

Bulletin de Noël 2017

Editorial

Ce dernier numéro du bulletin du GDR ThéMS de l'année 2017 fait suite à notre réunion annuelle qui a eu lieu à Metz les 16 et 17 Novembre. La réunion annuelle du GDR a maintenant un public fidèle et cette édition organisée par nos collègues messins était particulièrement réussie. Vous trouverez ci-joint un compte rendu des échanges que nous avons eu lors de la séance de table ronde dont certains à propos du contenu du bulletin. Nous souhaitons que son fonctionnement soit plus interactif et nous avons décidé comme vous l'avez peut-être noté, de faire un appel à contribution quelque temps avant chaque nouvelle édition du bulletin afin de donner à chacun(e) la possibilité d'informer notre communauté de réunions, soutenances, offres de thèse ou post-doc mais aussi de ses dernières recherches en envoyant simplement titre et auteurs de publications récemment acceptées. Ces dernières seront présentées dans la nouvelle rubrique Actualité éditoriale.

Nous vous encourageons à utiliser largement cette possibilité en 2018. N'oubliez donc pas dès la réception de l'appel à contribution au bulletin de transmettre toutes les informations du mois que vous souhaitez 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 et vous souhaite ses meilleurs vœux pour vos recherches en 2018 : Osman Atabek, Arnaud Leclerc, Sabine Morisset, Nadine Halberstadt, Thierry Stoecklin et Dominique Sugny

Dernières nouvelles du GDR

Journées du GDR

Journées du GDR ThéMS à Metz les 16 et 17 novembre 2017

Cette édition organisée à Metz par Ugo Ancarani, Francesca Ingrosso, Arnaud Leclerc, et leur équipe administrative a connu un franc succès. Merci à tous et à toutes.

Le programme scientifique de la réunion ainsi que les interventions peuvent être téléchargés sur le lien suivant jusqu'au 12 Janvier 2018.

<https://filesender.renater.fr/?s=download&token=d7d56d75-3e12-8d52-0d38-936954f484e4>

Lors de la table ronde, les sujets suivants ont été abordés :

Bulletin du GDR

Les propositions pour rendre son fonctionnement plus interactif ont été adoptées et vous recevrez systématiquement un appel à contribution quelques temps avant la parution de chaque numéro. Vous trouverez d'autre part une nouvelle rubrique dans notre bulletin intitulée Actualité éditoriale que vous êtes invité à enrichir.

Parité Femme/Homme au sein du GDR

Le GDR soutient la Charte de parité pour les conférences scientifiques. A l'occasion des Journées du GDR ThemS, la question de la place des femmes en Physique a été abordée lors d'une table ronde. En outre, suite à l'appel des organisateurs pour encourager la participation des femmes aux Journées, 5 des 22 exposés ont été donnés par des doctorantes, post-doctorantes, chercheuses ou enseignantes-chercheuses. Après un débat sur la proportion femmes/hommes dans notre GdR (autour de 25%, c'est-à-dire un peu mieux qu'en commission 04 du CNRS où elle est de 20% mais moins qu'en 13 où elle est de 37,5%), il est décidé d'organiser une introduction aux stéréotypes de genre lors des prochaines Journées du GdR, comme première étape qui pourrait nous aider à identifier les freins inconscients, extérieurs ou personnels, aux carrières des femmes.

Journées du GDR 2018

Les prochaines Journées du GdR auront lieu à Dijon, comme cela avait été prévu l'an dernier. Elles seront organisées par Grégoire Guillon, Pascal Honvault, Maxence Lepers et Dominique Sugny.

