PCCP Workshop 2019

24-25th of June

Université de Bordeaux

université de BORDEAUX

Unité de formation
de chimie
Université de Bordeaux

THE PCCP WOKSHOP

Organized within the framework of the **international Master program *Physical Chemistry & Chemical Physics*** of the University of Bordeaux, the PCCP workshop provides a unique communication platform that covers a wide range of subjects related to the various fields of physical chemistry, ranging from fundamental academic research to industrial applications. This important event is also a great opportunity for students to exchange with worldwide researchers in a convivial framework. Keynote speakers are invited to outline state-of-the-art and recent trends in various research fields. PCCP students are both involved in the organization of the workshop and in the scientific presentations, either through poster or oral communications.

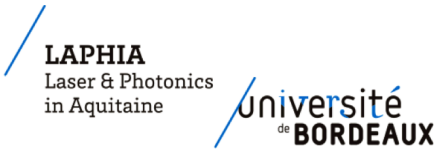
We hope you will enjoy the third edition of this workshop.

Cédric Crespos and Frédéric Castet

SPONSORS

Financial supports of the following institutions are acknowledged:

IDEX Bordeaux
Direction des Relations Internationales, University of Bordeaux
AMADEus Cluster of Excellence, University of Bordeaux
LAPHIA Cluster of Excellence, University of Bordeaux
Euskampus/IDEX Cross-border Lab. *QuantumChemPhys*
Institut des Sciences Moléculaires, University of Bordeaux/CNRS
Centre de Recherche Paul Pascal, CNRS
Région Nouvelle Aquitaine



SCHEDULE

Monday June 24

• 13h30	Welcome of the participants	
• 14h00	*Opening words*	**Laurent Servant** *Vice-president International, University of Bordeaux*
• 14h10	*Opening words*	**Daniel. E. Hall** *US Consul of Bordeaux*
• 14h20	*Presentation of the Dual diploma with Colorado School of Mines and Feedback from students*	**Neal Sullivan and Cédric Crespos** *Heads of the PCCP Master program at CSM and UB*
• 14h30	*Research in proton-conducting ceramics at the Colorado Fuel Cell Center*	**Neal Sullivan** *Colorado School of Mines, USA*
• 15h00	*Light on functionalized surfaces with advanced vibrational spectroscopies*	**Francesca Cecchet** *University of Namur, Belgium*
• 15h30	Break Poster session (First Year students of PCCP)	
• 16h00	*Microscopic single-particle analysis for atmospheric aerosol characterization*	**Chul-Un Ro** *Inha University, South Korea*
• 16h30	*Presentation of P&G, the various functions in R&D and the internship programs*	**Pierre Verstraete and Raúl Rodrigo Gómez** *Procter & Gamble Brussels Innovation Center*
• 17h00	*Flash communications – Part 1*	Second Year students of PCCP
• 18h00	End of the session	

Tuesday June 25

• 09h00	*Spatiotemporal control in minimal synthetic cells*	**Seraphine Wegner** *(Max Planck Institute for Polymer Research, Mainz, Germany*
• 09h30	*Examples of PCCP research @ Leiden: Understanding elementary catalytic processes at surfaces*	**Ludo Juurlink** *University of Leiden, Netherlands*
• 10h00	*Molecular interactions: matrix-isolation FTIR spectroscopy studies*	**Rosana Mariel Romano** *Universidad Nacional de La Plata, Argentina*
• 10h30	Break Poster session (First Year students of PCCP)	
• 11h00	*Presentation of the UB/Donostia Transborder Lab. QuantumChemPhys and Feedback from students*	**Ricardo Diez Muño and Pascal Larregaray** *Directors of the Transborder Lab.*
• 11h10	*Molecular dynamics and energy dissipation channels in gas/solid interfaces*	**Ricardo Diez Muño** *DIPC, San Sebastian, Spain*
• 11h40	*Current research activities at CFM*	**Andrés Arnau** *CFM, San Sebastian, Spain*
• 12h10	*Flash communications – Part 2*	Second Year students of PCCP
• 13h00	Lunch	
• 14h30	*Thermochromism in crystals and co-crystals – A quantum chemistry insight*	**Benoit Champagne** *University of Namur, Belgium*
• 15h00	*The Challenges of Developing a MOF-FF Compatible Interaction Model For Liquid Methanol and Cl- in Methanol*	**Siwarut Siwaipram** *VISTEC, Rayong, Thailand*
• 15h20	*Flash communications – Part 3*	Second Year students of PCCP
• 16h00	*Closing Words*	**Cédric Crespos** *Head of the PCCP master program*

