



Éditorial :

Ce premier numéro du bulletin du GDR *ThémS* de l'année académique 2017-2018 se situe peu de temps avant notre réunion annuelle qui aura lieu à Metz les 16 et 17 Novembre (<http://www.gdr-thems.cnrs.fr>). A cette occasion la participation de nos collègues doctorantes, post-doctorantes, chercheuses et enseignantes-chercheuses est particulièrement encouragée, de sorte que le programme scientifique reflète les engagements pris par le CNRS en signant la charte sur la parité proposée notamment par la Société Française de Physique (<https://www.sfpnet.fr/charte-de-parite-pour-les-conferences-scientifiques>).

Une table ronde sera organisée durant notre réunion afin d'échanger avec vous des améliorations que vous souhaiteriez pour notre bulletin. Toute suggestion sera la bienvenue.

Nous vous rappelons par ailleurs que l'intérêt de notre bulletin 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

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* Thème 3: Systèmes moléculaires environnés

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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 Thèmes 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

Bulletin du mois d'Octobre 2017

1. Dernières nouvelles du GDR

Congrès , Ecoles et Colloques

* Derniers jours pour s'inscrire aux **Journées Scientifiques du GDR Thèmes** qui se tiendront les **16 et 17 novembre 2017 à Metz**. (la date limite d'inscription est le mardi 10 Octobre 2017)

<http://www.gdr-thems.cnrs.fr>

*** 22nd International Few-Body Conference FB22 (9-13 July 2018, Caen, France)**

The next International Conference on Few-Body Problems in Physics (FB22) will be held in Caen, France from 9 to 13 July next year. This will be the 22nd edition of this conference series which began in 1959 in London and was most recently held in Chicago in 2015 and Fukuoka in 2012. Following tradition FB22 will be an interdisciplinary conference covering a very wide range of aspects of few-body problems in diverse fields of physics – both from the theoretical and experimental points of views, including:

- * Atomic and molecular physics.
- * Hadron physics and related high-energy physics.
- * Strange and exotic matter, including hypernuclear physics.
- * Few-nucleon systems.
- * Few-body aspects of nuclear physics and nuclear astrophysics.

<https://fb22-caen.sciencesconf.org/>

* Offres de thèses et de stage post doctoral

Thème 1:

* A Ph.D. (3 years) 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 successful 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 continue until the position is filled.

Thème 3:

Post doctoral position dedicated to High energy controlled attosecond pulses

Centre Lasers Intenses et Applications
UMR5107 - Université de Bordeaux - CNRS - CEA
351 Cours de la Libération – 33405 Talence Cedex



<http://www.celia.u-bordeaux1.fr>

Contact Person:

Pr Eric Mével (director of CELIA) or Dr Constance Valentin

Email: eric.mevel@u-bordeaux.fr; constance.valentin@u-bordeaux.fr

Phone: +33 (0)5 40 00 37 75; +33 (0)5 40 00 25 86

Practical information:

The post-doctoral position is granted for eighteen months. The monthly salary depends on the applicant qualification and is between 2,056-2,373 net euros for less than 2 years after Ph. D. defense applicants and 3,108 net euros after. Immediate starting is possible. We will review applications until the position is filled.

Key words:

High power short pulse laser, high order harmonic generation in gases, attosecond XUV pulses, temporal, spatial and polarization shaping, non linear processes, molecular dynamics.

Application deadline is December 31, 2017.

Project description:

The project takes place within the CIRCÉ (Correlation Induced Relaxation dynamics in Complex XUV-Excited molecules) ANR project associating the CELIA (Bordeaux), ILM (Lyon) and LPT (Toulouse) laboratories. The goal of the CIRCÉ project is to exploit the opportunities offered by controlled ultrashort extreme ultraviolet (XUV) pulses to investigate the role played by the many-body nature of molecular wavefunctions on the stability of complex molecular systems [1]. At Celia, development of well controlled XUV attosecond pulses is the milestone of this novel research domain. The open position is strongly linked to CELIA laboratory expertise, i.e. producing, characterizing and using high energy attosecond XUV pulses produced from multi-dimensionally shaped intense femtosecond laser pulses of a TW class laser system (ECLIPSE laser at CELIA) [2]. Post-compression of femtosecond pulses at the TW level was investigated and 10 fs, 10 mJ post-compressed pulses were achieved [3]. Source characteristics such as XUV tunability, stability, focusing and accordability of the XUV pulse duration will be studied before performing XUV pump-probe experiments.

Single-shot characterization is also possible to control CEP dependent spatio-temporal characteristics of attosecond pulses. Collaborative and complementary works at both experimental locations (CELIA and ILM laboratories) are planned. The applicant will also take benefit from collaborations with other groups worldwide.

Recent related publications:

[1] F. Lepine et al., *Attosecond molecular dynamics: fact or fiction?*, Nat. Phot. **8**, 195-204 (2014)

[2] A. Dubrouil et al., *Spatio-spectral structures in high-order harmonic beams generated with Terawatt 10-fs pulses*, Nat. Com. **5**, 4637 (2014)

[3] O. Hort et al., *Postcompression of high-energy terawatt-level femtosecond pulses and application to high-order harmonic generation*, JOSAB **32**, 1055-1062 (2015)

Competence requirements:

Experience in high harmonic generation, characterization of ultrashort laser pulses and VUV/XUV radiation in general will be appreciated. The applicant should be highly motivated and have a strong interest for state of the art laser technology and ultrafast science. Interests and skills in molecular physics will also be advantageous. The candidate must have the ability to work independently as well as a part of the research group.

