

## GK2022 Programme – Couvent des Jacobins, Rennes, August 28 – September 1 2022

Registration takes place in the main entry hall, and the welcome reception is in the South Gallery of the Cloister. All oral presentations take place in *La Nef*, while refreshments, lunches and posters are upstairs in *La Halle*.

### Sunday August 28, 2022

“Cocktail dinatoire” reception and registration at the Couvent des Jacobins from 18:00 to 21:00

### Monday August 29, 2022

08:00–09:00	Registration in the Entry Hall and time to put posters up in the Level 1 Hall	
09:00 (20')	Welcome and introduction	RSC Gas Kinetics Discussion Group and GK2022 Organising Committee
09:20 (15')	<b>Award of 2020 Polanyi medal to Dr Stephen J. Klippenstein</b>	GK Committee Chair, Christa Fittschen and GK2020 Chair, Matthias Olzmann
09:35 (45')	<b>Polanyi Lecture: Interpreting the Complexities of Chemically Reactive Environments</b>	Dr Stephen J. Klippenstein, Argonne National Laboratory, USA
10:20 (30')	Refreshments	
	<b>Atmospheric Chemistry I / Theoretical Kinetics I</b>	Session chair: Abdelwahid Mellouki
10:50 (30' + 10')	<b>Driving new developments in excited-state molecular dynamics through challenging photochemical applications</b>	Prof Basile Curchod, University of Bristol, UK
11:30 (15' + 5')	Direct Studies of Isoprene-Derived Four-Carbon Criegee Intermediate	Dr Rebecca Caravan, Argonne National Laboratory, USA
11:50 (15' + 5')	Atmospheric oxidation of a new green solvent 2,2,5,5-tetramethyloxolane	Ms Caterina Mapelli, University of York, UK
12:10	Tribute to Robert Lesclaux	Dr Abdelwahid Mellouki, CNRS Orléans, France
12:30 (90')	Lunch	
	<b>Combustion I</b>	Session chair: Laure Pillier
14:00 (30' + 10')	<b>Unravelling the Bimolecular Reactions of Hydroxyl Radicals</b>	Prof Aamir Farooq, KAUST, Saudi Arabia
14:40 (15' + 5')	OH Radical Reactions with Propargyl and Cyclopentadiene	Prof Fabien Goulay, University of West Virginia, USA
15:00 (15' + 5')	Pyrolysis of Methyl Formate: Elementary Steps and Overall Mechanism	Mr Johannes Wenz, KIT, Germany
15:20 (15' + 5')	Reactions of Propargylic Radicals with Molecular Oxygen: A Comprehensive Experimental and Computational Study	Mr Timo Pekkanen, University of Helsinki, Finland
15:40 (15' + 5')	Industrial Perspective on Automated Exploration of Chemical Reaction Networks	Dr Maike Bergeler, BASF, Germany
16:00 (30')	Refreshments	
	<b>Combustion II</b>	Session chair: Clemens Naumann
16:30 (15' + 5')	The many fates of alkyl radicals	Dr Rob Tranter, Argonne National Laboratory, USA
16:50 (15' + 5')	Probing O <sub>2</sub> -Dependence of Tetrahydrofuranyl Reactions via Isomer-Resolved Speciation	Ms Alanna Koritzke, University of Georgia, USA
17:10 (15' + 5')	Genetic Algorithm Optimization of A Theory-Based Low-Temperature Cyclopentane Oxidation Model for Improved Accuracy	Dr Maria Demireva, Sandia National Laboratories, Livermore CA, USA
17:30 (20')	Flash poster presentations	Chair: Lucile Rutkowski
17:50 (10')	IUPAC Atmospheric Chemical Kinetic Data Evaluation	Dr Tim Wallington, Ford Motor Company, Ann Arbor MI, USA
18:00 (90')	Poster session I + cocktail	