D'autres suggestions d'actions sont faites:

- Organiser une Ecole thématique du CNRS ou un tutoriel CECAM
- Organiser une réunion commune avec un GdR dont la thématique nous est proche (QDyn, CORREL)
- Prévoir une forme de participation au congrès 2019 de la SFP à Nantes

Points divers

Le Réseau Femto du CNRS (<http://reseau-femto.cnrs.fr/>) informe que toute personne intéressée par ce domaine de recherche peut s'abonner à sa liste de diffusion à l'adresse suivante :

https://listes.services.cnrs.fr/www/subrequest/reseau_femto

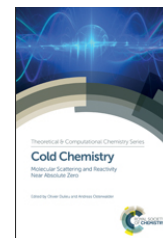
Actualité éditoriale

Livres

Parution du livre "Cold Chemistry : Molecular Scattering and Reactivity Near Absolute Zero"

Trois membres du GDR sont impliqués dans ce nouveau livre : Olivier Dulieu en est co-éditeur ; Maxence Lepers et Goulven Quémener y ont également contribué.

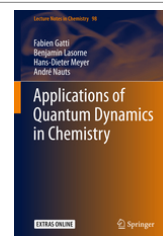
En savoir plus : Cold Chemistry : Molecular Scattering and Reactivity Near Absolute Zero, Olivier Dulieu, Andreas Osterwalder, The Royal Society of Chemistry (2018) ISBN 978-1-78262-597-1.



Parution du livre "Applications of Quantum Dynamics in Chemistry"

par Fabien Gatti, Benjamin Lasorne, Hans-Dieter Meyer and André Nauts

En savoir plus : <http://www.springer.com/gp/book/9783319539218>



Publications

Exotic states in the strong-field control of H_2^+ dissociation dynamics: from exceptional points to zero-width resonances

Arnaud Leclerc, David Viennot, Georges Jolicard, Roland Lefebvre and Osman Atabek, J. Phys. B, 50, 234002 (2017). *Special Issue: Jubilee Issue on Hydrogen: a Fundamental System in All States*

High Resolution Molecular Spectroscopy for Producing Ultracold Absolute Ground-State $^{23}\text{Na}^{87}\text{Rb}$ Molecules

Mingyang Guo, Romain Vexiau, Bing Zhu, Bo Lu, Nadia Bouloufa-Maafa, Olivier Dulieu, Dajun Wang, Phys. Rev. A, 96.052505 (2017)

Anisotropic polarizability of erbium atoms

Jan Hendrik Becher, Simon Baier, Kiyotaka Aikawa, Maxence Lepers, Jean-François Wyart, Olivier Dulieu, Francesca Ferlaino, Phys. Rev. A, accepted (arXiv:1710.07162)

Dynamic dipole polarizabilities of heteronuclear alkali dimers: optical response, trapping and control of ultracold molecules

R. Vexiau, D. Borsalino, M. Lepers, A. Orbán, M. Aymar, O. Dulieu & N. Bouloufa-Maafa, Int. J. Phys. Chem. 36, 709 (2017)

Annonces

Congrès, écoles et colloques

FB22 : International Conference on Few -Body Problems in Physics (9-13 juin 2018, Caen)

The next International Conference on Few-Body Problems in Physics 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 May 2015 and Fukuoka in August 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/>

MOLEC22 (26-31 août 2018, Dinard)

La vingt-deuxième édition du congrès « European Conference on the Dynamics of Molecular Systems » sera organisée à Dinard par nos collègues rennais du 26 au 31 août 2018. The aim of this conference series is to highlight experimental and theoretical aspects of atomic and molecular interactions. At MOLEC 2018, the focus will be on the following, non-exhaustive, list of topics:

- * Molecular collisions
- * Fundamental problems in molecular dynamics
- * Ultracold atoms and molecules
- * Molecular dynamics in condensed phases
- * Photon-matter interactions
- * Astrophysics and astrochemistry
- * Atmospheric chemistry
- * Femtochemistry
- * Coherent control of molecular processes

The conference format will be comprised of invited lectures, oral communications and poster presentations. For updated information, please visit

<https://molec2018.sciencesconf.org/>

MES : Molecular Electronic Structure (28-31 août 2018, Metz)

La prochaine édition de la conférence Molecular Electronic Structure (MES) sera organisée à Metz du 28 au 31 août 2018. The MES conference attracts about 100 scientists from all over the globe who work actively in the field of molecular electronic structure and related areas.

Previous editions were held in Cannakale, Turkey (2012), Amasya, Turkey (2014), and Buenos Aires, Argentina (2016).