MASTER STUDENTS ORAL COMMUNICATIONS

Part 1: Monday June 24

STUDENT NAME	Place of internship	TITLE	TIME
Loic Lecroart	Max-Planck-Institute für Biophysikalische Chemie, Göttingen	*Nonadiabatic molecular dynamic simulations of H scattering from O-covered Pt(111) surface*	17:00
Jessica Bowles	Centre for Sustaintable Chemical Technologies, University of Bath	*Polymerisation of a sugar-derived oxetane*	17:10
Guillermo Siliezar	ICMCB, University of Bordeaux	*Synthesis and sintering of fragile materials by Cool SPS (Spark Plasma Sintering).*	17:20
Charles Boury	Massachusetts Institute of Technology	*BaS-La2S3, a supporting electrolyte for molten salt electrolysis*	17:30

Part 2: Tuesday June 25

STUDENT NAME	Place of internship	TITLE	TIME
Florian Calzavara	ICMCB, University of Bordeaux	*Structure and properties of gallium-rich alkali and rare-earth germano-gallate glasses*	12:10
Jean Deviers	University of Namur	*MD then QM investigations of the second-order NLO responses of polymer chains: order-disorder effects*	12:20
Chloé Miossec	Department of Chemistry, Biology and Biotechnology, University of Perugia	*Experimental study of Vitreous Carbon Oxidation at High Temperatures*	12:20
Maxime Infuso	Centro de Física de Materiales, San Sebastián	*Laser induced femtochemistry on metal surfaces*	12:30

Part 3: Tuesday June 25

STUDENT NAME	Place of internship	TITLE	TIME
Steven Kerjosse	Institute of Chemistry, Leiden university	*Kaischew's approach, how to prepare curved and flat single crystals*	15:20
Theo Beigbeder	ISM, University of Bordeaux	*Construction of machine learning models for atomic forces prediction in monolayer and bulk MoS2*	15:30
Matthieu Wolf	Chemicum, University of Helsinki	*Determination of the saturation vapor pressure of monoterpenes using the COSMO-RS method and the possibility of second organic aerosol formation*	15:40
Florian Lochon	Quantum Nano-Photonics Lab. San Sebastián	*Characterization of noise in interferometric measurements*	15:50

MASTER STUDENTS POSTER COMMUNICATIONS

STUDENT NAME	Place of internship	TITLE	NUM
Francesca Lorenzutti	ICMCB, University of Bordeaux	*Synthesis and characterization of iron-based spin crossover material and its Au@SCO nanohybrids*	1
Appoline Simon	CRPP, University of Bordeaux	*Formulation and study of Pickering emulsions*	2
Nabila Zerrouki	Institute of Semiconductor Physics, Siberian Branch of the Russia Academy of Sciences	*The mechanical properties of partially fluorinated multigraphene films*	3
Alexis Manche	ICMCB, University of Bordeaux	*Synthesis and characterizations of new positive electrode materials of NASICON type for Li-ion batteries*	4
Coline Boyer	Laboratoire de Microanalyse, Sciences des Matériaux Anciens et du Patrimoine, University of Bordeaux	*Microanalysis techniques applied to the study of heritage materials*	5
Mateo Tunon de Lara	ICMCB, University of Bordeaux	*Synthesis of multifunctional nanoparticles for radiotherapy*	6
Thibault Yssartier	ISM, University of Bordeaux	*Bimodal Bright-Field/SHG Meso-Imaging: Application to Glass-Ceramics*	7
Keegan Mcgehee	ISM, University of Bordeaux	*CO_2 Addition Over Diols Promoted by Organic Bases: A DFT Investigation*	8
Alexis Maillard	CRPP, University of Bordeaux	*Photoinduced liquid-liquid phase transition kinetics via droplet based microfluidic*	9
Arthur Avignon	ISM, University of Bordeaux	*Theoretical simulation of the Eley-Rideal reaction*	10