Application

The application should include:

1. A cover letter with a brief description of qualifications, research interests, experiences, and motivation (max 2 pages).
2. Curriculum vitae.
3. Copies of relevant degree diploma(s).
4. At least one reference contact person.

2. En dehors du GDR:

Offres de thèse et de stages post doctoraux:

Thème 2:

The Dynamics at Surfaces department of Alec M. Wodtke at the Max-Planck-Institute for Biophysical Chemistry in Goettingen is looking for candidates to fill two open PhD positions.

The aim of the department is to gain a detailed understanding of the fundamental physical and chemical processes occurring at surfaces and providing benchmark data for testing and validation of theoretical models. Theoretical understanding of surface chemistry will eventually become a tool to design new chemical technology including: heterogeneous (photo) catalysts, photovoltaics, fuel cells and much more. To reach this goal, we require new ideas and new theories of molecular interactions at interfaces. Applying cutting-edge laser, molecular beam, and ultrahigh vacuum technology to design well-defined experiments that can catch molecules in the act of reacting, our group strives to provide benchmark measurements which set standards for the next generation of theoretical advance. In particular, we seek to discover the "rules" that govern the conversion of energy at interfaces. Although too small to see with the naked eye and too fast to follow except with the fastest pulsed lasers, energy conversion takes place one molecule at a time and one collision at a time. By isolating these individual energy conversion events and studying them, we are building the conceptual bridge connecting our macroscopic experience of energy conversion to the molecular world. Candidates will be involved in a recently founded highly ambitious research project aimed to investigate chemical reactions at surfaces on a picosecond time scale. The experimental work will involve the production of ultra-short atom pulses and the study of their interaction with photo-excited surfaces under ultra-high vacuum conditions using short-pulse lasers. Potential candidates should have bachelor or master degree in chemistry, physical chemistry, physics or a related subject. Experiences in working with high power short-pulse laser, optics, programming and vacuum technologies are advantageous. Candidates with bachelor degree will have the opportunity to receive their Master degree with the prospect to continue their research as a PhD student.

The payment and benefits for PhD candidates are based on the TVÖD guidelines. The position are supposed to be filled as soon as possible from October 2017.

Detailed information are available under the following link:

<http://www.mpibpc.mpg.de/15742085/30-17>

Post-doc (2 years) position in theory of molecule-surface interactions at Leiden University.

A post-doc (2 years) position is available starting November 1st 2017, in the theoretical chemistry group of Leiden University (NL).

The research of the post-doc will focus on applying the quantum-Monte Carlo (QMC) electronic structure method to molecules reacting with transition metal surfaces. First results for $H_2 + Cu(111)$ are encouraging, with the Diffusion Monte-Carlo barrier height differing from the semi-empirical SRP-DFT reference value by just 1.6 kcal/mol (see *J.Chem.Theory Comput.*13, 3208, 2017). We will be applying the QMC method to a few other systems, and will try to improve the accuracy of our implementation. The project is funded by NWO, under an NWO/EW TOP grant for Geert-Jan Kroes. The post-doc will be employed by Leiden University.

Requirements:

Applicants should have experience with quantum Monte-Carlo calculations in general, or with electronic structure calculations on molecules interacting with metal surfaces, or with dynamics calculations on such systems. The candidate should have a Ph.D. in Chemistry, Physics, or Applied Mathematics. Experience with using QMC, computer programming, and with running calculations on parallel computers will be counted as advantages. The position is open to all nationalities.

Appointment:

The appointment will be for an initial period of 1 year with extension possible to 2 years. The envisaged starting date is anywhere between 1 November 2017 and 1 March 2018.

Applications:

To be considered for the project, applicants should send an application letter and CV, and should arrange themselves that three letters of recommendation are sent to Prof. Dr. Geert-Jan Kroes, by email (g.j.kroes@chem.leidenuniv.nl), preferably by October 15. Note: it is not enough to provide the names of referees, the applicants should arrange and ensure themselves that letters of reference are sent. Selection of candidates will start on October 15, 2017 and will continue until the position is filled.

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Thème 3:

A PhD student position in the field of ultrafast photochemistry is open in the group of Prof. Eric Vauthey at Department of Physical Chemistry of the University of Geneva. Information about the research of the group can be found on the following webpage:

(<http://www.unige.ch/sciences/chifi/Vauthey>).

Topic: Ultrafast excited-state dynamics of molecular probes and of photochemical processes at liquid-liquid interfaces investigated using nonlinear optical spectroscopy. Information on this research area can be found in the following publications:

1) Fedoseeva, M.; Richert, S.; Vauthey, E., *Langmuir* **2012**, 28, 11291 2) Licari, G.; Brevet, P.-F.; Vauthey, E., *Phys. Chem. Chem. Phys.* **2016**, 18, 2981.

Profile: Master degree in chemistry or physics. Preference will be given to candidates with experience in ultrafast spectroscopy, interfaces or photochemistry. The position requires a high motivation to work in an interdisciplinary environment. The successful candidate will benefit from an excellent research infrastructure and will be exposed to a large variety research activities in the field of molecular excited- state dynamics and photochemistry.

Start: November 2017 or later **Duration:** 4 years (the first year is a trial period).
Salary: from SFr. 47'000.- per year.

Application: the application should include: - a letter of motivation - a curriculum vitae - the marks of all university classes - two letters of reference

Contact information:

Prof. Eric Vauthey Dpt. of Physical Chemistry 30, Quai Ernest-Ansermet CH-1211 Genève 4



GDR 3575 du CNRS ThéMS

Dynamique quantique dans les systèmes moléculaires. Théorie modélisation simulation.



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