GDR 3575 du CNRS ThéMS
Dynamique quantique dans les systèmes moléculaires. Théorie modélisation simulation.

Editorial :

Voici le deuxième et dernier numéro avant les vacances d'été du bulletin du GDR *ThéMS*. Son intérêt dépend fortement de votre implication. N'oubliez donc pas de transmettre toutes les informations du mois que vous souhaiterez faire connaître aux autres membres du GDR à vos correspondants du bulletin dont les coordonnées sont les suivantes :

* Thème 1: Systèmes moléculaires isolés
  Arnaud Leclerc : arnaud.leclerc@univ-lorraine.fr

* Thème 2: Systèmes moléculaires en présence de champs intenses
  Osman Atabek: osman.atabek@u-psud.fr
  Dominique Sugny : Dominique.Sugny@u-bourgogne.fr

* Thème 3: Systèmes moléculaires environnés
  Sabine Morisset: Sabine.Morisset@u-psud.fr

Vous êtes aussi encouragé à consulter le site du GDR (www.gdr-thems.cnrs.fr/) qui est actualisé régulièrement

Le comité de rédaction du bulletin du GDR Thems recevra avec plaisir tous vos commentaires et suggestions pour améliorer notre bulletin:

Osman Atabek, Arnaud Leclerc, Sabine Morisset, Nadine Halberstadt, Thierry Stoecklin et Dominique Sugny

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Bulletin du mois de Juin 2017

1. Dernières nouvelles du GDR

Appel urgent à candidature :

2 prises en charge complètes des frais afférant à la participation de deux étudiants motivés à l'école MCTDH organisé par Fabien Gatti à Paris-Saclay (25 Septembre- 20 Octobre): https://mctdh.sciencesconf.org/resource/page/id/1 sont proposées. Les étudiants intéressés sont appelés à soumettre leur candidature en envoyant un cv aux correspondants du thème 2 du GDR.

* Les ***Journées Scientifiques du GDR ThéMS*** se tiendront les **16 et 17 novembre 2017 à Metz**. Réservez la date dès à présent. L'appel à contributions sera lancé prochainement.

* Résultats de l'APPEL d'OFFRES 2017 pour le soutien aux conférences

Des subventions de 500 euros par congrès ont été accordées aux Congrès :

* MOLEC2018 : 22nd European Conference on the dynamics of molecular systems, Rennes, 26/08/2018 au 31/08/2018. (Alexandra Viel)

* Théorie et modélisation en Physico-Chimie : de la phase gazeuse vers la phase condensée, Lyon, 9 au 13 Octobre 2017. (Florent Calvo)

* Spectroscopy and Dynamics of Ozone and Related atmospheric species, Reims, 4-6 Octobre 2017. (Vladimir Tiouterev)

* Résultats de l'APPEL d'OFFRES 2017 pour des visites entre équipes du GDR THEMS

Une subvention de 300 euros a été accordée pour un échange entre Arnaud Leclerc et Daniel Pelaez Ruiz.

*** Offres de thèses et de stage post odctoral**

Thème 1:

* A Ph.D. (3 years) position position is available starting September-October 2017, in the theoretical chemistry group of the institut des sciences moléculaires at the University of Bordeaux. The research project will be dedicated to the theoretical study of Interactions of cold and trapped negative hydrogen molecular ions in ion traps. Both the radiative association and the inelastic processes will be considered. This research project (Cold HMINUS) is funded by the French Agence Nationale de la Recherche and by the Austrian Science Fund (FWF). It gathers the experimental team of Roland Wester in Innsbruck and the theoretical teams of Olivier Dulieu in Orsay and Thierry Stoecklin in Bordeaux. The sucessful candidate will then benefit from this collaborative environment.

Requirements:

Applicants for the Ph.D. position should have a MSc degree or equivalent degree in Physics, Chemical Physics, or Applied Mathematics. Experience with computational research and/or computer programming will be counted as advantages. The position is open to all nationalities. Applicants should have experience with either electronic structure calculations or quantum dynamics calculations.

Appointment:

The appointment will be for an initial period of 3 years. The envisaged starting date is anywhere between 1 September 2017 and 1 October 2018.

Applications:

To be considered for the project, applicants should send an application letter and CV, and should arrange themselves that two letters of recommendation are sent to Dr. Thierry Stoecklin, by email (thierry.stoecklin@u-bordeaux.fr) Selection of candidates will start on July 15, 2017 and will continue until the position is filled.

2. En dehors du GDR:

Congrés , Ecoles et Colloques

Thème 1:

*** 3-d International Workshop"Spectroscopy and Dynamics of Ozone and Related Atmospheric Species"** October 4-6, 2017 - Reims, France

Contributions will take the form of oral presentations and will cover the following topics:

- Laboratory measurements (IR , MW, UV ranges) and spectral analyses of ozone and of molecules involved in the ozone atmospheric cycle.

- Electronic structure calculations, potential-energy, dipole moment surfaces and non-adiabatic effects in ozone.

- Theoretical models for describing the ozone rovibrational states.

