



# MLQC4Dyn - Week 4

**Monday September 26 :**

## Approches quantiques dépendantes et indépendantes du temps

**Chair: Nadine Halberstadt**

- 9:00 - 9:30**      **Onsite registration - coffee**
- 9:30 - 9:40**      **Welcome and introduction by the organizers**
- 9:40 - 10:10**      **Fabien Gatti - ISMO, Université Paris-Saclay**  
*Quantum Dynamics with motions of large amplitude*
- 10:10 - 10:40**      **Grégoire Guillon- LICB, Université de Bourgogne**  
*Dynamics in dilute media: quantum clusters & molecular encounters - How may AI help circumvent roadblocks?*
- 10:40-11:00**      **Coffee Break**
- 11:00 - 11:30**      **Dominique Sugny - LICB, Université de Bourgogne**  
*Quantum control in Molecular dynamics: Application to Molecular Rotation and Quantum Technologies*
- 11:30-12:00**      **Ioan Schneider- LOMC, Université du Havre**  
*Études théoriques des collisions électron/cation moléculaires à basse énergie*
- 12:00 - 14:00**      **Lunch Break**
- Chair: Grégoire Guillon**
- 14:00 - 14:40**      **Bruno Senjean - ICGM, Université de Montpellier**  
*Quantum Computing applied to Quantum Chemistry*
- 14:40 - 15:00**      **Coffee break**
- 15:00 - 15:30**      **lei.shi - ISMO, Université Paris-Saclay**  
*Quantum dynamic simulation for H atom scattering from graphene surface*
- 15:30 - 16:00**      **Aliezer Martinez-Mesa- LCAR, Université Paul Sabatier**  
Hydrogen storage in nanoporous materials
- 16:00 - 18:00**      **Group discussions / Round tables**
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Tuesday September 27

## Méthodes pour les approches théoriques des systèmes ouverts

Chair: David Lauvergnat

09:30 - 10:00

Coffee

10:00 - 10:10

Introduction by the organizers

10:10 - 11:00

**Michèle Desouter-Lecomte** - LCP, Université Paris-Sud

*A tribute to Chris Meyer*

11:00-11:20

Coffee break

11:20 - 12:00

**Roberto Marquardt** - LCQ, Université de Strasbourg

*Dynamique quantique de la diffusion thermique d'adsorbats*

12:00 - 14:00

Lunch break

Chair: Fabien Gati

14:00 - 14:40

**Daniel Pelaez-Ruiz** - ISMO, Université Paris-Saclay

*Overview of the recent approaches for the representation of multidimensional operators -*

14:40 - 15:20

**Goulven Quémener**- LAC, Université Paris-Saclay

*Ultracold molecules for collisions, chemistry and control*

15:20 - 15:40

Coffee break

15:40 - 16:20

**Christophe Tremblay**- LPCT, Université de Lorraine

*Stochastic Dissipative Quantum Dynamics*

16:20 - 18:00

Group discussions / Round tables

19:30 - 21:30

Social diner

## Wednesday September 28

### Propriétés électroniques pour la dynamique

	<b>Chair: Ioan Schneider</b>
<b>9:30 - 9:50</b>	<b>Coffee</b>
<b>9:50 - 10:00</b>	<b>Introduction by the organizers</b>
<b>10:00 - 10:40</b>	<b>Mathias Rapacioli - LCPQ, Université Paul Sabatier</b> <i>Some developments for DFTB dynamics and PES exploration</i>
<b>10:40-11:00</b>	<b>Coffee break</b>
<b>11:00 - 11:30</b>	<b>Alexandre Voute- LAC, ISMO, Université Paris-Saclay</b> <i>Cold collisions beyond the Born-Oppenheimer approximation</i>
<b>11:30-12:00</b>	<b>Llinersy Uranga-Pina- LUPM, Université de Montpellier</b> <i>Quantum trajectory modeling of ultrafast molecular dynamics</i>
<b>12:00 - 14:00</b>	<b>Lunch break</b>
	<b>Chair: Goulven Quemener</b>
<b>14:00 - 14:40</b>	<b>Majdi Hochlaf - Université Gustave Eiffel</b> <i>Towards the identification of middle size molecular ions in the gaz phase: Theory, applications and experiment</i>
<b>14:40: 15:00</b>	<b>Coffee break</b>
<b>15:00 - 15:30</b>	<b>A.Rivero Santamaria - PhLAM, Université de Lille</b> <i>High-Dimensional Atomistic Neural Network Potentials to Study Gas- Surface Interactions. Study case: O2 Scattering from Highly Oriented Pyrolytic Graphite.</i>
<b>15:30 - 16:00</b>	<b>Amrenda Pradey- LAC, Université de Paris-Saclay</b> <i>Calculations of atomic and molecular properties of Rb for ultracold molecule collisions</i>
<b>16:00 - 19:00</b>	<b>Group discussions / Round tables</b>

Thursday September 29

## Méthodes semi classiques et approches mixtes

Chair: Laurent Wiesenfeld

9:00 - 9:30

Coffee

9:30 - 9:40

Introduction by the organizers

9:40- 10:20

Stefan Willitsch - University of Basel

*Cold molecular ions in traps: From molecular quantum technologies to precise mechanistic studies of chemical reactions*

10:20 - 11:00

Mario Barbatti - ICR, Université d'Aix-Marseille

*Dynamics for Modeling Molecular Photoprocesses*

11:00 - 11:20

Coffee break

11:20 - 12:00

Nadine Halberstadt - LCAR, Université Paul Sabatier

*Dynamique de dopants dans un environnement très quantique, les nanogouttes d'hélium superfluide*

12:00 - 14:00

Lunch break

Chair: Mathias Rapacioli

14:00 - 14:40

Lucien Dupuy - LUPM, Université de Montpellier

*Multidimensional tunneling from an hybrid quantum-classical trajectory approach*

14:40 - 15:00

Coffee break

15:00 - 15:30

Natasa Nadoveza - ISMO, Université Paris-Saclay

*Analytical high-dimensional operators in Canonical Polyadic Finite Basis Representation (CP-FBR) Natasa Nadoveza, Ramon L. Panades-Barrueta, Lei Shi, Fabien Gatti, and Daniel Pelaez.*

15:30 - 16:00

Guillaume Dhont - LPCA, Université du Littoral Côte d'Opale

*High-resolution spectroscopy and reactivity of molecules of atmospheric interest*

16:00 - 19:00

Dario Roca, Pavlo Dral, Majdi Hochlaf, Bruno Senjan, Mario Barbatti

Concluding remarks-Round table

19:30 - 21:30

Conference diner

