PCCP Light S&T Graduate Program

PCCP Workshop 2022

23-24th of June

Université de Bordeaux

université de BORDEAUX

Unité de formation de chimie
Université de Bordeaux

THE PCCP WOKSHOP

Dear students and colleagues,

We are pleased to welcome you to the 4th workshop 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.

We are particularly happy of being able to welcome you in person to Bordeaux, after the cancellation of the two last editions imposed by the pandemics.

I wish you an inspiring symposium with lots of interesting science and fruitful discussions.

Frédéric Castet

SPONSORS

Financial supports of the following institutions are acknowledged:

Collège Sciences & Technologies, University of Bordeaux
EUR LIGHT, University of Bordeaux
Euskampus/IDEX Cross-border Lab. *QuantumChemPhys*
Institut des Sciences Moléculaires, University of Bordeaux/CNRS
Institut de Chimie de la Matière Condensée de Bordeaux, University of Bordeaux/CNRS
Centre de Recherche Paul Pascal, CNRS

VENUE

The workshop will take place in the building B6 (Tram station "François Bordes") of the campus of Sciences & Technologies of the University of Bordeaux.

POSTER SESSIONS

Poster sessions will take place during the coffee breaks. To maximize the interaction and exchange around posters, we recommend to hang your poster on the supports provided at your arrival at the conference place.

SCHEDULE

Thursday June 23, morning

• 9h00	Welcome of the participants	
• 09h10	*Opening words*	**Frédéric Castet** *Head of the PCCP master program*
• 09h20	*Influence of Various Lipid Building Blocks on the Second-Order Nonlinear Optical Responses of an Embedded Di-8-ANEPPS Probe*	**Charlotte Bouquiaux** *University of Namur, Belgium*
• 09h50	*CO oxidation on Ru(0001): unraveling the changes in molecular orbitals*	**Auguste Tetenoire** (PCCP 2018)
• 10h00	*Control of low-energy ND3-HD collisions*	**Pierre Sustar** (PCCP 2022)
• 10h10	*Optical properties of plasmonic oxide nanoparticles for intelligent glazing application*	**Florian Lochon** (PCCP 2019)
• 10h20	*Study of glassy boron oxide B2O3 structural features through statistical ensemble of crystalline microstates*	**Laszlo Wolf** (PCCP/CSM 2022)
• 10h30	Coffee Break (with posters from first-year PCCP students)	
• 11h00	*Presentation of the Light UB Grads*	**Véronique Jubéra** *Head of Light UB Grads for the Chemistry department*
• 11h10	*Presentation of the UB/Donostia Transborder Lab. QuantumChemPhys*	**Pascal Larregaray** *Director of QuantumChemPhys*
• 11h20	*Rationalization and tuning of doublet emission in organic radicals*	**Claire Tonnelé** *DIPC, San Sebastian, Spain*
• 11h50	*Tracking the degradation of organic chlorine compounds from reactive molecular dynamics simulations*	**Matthieu Wolf** (PCCP 2019)
• 12h00	*H-atom scattering from p(2x2) O on Pt(111): Resolving the nonadiabatic puzzle*	**Loïc Lecroart** (PCCP 2019)
• 12h10	*Exploring the optical properties of perovskite single nanocrystals*	**Elise Prin** (PCCP 2021)
• 12h20	*Towards molecular nanophotonics: preparation and investigation of fluorescent molecular based nanoparticles*	**Eleonore Kurek** (LIGHT 2022)
• 12h30	Lunch	

Thursday June 23, afternoon

• 14h30	*Molecular Modelling and Machine Learning for the Chemical Industry*	**Rémi Petuya** *Nextmol, Barcelona*
• 15h00	*Dissociation of O2 on Cu(111) studied with a screened hybrid density functional*	**Laura Viaud** (PCCP 2022)
• 15h10	*Multi scale modelling of solid electrolytes for next gen Li-ion batteries*	**Bassey Oboho** (PCCP 2021)
• 15h20	*Study of different SERS substrates for application to sub-micron aerosol analysis*	**Chloé Sanz** (PCCP 2022)
• 15h30	*Is ethylene (C2H4) present in the atmosphere of Hot Jupiter exoplanets*	**Solène Perot** (PCCP 2021)
• 15h40	*Determination of Vibrational Circular Dichroism spectra of fluxional molecules through classical polarisable molecular dynamics*	**Jessica Bowles** (PCCP 2019)
• 15h50	Coffee Break (with posters from first-year PCCP students)	
• 16h20	*Computational study of the electrically-stimulated isomerization of an indolinooxazolidine core including a bithiophene moiety*	**Lucie Combrouze** (PCCP 2022)
• 16h30	*Molecular simulation of CH4 adsorption in kerogens: effects of maturity and poromechanics*	**Kevin Potier** (PCCP 2020)
• 16h40	*Adsorption and desorption studies of CO on Cu(211)*	**Pierre Loora** (PCCP 2022)
• 16h50	Presentation of the PCCP association	
• 17h00	PCCP students from abroad	
• 17h00 • 17h05 • 17h10 • 17h15 • 17h20	*Flash communication* *Flash communication* *Flash communication* *Flash communication* *Flash communication*	**Evangelia Charvati** (PCCP 2018) **Chloé Miossec** (PCCP 2019) **Charles Boury** (PCCP 2019) **Francesca Lorenzutti** (PCCP 2020) **Jean Deviers** (PCCP 2019)
• 17h25	End of the session	