INVITED TALKS

Light on functionalized surfaces with advanced vibrational spectroscopies

Francesca Cecchet

Research Associate of the Belgian National Fund for the Scientific Research F.R.S.-FNRS
Laboratory of Lasers and Spectroscopy (LLS), Namur Institute of Structured Matter (NISM), NAmur Institute for LIfe Sciences (NARILIS), University of Namur, Belgium, francesca.cecchet@unamur.be

Molecular vibrations are unique chemical fingerprints, which provide deep physicochemical information of matter and its environment. In this talk, we will see how nanoscale molecular films adsorbed on surfaces can be investigated through their vibrational response. We will give a general overview of the most known vibrational techniques, namely infrared (IR) spectroscopy and Raman scattering applied to the study of functionalized surfaces, and then we will focus on more advanced vibrational spectroscopies, which are based on nonlinear optical (NLO) phenomena. We will point out the unique advantages of vibrational NLO spectroscopies, and we will show their main research applications and achievements. More in details, we will discuss the research topics that we develop in our laboratory with a vibrational NLO spectroscopy, called sum-frequency generation (SFG) [1], to investigate nano-(bio)-interfaces (Figure) [2].

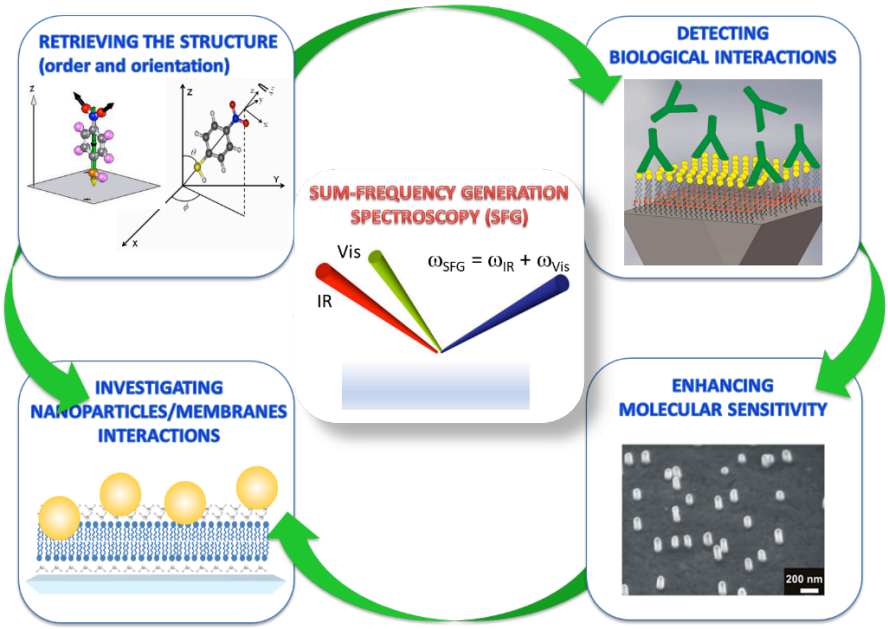


Figure. *Schematic representation of the SFG technique - a vibrational NLO spectroscopy based on the mixing of three photons (infrared-IR, visible-Vis and sum-frequency generated-SFG) -, and of some research topics we investigate in the field of the nano-(bio)-interfaces.*

[1] Y.R. Shen, *Fundamentals of Sum-Frequency Spectroscopy*, **2016**, Cambridge University Press
[2] C. Molinaro, F. Cecchet *Sensors and Actuators B: Chemical* 289, **2019**, 169-174; D. Lis, F. Cecchet *ChemPhysChem* 17, **2016**, 2645-2649; D. Lis, Y. Caudano, M. Henry, S. Demoustier-Champagne, E. Ferain, F. Cecchet *Advanced Optical Materials*, 1, **2013**, 244-255; D. Lis, J. Guthmuller, B. Champagne, C. Humbert, B. Busson, A. Peremans, F. Cecchet *ChemPhysChem* 14, **2013**, 1227-1236.

