

Workshop on « Quo vadis theoretical modeling of gas-phase reactions: applications in atmospheric chemistry and climate change »

Workshop Agenda

June 20, 2023 09:00 - 22:30 CEST / Amphi 2301 OU RH (Jardin Botanique)
Montpellier, France

09h00 – 09h30 Onsite registration (Welcome coffee)
09h30 – 09h40 Presentation of the MAK'IT program and venue by MAK'IT

“Atmospheric science and climate action”

Chairwoman : Dr. Bibiana BILBAO

(Professor at the Environmental Studies Department, Simón Bolívar University in Venezuela, and an active Cobra Collective CIC (Community Interest Company), UK member)

09h40 – 09h50 Introduction by the organizers (1st part)
09h50 – 10h30 Dr. Abir HADDAD (virtual)
(Legal Futurist, Founder and director of Institute for Legal Transformation (Bonn), Adjunct Professor, Universität zu Köln)
[Key note talk : "Scarce Global Water Resources: A new methodological interdisciplinary approach to create sustainable regulatory frameworks for future generations by combining comparative law methods and futurism"](#)
10h30 – 10h50 Discussion
10h50 – 11h05 Coffee break
11h05 – 11h45 Dr. Rebecca GARLAND (virtual)
(Professor, University of Pretoria, South-Africa, specialist on atmospheric chemistry with a focus on air quality, climate change, and science-policy linkages)
[Key note talk : "Improving the quantitative evidence base for air quality management in a data scarce region: perspectives from South Africa"](#)
11h45 – 12h05 Discussion
12h05 – 13h30 Reception (lunch)

“Theoretical modeling of gas-phase reactions in different atmospheres”

13h30 – 13h40 Introduction by the organizers (2nd part)

Subsession : “Reactions in planetary atmospheres”

Chairwoman : Dr. Nadine HALBERSTADT

(CNRS Researcher, LCAR-FERMI, University Paul Sabatier, France)

13h40 – 14h10 Dr. Sergey YURCHENKO
(Professor, University College London, UK)
[Title : “Computing molecular line lists for atmospheric applications: completeness versus accuracy”](#)
14h10 – 14h40 Dr. Alejandro RIVERO-SANTAMARIA
(Professor, Laboratoire PhLAM, Université de Lille, France)
[Title : "Ab Initio Molecular Dynamics calculation on NO oxidation over graphite oxides"](#)
14h40 – 15h10 Dr. Jean Christophe TREMBLAY (virtual)
(Professor, University of Lorraine, France)
[Title : "Stochastic Simulations of Energy Exchange at Surfaces"](#)
15h10 – 15h40 Dr. Maikel BALLESTER-FURONES (virtual)
(Professor, Universidade Federal de Juiz de Fora, Brasil)
[Title : "Vibrational relaxation and recrossing effects in the OH + SO → H + SO₂ reaction"](#)

- 15h40 – 16h00 Coffee break
Subsession : “Photochemical reactions: Non-adiabatic dynamics”
Chairman : Dr. Sergey YURCHENKO
(Professor, University College London, UK)
- 16h00 – 16h30 Dr. Sebastian FERNANDEZ-ALBERTI (virtual)
(Professor, Universidad Nacional de Quilmes, Argentina)
[Title : “Vibrational Funnels for Energy Transfer during Internal Conversion in Organic Chromophores”](#)
- 16h30 – 17h00 Dr. Benjamin LASORNE
(CNRS Researcher, Institut Charles Gerhardt Montpellier, France)
[Title : “Variational error in molecular quantum dynamics - a dialog between maths and chemistry”](#)
- 17h00 – 17h30 Dr. Basile CURCHOD (virtual)
(Professor, University of Bristol, UK)
[Title : “Photochemistry from a theoretical and computational perspective”](#)
- 17h30 – 18h30 Cocktail & Poster Session
- 20h00 – 22h30 Social Dinner

*June 21, 2023 09:15 - 12:30 CEST / Amphi 2301 OU RH (Jardin Botanique)
Montpellier, France*

Subsession : “High resolution spectroscopy and reaction dynamics”

- 09h00 – 09h30 Welcome coffee
Chairman : Dr. Benjamin LASORNE
(CNRS Researcher, Institut Charles Gerhardt Montpellier, France)
- 09h30 – 10h00 Dr. Ha TRAN (virtual)
(CNRS Resercher, Laboratoire de Météorologie Dynamique Paris)
[Title : “Collisional effects on the spectral shape and atmospheric remote sensing”](#)
- 10h00 – 10h30 Dr. Nadine HALBERSTADT
(CNRS Researcher, LCAR-FERMI, University Paul Sabatier, France)
[Title : “Dynamics of superfluid helium nanodroplets”](#)
- 10h30 – 11h00 Dr. Marta I. HERNANDEZ-HERNANDEZ
(Researcher, CSIC Madrid, Spain)
[Title : “Attachment of hydrogen molecules to atomic ions: role of the hydrogen rotational states”](#)
- 11h00 – 11h20 Coffee break
- 11h20 – 11h50 Dr. Lidice CRUZ-RODRIGUEZ (virtual)
(Research Fellow, University College London, UK / Assistant Professor, University of Havana)
[Title : “Forward and hybrid path-integral approaches in photoelectron holography”](#)
- 11h50 – 12h20 Dr. Pascal LARREGARAY
(Professor, Diputy director, Institut des Sciences Moléculaires, Université de Bordeaux, France)
[Title : “Recent applications of the statistical approach of reaction dynamics”](#)
- 12h20 – 12h30 Concluding Remarks