The dedicated webpage is: <https://mesm.event.univ-lorraine.fr/>

and the conference contact email is: mes2018-contact@univ-lorraine.fr

Ecole « Mathematics in electronic structure theory of the GDR CORREL » (16-18 avril 2018, Paris)

We are glad to announce the second edition of the Mini-school that will be held in Paris (Jussieu campus) on the 16th, 17th and 18th of April 2018. The lectures delivered are intended to be of interest to any person working in the field of electronic structure theory and molecular dynamics and willing to discover or deepen the mathematical aspects of the methods. Master and PhD students, post-docs and any academic are welcome! To provide a detailed presentation of subjects, we have chosen to give a good amount of time to each lecturer. At this new edition two 9h-long lectures will be proposed:

- 1) "Stochastic methods for electronic structure theory and molecular dynamics" (9 hours)
by Tony Lelièvre, Ecole des Ponts and INRIA, Paris, France
- 2) "Fourier and Laplace transforms, and applications" (9 hours)
by Eric Cancès, Ecole des Ponts and INRIA, Paris, France

If you are interested and willing to participate, please register by sending an email at minischool2018@lct.jussieu.fr and indicate:

- your name and affiliation;
- whether you want to participate in group lunches the 3 days;
- whether you are a CNRS staff.

Important: To facilitate the participation of young researchers, no registration fees will be asked. We may also help with housing in student-type accommodation depending on the demands. If you are not registered to the GDR CORREL, we also invite you to do so on our web site: <http://gdrcorelec.ups-tlse.fr/NouvelUtilisateur.py> in order to be informed about the different events.

If you have any questions, do not hesitate to send an email to: minischool2018@lct.jussieu.fr

Atelier « Long range interactions in quantum systems » (25-28 juin 2018, Hannover, Allemagne)

This is the fifth in a series of conferences that is scheduled to run annually to biannually. The previous workshops were held in Stuttgart, Germany 2013, Palaiseau, France 2014, Naples, Italy 2016, Bad Honnef Germany 2017. For more information please visit

<https://www.for2247.uni-hannover.de/18workshop.html>

Registration and Abstract Submission via this website will open in January 2018. The 2018 workshop will focus on dipolar few and many-body quantum systems enriched by a discussion of a wider range of long-range interactions.

Quantum Technology Conference (EPE104) at Photonics Europe (22-26 avril 2018, Strasbourg)

You can submit an abstract online at <http://www.spie.org/EPE104>

Offres de thèses

Bonn, Allemagne (Thème 1)

Computational chemistry

The group of Prof. Dr. Barbara Kirchner has currently a PhD position open in computational chemistry.

The position is part of the following network:

<https://lnkd.in/g/hrS2vZ>; <http://etn-socrates.eu/>; (<https://lnkd.in/gt3tDDh>)

If the applicant wants to know about what we are doing:

<https://lnkd.in/g/yA7zF9>; <https://lnkd.in/g/B9fV8w>

Interested candidates can contact Prof. Kirchner via email (kirchner@thch.uni-bonn.de).

Leiden, NL (Thème 3)

Theoretical chemistry

A Ph.D. (4 years) position is available starting February 1st 2018, in the theoretical chemistry group of Leiden University (NL). The research will address a number of issues in dynamics of molecules reacting on metal surfaces. Goals are to establish what effects surface phonons and electron-hole pair excitation may have on the dynamics of reactive scattering of H₂ from metal surfaces. We will also attempt to determine accurate reaction barrier heights for the reaction of polyatomic molecules with metal surfaces, through ab initio molecular dynamics and the specific reaction parameter (SRP) approach to density functional theory. Furthermore, we will investigate the transferability of SRP density functionals among systems in which one and the same molecule interacts with smooth low index surfaces and with defected surfaces of one and the same metal. The project is funded by NWO, under a CW-TOP grant for Geert-Jan Kroes. The Ph.D. student will be employed by Leiden University.

Requirements: Applicants for the Ph.D. position should have a MSc or equivalent degree in Chemistry, Physics, or Applied Mathematics. Experience with computational research and/or computer programming will be counted as an advantage. The position is open to all nationalities.

