamila Dhiflaoui[1], Józef E. Sienkiewicz[2], and **Hamid Berriche**[2, 3, 1, *]

[1]*Faculty of Science of Monastir, Laboratory of Interfaces and Advanced Materials LR11ES55, Physics Department, University of Monastir, 5019 Monastir, Tunisia*
[2]*Faculty of Applied Physics and Mathematics, Gdan´sk University of Technology, Narutowicza 11/12, 80-233 Gdan´sk, Poland.*
[3]*Mathematics and Physics Department, School of Arts and Sciences, American University of Ras Al Khaimah, Ras Al-Khaimah, United Arab Emirates.*

hamid.berriche@aurak.ac.ae

In this study, we present a high-level theoretical investigation of the electronic structure and nonadiabatic dynamics of the LiS molecule. High-precision adiabatic potential energy curves (PECs) for the lowest electronic states were computed using multireference configuration interaction with Davidson correction (MRCI+Q). In addition, we determine the permanent (PDMs) and transition (TDMs) dipole moments, as well as the radiative lifetimes of vibrational levels to characterize the molecule's spectroscopic and dynamical properties. The nonadiabatic radial coupling *ab initio* matrix elements were obtained from the *ab initio* adiabatic PECs using the finite difference method between the ($X^2\Pi$–$2^2\Pi$) and ($2^2\Pi$–$3^2\Pi$) adiabatic states. The first-order adiabatic correction was also evaluated, and its effects on the spectroscopic constants and vibrational energy levels were analyzed for both the $X^2\Pi$ and $2^2\Pi$ states. This work advanced the theoretical framework for modeling diatomic systems in which nonadiabatic effects may be significant, with implications for precision spectroscopy and molecular dynamics.

References

[1] Sana Akkari, Wissem Zrafi, Mohamed Bejaoui, Hela Ladjimi, Jamila Dhiflaoui, Józef E. Sienkiewicz[2], and Hamid Berriche, *Phys. Chem. Chem. Phys.*, 2026, 28, 4790–4805
[2] N. Mabrouk, W. Zrafi and H. Berriche, Mol. Phys., 2020, 118, e1605098.
[3] H. Hendaoui, R. Linguerri, G. Chambaud, N.-E. Jaidane and M. Hochlaf, Mol. Phys., 2019, 117, 1653.
[4] M. Brewster and L. Ziurys, Chem. Phys. Lett., 2001, 349, 249.
[5] B. Mehnen, S. Akkari, W. Zrafi, I. Jendoubi, M. Bejaoui, N. Bulut, H. Berriche and M. Hochlaf, J. Quant. Spectrosc. Radiat. Transfer, 2024, 322, 109014.

Comprehensive Ab Initio Characterization of CO Electronic States for Quantum Dynamics and Reactive Scattering Applications

Benjamin A. Ikuesan,[(a), (b)] *Patryk Jasik*,[(a),(c)] , *Niyazi Bulut*[(a),(e)], *Józef E. Sienkiewicz*[(a),(d)]

[(a)]*Institute of Physics and Applied Computer Science, Faculty of Applied Physics and Mathematics, Gdańsk Tech,* [(b)]*Doctoral School, Gdańsk Tech,* [(c)]*BioTechMed Center, Gdańsk Tech,* [(d)]*Advanced Materials Center, Gdańsk Tech, Poland*
[(e)]*Physics Department, Faculty of Science, Firat University, 23119 Elazig, Türkiye*
Email: benikues@pg.edu.pl

Carbon monoxide (CO) is a fundamental molecule in molecular spectroscopy and astrochemistry, where accurate electronic-structure data are required for interpreting laboratory and astrophysical spectra. In this work, we present a comprehensive ab initio characterization of the complete set of eighteen adiabatic electronic states of CO correlating with the first dissociation limit, C(^{3}P) + O(^{3}P). The investigated states include singlet, triplet, and quintet states of $\Sigma^{\pm}$, Π, and Δ symmetries. Potential-energy curves were computed using state-averaged CASSCF followed by MRCI with Davidson correction, together with large augmented correlation consistent basis sets. Basis-set convergence was assessed through complete-basis-set extrapolation, providing an estimate of the remaining uncertainty in the calculated electronic energies.[1,2]

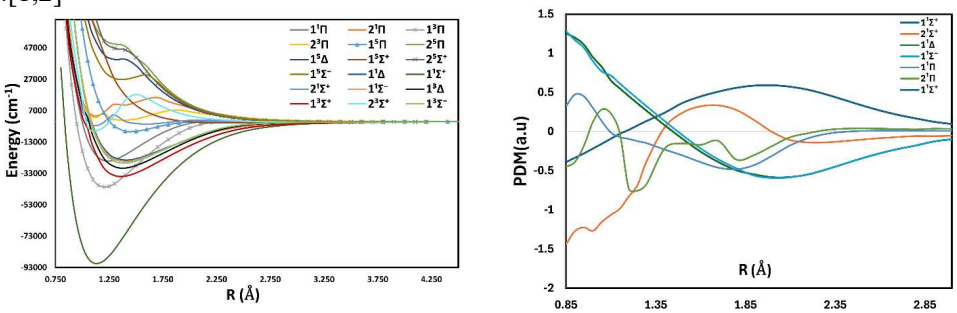


Figure 1. (left) The selected PECs of the CO molecule. (right) Permanent dipole moment for the singlet states of CO

From the calculated potential energy curves, spectroscopic constants were derived for the bound and weakly bound states and compared with available experimental and theoretical values. The results show good agreement for the well-characterized low-lying states and provide additional predictions for higher-lying and less studied electronic states, including quintet states that are often omitted in earlier studies. Permanent dipole-moment functions were also computed along the internuclear distance for all eighteen states, giving complementary information on the evolution of the electronic charge distribution[1,2]
The resulting dataset provides a consistent theoretical reference for CO electronic states associated with the first dissociation asymptote.

References

[1] S. Ryzner, M. I. Malicka, A. N. Heays, R. W. Field, N. de Oliveira, W. Szajna, W. Ubachs, R. Hakalla, *J. Mol. Spectrosc.*, 2021, **379**, 111528.

[2] M. I. Malicka, S. Ryzner, A. N. Heays, N. de Oliveira, R. W. Field, W. Ubachs, R. Hakalla, *J. Quant. Spectrosc. Radiat. Transf.*, 2020, **247**, 106939.