## Tuesday August 30, 2022

	<b>Heterogeneous and Gas-particle chemistry I</b>	Session chair: Sébastien Le Picard
09:00 (30' + 10')	<b>Are average cloud droplet properties sufficient? - The role of drop-resolved properties in predicting oxidant budgets in the atmospheric multiphase system:</b>	Dr Barbara Ervens, University of Clermont Auvergne, France
09:40 (15' + 5')	Rate constants of iron chemistry behind the flame-assisted iron oxide nanoparticle synthesis	Prof Igor Rahinov, The Open University of Israel
10:00 (15' + 5')	Experimental characterization of the chemical species governing the soot nucleation process in flames by coupling ToF-SIMS and Raman spectroscopy	Ms Jessy Elias, University of Lille, France
10:20 (30')	Refreshments	
	<b>Heterogeneous and Gas-particle chemistry II / Atmospheric Chemistry II</b>	Session chair: María Antañolo
10:50 (15' + 5')	Uptake and Dynamics of OH Radicals at Organic-Aerosol-Surface Proxies	Dr Daniel Moon, Heriot Watt University, Edinburgh, UK
11:10 (15' + 5')	Iodide oxidation at the gas/water interface as a function of temperature	Mr Antoine Roose, Paul Scherrer Institute, Switzerland
11:30 (15' + 5')	Kinetics and Mechanisms of Aqueous-Phase Photosensitized Reactions of Imidazole-2-carboxaldehyde and 3,4-Dimethoxybenzaldehyde with $\alpha,\beta$ -Unsaturated Carbonyl Compounds	Dr Thomas Schaefer, Leibniz Institute for Tropospheric Research – TROPOS, Leipzig, Germany
11:50 (15' + 5')	Kinetic and mechanistic experimental study of the reactivity of $\alpha$ and $\beta$ -phellandrene with the $\text{NO}_3$ radical	Mr Sergio Harb, LISA, UPEC, Paris
12:10 (15' + 5')	Atmospheric Chemistry of Perfluoroheptenes ( $\text{C}_7\text{F}_{14}$ ): Isomer Specific OH Reaction Rate Coefficients, Infrared Spectra, and Climate Metrics	Dr Aparajeo Chattopadhyay, NOAA University of Colorado Boulder, USA
12:30 (90')	Lunch	
	<b>Theoretical Kinetics II / Astrochemistry I</b>	Session chair: Luc Vereecken
14:00 (30' + 10')	<b>Circumstellar Chemistry</b>	Prof John Plane, University of Leeds, UK
14:40 (15' + 5')	Radiative Association for NaCl, Including Non-Adiabatic Coupling	Dr Martina Šimsová, Luleå University of Technology, Sweden
15:00 (15' + 5')	Fine and hyperfine excitation of CCS isotopologues induced by collisions with He	Ms Amélie Godard Palluet, Université de Rennes 1, France
15:20 (20')	Flash poster presentations	Chair: Lucile Rutkowski
15:40 (8' + 2')	Special poster introduction: Application of the theoretical SVECV-f12 protocol to the prediction of energy barriers, enthalpies of atomization and formation, and special problems related to the N-F bond in high-energy species	Prof Oscar Ventura, Universidad de la República (UdelaR), Uruguay
15:50 (100')	Posters + refreshments	
17:30	End of poster session – please walk to Reception	
<b>18:00</b>	<b>Reception at the Hôtel de Ville de Rennes</b>	

**Wednesday August 31, 2022**

	<b>Elementary processes I</b>	Session chair: Bénédicte Picquet-Varrault
09:00 (30' + 10')	<b>New Observations of Old Reactions</b>	Prof Paul Seakins, University of Leeds, UK
09:40 (15' + 5')	State selective investigation of the $\text{HBr}^+ + \text{H/DCI}$ reaction	Mr Dominik Plamper, Philipps-Universität Marburg, Germany
10:00 (15' + 5')	Crossed molecular beams and theoretical studies of the $\text{O}(^3\text{P}) + 1,2\text{-butadiene}$ reaction	Dr Gianmarco Vanuzzo, Università degli studi di Perugia, Italy
10:20 (30')	Refreshments	
10:50 (15' + 5')	Destruction routes of interstellar complex organic molecules by collisions with $\text{He}^+$	Ms Emília Valença Ferreira De Aragão, Università degli studi di Perugia, Italy
11:10 (15' + 5')	Product branching fraction measurements at low temperature for the reaction of the CN radical with propene	Ms Myriam Drissi, Université de Rennes 1, France
11:30	End of sessions – please collect your lunch box and go directly to Place des Lices for excursion	
<b>12:00 sharp</b>	<b>Departure of buses for Mont St Michel (Place des Lices)</b>	
20:30 (approx.)	Return of buses from Mont St Michel	

**Excursion**

We will leave promptly at 12:00 Wednesday August 31 by coach from the Place des Lices which is just a short walk from the Couvent via the Place Ste Anne and Rue St Michel, members of GK2022 Staff will guide you. Lunch boxes are provided for everyone who is registered whether you are going on the excursion or not, and should be collected directly outside La Nef in the entry hall at the end of the morning session. You can eat your lunch quickly while waiting outside for the coach, or on arrival at Mont St Michel (around 13:00) but the coach company would prefer you not to eat in the coaches.