- Ozone dynamics: formation, decomposition, and photodissociation.

- Isotopic effects in ozone.

- Chemical reactivity along the ozone cycle, in situ atmospheric balloon and satellite measurements.

- Databases related to ozone spectroscopy and dynamics.

Abstract submission until July 10th, 2017 , Inscription until September 10th, 2017

www.univ-reims.fr/ozone2017

***2nd European Conference on Physical Chemistry ECPC'17**

24-27 septembre 2017 - Borgo, France

The 2nd European Conference on Physical Chemistry, sponsored by the Division of Physical Chemistry of EuCheMS, will be held during September 24-27, 2017 at Borgo in Corsica (France). ECPC is an international interdisciplinary conference uniting physical chemists from different fields:

-Photochemistry

-Magnetism and Magnetic Resonance

-Nanosciences

-Modelling and Simulation

-Optical and Neutronic Spectroscopies

-Electrochemistry

-Analytical Chemistry

-Radiation Chemistry and Radiochemistry

Registration until June 30th 2017 ecpc17.com

* **16th International Congress of Quantum Chemistry** June 18-23, 2018 - Menton, France

The International Congress of Quantum Chemistry (ICQC) has been held every three years under the auspices of the International Academy of Quantum Molecular Science (IAQMS) since 1973. It brings together the international community of theoretical chemists in the form of a one-week conference aimed at presenting the state of the art and latest advances in terms of developments and applications in the field of theoretical and computational chemistry. The 16th ICQC will be held in 'le Palais de l'Europe' in the town of Menton, France, from Monday June 18th afternoon to Saturday June 23rd early afternoon, 2018. A single-session format will allow the audience to follow the entire program. Every talk will be invited and all other contributions will be presented as posters.

Pre-registration open : icqc16.sciencesconf.org

*** Conference on Quantum Information and Quantum Control VII** , August 28 to September 1, 2017 , Toronto, Canada

CQIQC-VII is the seventh in the series of biennial conferences jointly organized by the Toronto Center for Quantum Information & Quantum Control and the Fields Institute, which aim to bring together researchers from a broad set of areas ranging from quantum cryptography and computation to quantum control to quantum foundations to device fabrication, in a setting which encourages discussion and can help stimulate new collaborations and interactions.

Submissions until June 30th, 2017 www.fields.utoronto.ca/activities/17-18/CQIQCVII

Thème 2:

*** International Conference on Quantum Simulation, ICQSIM 2017**, that will take place at Ecole Normale Supérieure in Paris, France, from the 13th to the 17th of

November, 2017.

ICQSIM 2017 will present an up-to-date perspective on the thriving field of quantum simulation. The scientific program will combine invited tutorial talks by prominent specialists of the field, contributed talks, poster presentations and a round table discussion. The conference is organized jointly by the European integrating project RySQ, and the French networks SIRTEQ and GDR Atomes Froids.

Website : https://icqsim2017.sciencesconf.org/
Deadline for abstract submission: 10 July 2017

*** DIADEMS & SIRTEQ Quantum Technologies Workshop, 14-15 Sept. 2017, Paris-Palaiseau (France)**
The European FP7 project DIADEMS (DIAmond Devices Enabled Metrology and Sensing) and the French regional project SIRTEQ (Science and Engineering for Quantum Technologies in the French region of Ile-de-France) are organising a joint industry-orientated workshop bringing together some of the most prominent stakeholders in the field of Quantum Technologies. The event will take place on 14 15 September 2017 at Thales Research & Technology, in Palaiseau (Parisian area), France. The objective of this workshop is to provide a platform for knowledge exchange, discussion and networking between academic and industrial communities interested in the huge potential of quantum technologies, and to help them build collaborations in view of the upcoming Quantum Technology Flagship. Therefore, both academic and industrial participants are most welcome.

The event will cover the four pillars of the QT Flagship, while putting additional focus on enabling technologies.

REGISTER NOW: To register to the workshop (deadline: 15 June 2017), please go to the event website, where you can also find complementary information, as well as the preliminary program.
https://cmt.eurtd.com/events/event/view/18354/diadems-sirteq-quantum-technologies-workshop
To find out more about the organising projects, visit their respective project websites: DIADEMS, SIRTEQ (coming soon).

* **Advanced Optical Spectroscopies** in Paris-Saclay» (AOSPS2017) qui auront lieu les 29 et 30 novembre 2017 à l'Université Paris Sud.
Ces journées sont organisées dans le cadre du projet "Multi-scale physical chemistry" (PhyChiM^3) élaboré au printemps 2016, en réponse à l'appel à projet "Initiatives de Recherche Stratégiques 2016" (IRS) de l'IDEX Paris-Saclay. Elles sont financées par les départements de Chimie et SDV de l'IDEX.
Ces journées ont pour but de rassembler l'ensemble de la communauté scientifique autour des thématiques abordées par le projet PhyChiM^3 :

- **La spectroscopie bi-dimensionnelle**

- **Le dichroïsme circulaire**
- **La dynamique conformationnelle des systèmes complexes**

Ces journées ont pour objectif de favoriser les échanges et la réflexion sur les récentes avancées expérimentales et théoriques autour de ces thématiques. Elles seront aussi l'occasion de donner un aperçu des activités du campus Paris-Saclay, afin d'amorcer de nouvelles collaborations.