Appointment: The appointment will be for an initial period of 1 year with extension possible to 4 years, which is the standard time allotted to Ph.D. research in The Netherlands. The envisaged starting date is 1 February 2018, with flexibility towards later starts.

Applications: To be considered for the project, applicants should send an application letter and CV, and should ensure themselves that two letters of recommendation are sent to Prof. Dr. Geert-Jan Kroes, by email (g.j.kroes@chem.leidenuniv.nl). Selection of candidates will start on December 17, 2017 and will continue until the position is filled.

Basel, Suisse (Thème 3)

Computational chemistry

Applications are invited for PhD positions in theoretical and computational chemistry in the group of Markus Meuwly in the Department of Chemistry at the University of Basel, Switzerland. The appointment is within the established National Competence Center of Research (NCCR) on Molecular and Ultrafast Science and Technology, see <http://www.nccr-must.ch/home.html>

Candidates should have a degree in Chemistry, Physics, Mathematics, or related fields. The main theme of our research is to develop and apply state-of-the-art computational tools to characterize and understand the structure and dynamics of molecular systems in the gas- and condensed phase through direct contact with experiments. In particular we use and implement methods to accurately represent intermolecular interactions and use them in classical molecular dynamics and quantum dynamics simulations, depending on the system of interest. For more information see <http://www.chemie.unibas.ch/~meuwly/>

Offres de stages post doctoraux

Toulouse (Thème 1)

A two years' post doctoral fellowship is currently available at LCPQ (Laboratoire de Chimie et Physique Quantiques, Université Paul Sabatier, Toulouse, France) within the framework of the ANR-16CE290025 PACHYNO (Probing the diversity of Astrophysically relevant Carbon and HYdrogen NanOparticles, <http://www.lcpq.ups-tlse.fr/anr-pachyno/>) coordinated by C. Falvo (ISMO, Orsay). The project relies on the best use of state-of-the-art computational and experimental approaches and their synergy to study the spectroscopic response of hydrocarbon molecules present in the interstellar medium. It involves teams at ISMO (Orsay, C. Falvo & Th. Pino), LiPhy (Grenoble, F. Calvo) and LCPQ (Toulouse, A. Simon). The applicant should have a solid background in physics and chemistry with experience in computer simulation and quantum chemistry, and possess a solid track record of research accomplishments. Experience in using computational tools (elaboration of scripts in bash, python...) to run extensive simulation and post processing is required. Knowledge in astrochemistry is a plus, but is not required. The ability for programming (the deMonNano code is in Fortran language) is also a plus, but is not mandatory.

The starting date is January 1st, 2018, but can be adapted. The salary should be about 2.5 k€ per month. Applications should be sent by email to Aude Simon (aude.simon@irsamc.ups-tlse.fr). They should include:

- 1- An up-to-date CV with publication list
 - 2- Two letters of reference from academic supervisors or current employers (to be sent via email directly to aude.simon@irsamc.ups-tlse.fr)
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Paris-Saclay (thème 2)

Post-doc position in laser spectroscopy

A post-doctoral position in the field of complex molecules is open in the "BioMolecular Group" at Paris-Saclay University (Dr. Michel Mons and Dr. Eric Gloaguen), France.

Topic: Laser spectroscopy of isolated flexible molecules:

IR/UV double resonance spectroscopy ; pico- and femto-second pump-probe dynamics experiments.

Hamburg (thème 3)

A 3 years PhD position in Theoretical Chemistry is available in the group of Carmen Herrmann at the University of Hamburg. Research will focus on the interplay between electron transport through molecular junctions and spin degrees of freedom. The successful candidate will study and optimize phenomena such a magnetoresistance with first-principles methods, and develop further the required computational techniques. Applicants should have a strong interest in theoretical chemistry, a master's degree or equivalent in chemistry, physics, nanoscience, or a related subject, and good basic knowledge of theoretical chemistry or solid state physics. The successful candidate is expected to assist in teaching in the Chemistry Department, which makes practical experience in chemistry a strong plus. Solid English skills (both written and oral) are mandatory, knowledge of (or the willingness to learn) German is a plus. Applicants are asked to send (1) a CV, (2) a brief statement of research interests, (3) contact data for at least one reference, and (4) a copy of their master's degree (or a letter from their university or supervisor stating their anticipated graduation date and a copy of their last university degree) by email to carmen.herrmann@chemie.uni-hamburg.de.