On arrival there is a pleasant walk (20 minutes) to the Mont, and then we have a tour of (a part of) the Mont St Michel Bay on foot, accompanied by guides (we will be in several groups). The Bay is a remarkable natural environment rich in wildlife and shaped by a big tidal range, and the guided exploration will also give us the chance to admire the Mont from a different angle. The walk is best done barefoot (or with waterproof sandals but they tend to come off in the wet sand!). The company of guides recommends that you dress casually (shorts...) and that you bring a few things with you:

- A backpack (or bag) for your shoes etc
- A raincoat
- A bottle of water (provided when you leave the coaches, along with a snack in lieu of afternoon tea)
- A towel to dry your feet (but the sun will also do the job...)
- Sunscreen
- Headgear
- Sunglasses

The tour of the Bay will be followed by time to explore the Mont itself, and included is a visit to the Abbey which is timed, information will be given by GK2022 staff on arrival.

We expect to arrive back in Rennes around 20:30.

**Thursday September 1, 2022**

	<b>Astrochemistry II</b>	Session chair: Julia Lehman
09:00 (30' + 10')	<b>Interstellar molecular ions: reaction kinetics and photo-processes in cold traps</b>	Prof Roland Wester, University of Innsbruck, Austria
09:40 (15' + 5')	Low Temperature Study of the Reactions of NH <sub>2</sub> with CH <sub>2</sub> O and NO	Dr Kevin Douglas, University of Leeds, UK
10:00 (15' + 5')	Investigating ion-molecule reactions at low temperature with uniform supersonic flows	Dr Ludovic Biennier, Université de Rennes 1, France
10:20 (30')	Refreshments	
10:50 (15' + 5')	Gas-phase formation of interstellar methyl cyanide: review and new theoretical calculations	Ms Lisa Giani, Université Grenoble Alpes, France
11:10 (15' + 5')	A cryogenic ion trap for studying ion-radical reactions	Ms Chloe Miossec, Universities of Oxford and Liverpool, UK
11:30 (15' + 5')	Low Temperature Kinetics of the OH + CO Reaction: A Gas Phase Source of Interstellar CO <sub>2</sub> ?	Prof Mitchio Okumura, Caltech, Pasadena CA USA
	<b>Atmospheric Chemistry III</b>	Session chair: Daniel Stone
11:50 (15' + 5')	Absolute Absorption Cross-Section of C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> Radical and Kinetics of Its Self-Reaction: Rate Constant and Branching Ratio	Ms Cuihong Zhang, Université de Lille, France
12:10 (15' + 5')	Reaction of Furan Compounds Emitted from Biomass Burning with the Major Night time Oxidant (NO <sub>3</sub> Radical): Rate Coefficient Measurements & Product Characterization	Ms Fatima Al Ali, Université Littoral Côte D'Opale and IMT Université de Lille, France
12:30 (90')	Lunch	
14:00 (15' + 5')	Benzene autoxidation? Semi-empirical model building anchored on lab experiments and quantum chemical computations	Prof Matti Rissanen, Tampere University, Finland
14:20 (15' + 5')	A Broad View of Structure-Activity Relationship Performance for Alkanes and Haloalkanes	Dr Max McGillen, CNRS Orléans, France
	<b>Combustion III</b>	Session chair: Ravi Fernandes
14:40 (15' + 5')	A combined experimental and theoretical modeling study on diethoxymethane pyrolysis: unraveling the impact of adding carbon-carbon bonds to oxymethylene ethers	Mr Kevin De Ras, Ghent University, Belgium
15:00 (15' + 5')	Experimental and Theoretical Investigation of Thermal Decomposition of Methyl-2-methyl Butanoate Behind Reflected Shock Waves	Mr Subhadarsi Nayak, Indian Institute of Technology, Madras, India
15:20 (15' + 5')	Revealing H-Abstraction Reactions with Oxygenated Fuels in Shock Tubes by Atomic Resonance Absorption Spectrometry	Ms Fabienne Werner, German Aerospace Center (DLR), Stuttgart, Germany
15:40 (35')	Refreshments	
16:15 (15')	<b>Award of 2022 Polanyi medal to Dr Frédérique Battin-Leclerc</b>	GK Committee Chair, Christa Fittschen and GK2022 Chair, Ian Sims
16:30 (45')	<b>Polanyi Lecture: Chemistry of fuel low-temperature oxidation: recent progress and open questions</b>	Dr Frédérique Battin-Leclerc, CNRS - Université de Lorraine, France
17:15	End of sessions – please be on time for transport to dinner	
<b>18:15-18:30</b>	<b>Buses leave from Place des Lices for Gala dinner at the Chateau d'Apigné</b>	
23:45	Approximate return time	

**Friday September 2, 2022**

Informal tours of the experimental facilities of the Department of Molecular Physics (Laboratory Astrophysics) of the Institut de Physique Rennes will be offered on the morning of September 2 from 10:00 for those who are interested and can stay over. Instructions on how to make your way by public transport will be provided during the meeting, with sign-up at registration and during the meeting.