Thermochromism in crystals and co-crystals – A quantum chemistry insight

Benoît Champagne,[1,*] Andrea Carletta,[1] Tom Leyssens,[2] Jean Quertinmont,[1] Johan Wouters,[1] and Freddy Zutterman,[1]

[1] *Namur Institute of Structured Matter, University of Namur, 61 Rue de Bruxelles, B-5000 Namur, Belgium*

[2] *Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, 1 Place Louis Pasteur, B-1348 Louvain-La-Neuve, Belgium.*

email: benoit.champagne@unamur.be

Photochromic and thermochromic compounds are widely studied because of their potential applications in sensing devices. Still, most of these studies rely on characterizations performed in solutions whereas there is a need for understanding and optimizing their properties in the solid state. Salicylideneanilines (or anils), which are characterized by a tautomer equilibrium, between an enol and a keto form of different colors, present remarkable thermochromic and photochromic properties [1-2]. The enol form is usually the most stable but appropriate choice of substituents and conditions (solvent, crystal, host compound) can modify the thermodynamics and kinetics of the transformation [3]. One strategy to optimize the switching behavior and the related optical properties consists in forming co-crystals. In this presentation we discuss the quantum chemistry components of a multidisciplinary approach, which also includes synthesis of the chromophores, crystal formation, and physico-chemical characterizations. In particular, our latest achievements towards describing the structure-property relationships of co-crystals of anils with co-formers (featuring H-and X-bonding interactions) will be discussed. This encompasses i) the prediction of the crystal structures and of the key geometrical parameters, ii) the evaluation of the relative energy of the different keto and enol forms, iii) the simulation of the NMR signatures, to help in determining the enol-keto equilibrium constant in the solid state, and iv) the prediction of the UV/visible absorption spectra. In all cases, the focus is set on analyzing the effects of the interactions in the solid state between the chromophore and the co-former. Different methods are employed, from embedding techniques to periodic boundary conditions approaches. Compounds from the anil family (see Figure) are selected to illustrate these issues, owing to the availability of experimental data [4].

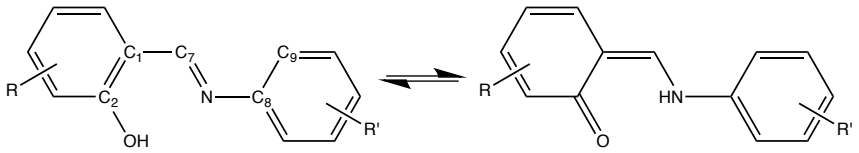


Figure. General structure of the anil derivatives. The compounds under investigation are (E)-2-methoxy-6-(pyridine-3-yliminomethyl)phenol, N-(5-chloro-2-hydroxybenzylidene)-aniline, and N-(5-chloro-2-hydroxybenzylidene)-hydroxyaniline

[1] Hadjoudis, E. Mavridis, I.M. Chem. Soc. Rev. **2004**, 33, 579−588.
[2] Antonov, L. Tautomerism: Methods and Theories. Wiley-VCH Press, Weinheim **2013**; Antonov, L. Tautomerism: Concepts and Applications in Science and Technology. WILEY-VCH Press, Weinheim **2016**.
[3] *e.g.* Zutterman, F. Louant, O. Mercier, G. Leyssens, T. Champagne, B. J. Phys. Chem. A **2018**, 122, 5370-5374.
[4] Carletta, A. Buol, X. Leyssens, T. Champagne, B. Wouters, J. J. Phys. Chem. C **2016**, 120, 10001-10008; Quertinmont, J. Carletta, A. Tumanov, N.A. Leyssens, T. Wouters, J. Champagne, B. J. Phys. Chem. C **2017**, 121, 6898-6908; Quertinmont, J. Leyssens, T. Wouters, J. Champagne, B. Crystals **2018**, 8, 125.

Microscopic single-particle analysis for atmospheric aerosol characterization

Chul-Un Ro

Department of Chemistry, Inha University, 100 Inha-ro, Namgu, Incheon, 402-751, Korea
curo@inha.ac.kr

The physicochemical characterization of atmospheric aerosols is of great interest because of their multiple roles in atmospheric processes and their diverse impact on environments. Microscopic single-particle analysis can provide information on morphology and internal mixing state of individual aerosol particles, which is essential for atmospheric aerosol study. In addition, elemental and molecular compositions, surface compositions, functional groups and hygroscopic property of individual particles can be investigated using various microscopic single-particle analytical techniques.