Application deadline: November 3rd 2017 or until the position is filled.

Earliest starting date: January 1st 2018.

<http://www.chemie.uni-hamburg.de/ac/herrmann/index.html>.

Postes permanents

Orsay (section 30)

Ouverture d'un poste de Professeur en 30ème section. Voici les profils qui devraient être concernés :

- PR « Optique et milieux dilués » Procédure 46-3

Poste avec le profil de la section 30.

Laboratoires concernés: tous les laboratoires relevant de la section 30

- MdC « Interaction matière rayonnement à hautes résolutions »

Dans le domaine des milieux gouvernés par le comportement individuel des atomes et des molécules, se développent dans les laboratoires de Paris-Sud relevant de la section 30 des outils expérimentaux et théoriques dont les performances en termes de résolutions (spatiale, temporelle ou spectrale) permettent de sonder et de manipuler la matière avec des niveaux de finesse qui ouvrent de nouvelles perspectives. On peut citer entre autres la physique ultra-rapide, les développements en spectroscopie très haute résolution temporelle ou fréquentielle, l'étude des plasmas hors équilibre, la spectro-imagerie multidimensionnelle, et la technologie quantique.

Laboratoires concernés: tous les laboratoires relevant de la section 30

Université Paris Est Créteil

A Maitre de conference position will be open at University Paris East Créteil (UPEC) in 2018.

Job profile: Observation of the Earth's atmosphere from molecular spectroscopy to satellite data exploitation. Key words: Molecular spectroscopy, molecular physics, optics, atmospheric sounding, Earth observation

Description:

Scientific context: Remote sensing of the chemical composition of Earth's atmosphere from space has seen major progress over the past decade, in particular by increasing the number of detectable species in the troposphere and providing higher sensitivity. Today, satellite observations allow for unprecedented atmospheric monitoring leading to a better understanding of the atmospheric system. LISA's team SpecAt is deeply involved in the scientific exploitation of satellite missions, and has acquired internationally recognized expertise in the fields of spectroscopy and the development of innovative methods for satellite data inversion.

Future space missions, such as IASI-NG, TROPOMI, MICROCARB, Sentinel 4 & 5, etc., aim to embark instruments with unrivaled performances. This new generation of instruments allows for detection and quantification of new atmospheric species of interest for air quality and / or climate. However, the objectives of these missions often touch the frontier of knowledge in molecular spectroscopy. Accurate spectroscopic data are essential for the retrieval of atmospheric mixing ratios with highest precision. In order to meet this challenge and make the best use of the potential of the new instruments, a synergy between spectroscopy and satellite observations has to be developed.

Needs: LISA's team SpecAt includes specialists in high-resolution molecular spectroscopy (theoretical and experimental) and atmospheric physics. Its needs concern the development of a research activity at the interface between remote sensing and molecular spectroscopy. This will effectively respond to the demands and expectations of the atmospheric community in the next decade.

The future teacher-researcher is expected to strengthen the bridges between spectroscopy and remote sensing of the Earth's atmosphere. He/she will contribute to improving the quantification and accuracy of measurements of atmospheric species either by (i) spectroscopic studies, or (ii) the development of radiative transfer codes and inversion methods. He/she is expected to contribute to the synergy between both fields.

Required skills: The ideal candidate will possess either (i) excellent knowledge of experimental and/or theoretical tools required for spectroscopic analysis of high resolution molecular spectra, or (ii) an excellent knowledge of atmospheric inversion methods.

URGENT: For foreign candidates: Please be aware of the French qualification procedure where inscription is needed before October 24th 2017 (documents can be send in later). Please consult https://www.galaxie.enseignementsup-recherche.gouv.fr/ensup/cand_qualification_droit_commun.htm

Contact:

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