Les sessions s'articuleront autour de 5 conférences plénières d'invités de renommée internationale :

· Thomas Baumert (Kassel)
· Valérie Blanchet (Bordeaux)
· Tobias Brixner (Würzburg)
· Rienk van Grondelle (Amsterdam)
· Jennifer Ogilvie (Michigan).

Nous vous invitons à vous inscrire et soumettre vos contributions dès à présent sur le site :
http://iramis.cea.fr/meetings/2DDC2017/index.php

Nous souhaitons favoriser la participation des jeunes chercheurs à présenter leurs travaux. L'inscription est gratuite et comprend les déjeuners.

Nous comptons sur votre participation.

Thème 3 :

* **Paris-Est Summer School " Environmental physics: theory and instrumentation**." From July 3th through July 13th 2017.

http://summerschool.u-pec.fr/welcome/

* **2017 meeting of the Southern Universities Spectroscopy and Dynamics group** to be held in Bristol across the 7th-8th of September

http://www.bristoldynamics.com/susdg2017/

3) **The 22nd European Conference on Dynamics of Molecular Systems, MOLEC 2018**, will be held

in the sea-side resort of Dinard, France, from the 26th to the 31st of August 2018 : https://molec2018.sciencesconf.org

Offres de thèse et de stages post doctoraux:

Thème 2 :

A postdoctoral position is available in the group of Uwe Thumm for a young theorist with experience in theoretical AMO physics or theoretical surface/nanoplasmonic physics at the KSU physics department. Uwe Thum is looking for a talented AMO researcher to work in the area of intense-field light-induced ultrafast dynamical processes in matter who will vigorously participate in emerging research on *time-resolved photonic interactions with surfaces and plasmonic nanoparticles*. The preferred start date is September 1, 2017.

Thème 3 :

1) Electron-Molecule Collisions: Study of the Reactive Mechanisms and Applications.

Doctoral School: Physics, Engineering, Materials, Energy (PSIME), Normandie Université.

Research group: 'Reactive Processes', LOMC-UMR-6294, Université du Havre Normandie.

Supervisor: Ioan F. SCHNEIDER, Université du Havre Normandie
: ioan.schneider@univ-lehavre.fr
Co-supervisor: Arnaud BULTEL, CORIA-UMR-6614, Université de Rouen Normandie.

Sponsor: Normandy region (La Région Normandie).

Key words: reactive collisions, dissociative recombination, rate coefficients, quantum methods, plasmas, kinetics, collisional-radiative model.

Context and motivation:
The electronic collisions are major processes in the plasmas of hypersonic entries of spacecrafts in the planetary atmospheres, in the edge of the fusion plasmas, in the interstellar molecular clouds, flames and ionic propulsion plasmas [1]. Sophisticated experiments measuring the rate coefficients of these processes are supported and extended by quantum state-to-state computations, in order to deeply understand the role of these collisions in the kinetics and hydrodynamics of the invoked environments, and in order to fill the data bases (NIST, ADAS, UMIST, KIDA, etc.) in view of detailed modelling.

Objectives of the doctoral work:
We will study the collisions between electrons and molecules – neutral and ionized - in particular the Hydrogen (molecular benchmark), the hydrides – containing Oxygen, Carbon, Argon, metalic elements, etc. – and species containing halogenes or Sulphur. Three activities will be simultaneously developped. The first one will be the production of molecular structure data – potential energy curves and inter-channel

couplings – by using quantum chemistry and R-matrix methods. The second one will be the modelling of the reactional dynamics (recombination, attachement, dissociation,ionization, excitation) by collisional methods and theoretical spectroscopy methods. And finally the third will be
that of the use of the rate coefficients in the kinetic models.

Methodological details:
Many of the reactions invoked occur simultaneously and, consequently, are in mutual competition. They are complex processes, where the super-excited states amplify resonantly the excitation, the ionization and the dissociation. Several fragmentation continua – electron/molecule, atom/atom, etc. and several infinite series of bound states overlap. Our methods are the only capable to manage this complexity, and to link it to the kinetic models. They are based on the Multichannel Quantum Defect Theory (MQDT) [2-6], on the R-matrix theory [7] and on the Configuration Interaction theory [8]. The kinetics driven by these processes will be described by collisional-radiative models [9].

Collaborations :
In France:
Laboratories CORIA (Rouen), LSPM (Villetaneuse), Aimé Cotton (Orsay), LPP (Ecole Polytechnique), Ecole Centrale de Paris, IPAG (Grenoble), LUPM (Montpellier).
Abroad:
University College London, University of Central Florida Orlando, University of California – Davis, Max-Planck-Institut für Kernphysik - Heidelberg, Stockholm University, Politecnico and Aldo Moro University - Bari, University of Calcutta, University of Douala, University of Burundi, Politehnica University and West University of Timisoara, Tunis El Manar University.

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