In this talk, some microscopic single-particle analytical techniques developed by and used in our laboratory, such as a quantitative energy-dispersive electron probe X-ray microanalysis (ED-EPMA), attenuated total reflectance FTIR (ATR-FTIR) imaging technique, Raman microspectrometry (RMS), and hygroscopic measurement systems based on optical microscopy and in-situ RMS, will be presented. The potential of combined use of microscopic single-particle analytical techniques for more detailed aerosol characterization is also emphasized as any single analytical technique cannot provide multimodal information on physicochemical properties of aerosols.

The Challenges of Developing a MOF-FF Compatible Interaction Model For Liquid Methanol and Cl^- in Methanol

Siwarut Siwaipram[a,b], Philippe A. Bopp[c], Jean-Christophe Soetens[d], Rochus Schmid[a] and Sareeya Bureekaew[b]

[a]Computational Materials Chemistry, Ruhr-Universität Bochum, DE-44801 Bochum
[b]Department of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong, Thailand
[c]Department of Materials Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC), Rayong, Thailand
[d]ISM Bât A12, Université de Bordeaux, 351 Cours de la Libération, FR-33405 Talence

Corresponding author: *s15_siwarut.s@vistec.ac.th*

The MOF-FF interaction model[1] has been specifically developed and then widely employed in molecular simulations of Metal-Organic-Frameworks (MOFs)[2], in particular flexible ones. These modify their unit cell volume according to external conditions and/or their loading with guest molecules of various types[3]. Some of the options taken when developing MOF-FF make it, however, difficult to combine it with the existing models developed e.g. for the liquids that may be present as guests inside the MOF. In the present work, we develop a model for liquid methanol compatible with the constraints of MOF-FF and test it with respect to bulk properties such as liquid density, diffusion coefficient and compressibility coefficient, which might be important in simulation studies of a flexible MOF immersed in this liquid. Since some of MOF frameworks are electrically charged, counterions such as Cl^- anion will be present and their interactions with the liquid must also be considered.

Keywords: Metal-organic frameworks, Force fields development, Molecular dynamics, Liquid methanol simulation, Methanol – Cl^- solution.

References

[1] Bureekaew, S.; Amirjalayer, S.; Tafipolsky, M.; Spickermann, C.; Roy, T.; Schmid, R. Phys status solidi 2013, 250(6), 1128–41.
[2] Horike, S., Shimomura, S. and Kitagawa, S., Nature chemistry 2009, 1(9), p.695.
[3] Kitagawa, S. and Matsuda, R., Chemistry of coordination space of porous coordination polymers. Coordination Chemistry Reviews 2007, 251(21-24), pp.2490-2509.
[4] Obeidat, A.; Abu-Ghazleh, H. AIP Advances 2018, 8(6), 065203
[5] Dortmund Data Bank l Density of Methanol and Diffusion Coefficient. DDBST GmbH. 2018.
[6] Kulschewski, T.; Pleiss, J. Molecular Simulation 2013, 39, 754–767.

Spatiotemporal control in minimal synthetic cells

Dr. Seraphine V. Wegner

Max Planck Institute for Polymer Research

Many of the emerging functions that are perceived as life require spatiotemporal regulation of molecular events at the microscopic and mesoscopic scale. Hence, in the quest to assemble minimal synthetic cells with life like functions from molecular building blocks, the spatiotemporal regulation of molecular interactions and coupled events is of central importance. Protein patterns and gradients, cell migration, tissue formation and cellular signaling are just a few examples of processes, where the dynamic spatiotemporal control is an essential ingredient for function. In this talk I will present strategies of how such spatiotemporal control can be achieved in minimal synthetic cells using photoswitchable protein interactions and how spatiotemporal control can lead to cell mimetic behavior in synthetic systems assembled from molecules from the bottom-up. This on one hand provides insight into underlying design principles of life and on the other hand allows integrating these concepts into cellular systems in the context of synthetic biology.