Friday June 24, morning

• 09h00	*Opening words*	**Laurent Servant** *Vice-president in charge of international networks*
• 09h10	*Opening words*	**Alexander Lipscomb** *US Consul of Bordeaux*
• 09h20	*Effect of fluorination on Disordered Rock-salt for cathodes in high energy density Li-ion batteries*	**Makenzie Parimuha** (PCCP/CSM 2022)
• 09h30	*Optimizing post-processing of 316L parts fabricated by extrusion-based additive manufacturing (EAM) process*	**Daniel Gifford** (PCCP/CSM 2022)
• 09h40	*Science and design of microstructures*	**Eugénie Pariente** (PCCP/CSM 2022)
• 09h50	*Synthesis and analysis of Dansyl Diazaborines adsorbed onto an hydrogel*	**Matthieu Soula** (PCCP/CSM 2022)
• 10h00	*My personal experience at Procter & Gamble and a career opportunity for you too*	**Coralie Naudin** *Procter & Gamble, Brussels, Belgium*
• 10h30	Coffee Break (with posters from first-year PCCP students)	
• 11h00	*Magnetic materials for photonic applications: Borontungstate and rare earth ions glasses*	**Leonardo Vieira Albino** *ICMCB, Bordeaux*
• 11h30	*On-chip heating effects in electronic measurements at cryogenic temperatures*	**Antoine Castagnède** (PCCP/CSM 2022)
• 11h40	*Chemical nano welding of Cu@Ni bimetallic nanowires for transparent electrodes*	**Anđela Križan** (PCCP 2021)
• 11h50	*Spectroscopic investigation on natural gas hydrate: from geo- to nanoscale*	**Semen Vasin** (PCCP 2022)
• 12h00	*Deciphering of the critical physicochemical parameters promoting the efficient diffusion of nanoparticles in tumor models*	**Apolline Simon** (PCCP 2020)
• 12h10	*3D localization of proteins in focal adhesions*	**Violeta Milanovic** (PCCP 2021)
• 12h20	*Closing Words*	**Cédric Crespos** *Head of the Master in Chemistry*
• 12h30	End of the session	

POSTER COMMUNICATIONS

STUDENT NAME	Place of internship	TITLE	NUM
Hanae Boulehjour	CRPP Bordeaux	*Coordination polymers based on the Pyrazine Ligand: towards the synthesis of the two-dimensional network [V(Pyz)2(OTf)2]*	1
Audrey Dolosor	ISM Bordeaux	*Simulation of the nonlinear optical properties of chiral molecular probes*	2
Chloé Flandrin	ICMCB Bordeaux	*Study and Optimisation of [Fe(Htrz)2(trz)](BF4) Synthesis by Batch or Flow Assisted by Supercritical CO2*	3
Jouke Fleege	CRPP Bordeaux	*Preparing micron-sized Silica-Polystyrene composite particles by seeded dispersion polymerisation in absolute alcoholic medium*	4
Inness Kamugisha	ISM Bordeaux	*Atomic Force microscopy in Environmental cell Applications to atmospheric and geochemistry*	5
Pierre-Alexis Kucharski	ISM Bordeaux	*Solvation of Li+ ion by Ethylene Carbonate, Dimethyl Carbonate and their mixture using Molecular Dynamics Simulation at 323K*	6
Maëva Louis	ISM Bordeaux	*Experimental astrochemistry: Analysis of inelastic collisions of hdo with n-h2 and ne*	7
Nikolay Nikolov	ISM Bordeaux	*Deep eutectic solvents for CO2 capture*	8
Samuel Proctor	ISM Bordeaux	*Theoretical description of collision dynamics of hydrogen atoms with W(100) and W(110) surfaces*	9
Julien Renaudeau	LOF Bordeaux	*Viscosity measurements using molecular rotors*	10
Kyriaki Samioti	CRPP Bordeaux	*Inkjet Printing of Polymer Nanocomposites for High Energy Storage*	11
Marie Tardieux	ISM Bordeaux	*Dynamics of nitrogen scattering on W(100) : the role of Van der Waals interactions in the Eley-Rideal mechanism*	12
Noémie Veyret	CBMN Bordeaux	*Determination of the binding affinity of synthetic compounds for microvesicles. A MicroScale Thermophoresis study*	13
Vincent Lazeran	CRPP Bordeaux	*Absorption of light in dilute plasmonic composite water droplets*	14

INVITED TALK 1

Influence of Various Lipid Building Blocks on the Second-Order Nonlinear Optical Responses of an Embedded Di-8-ANEPPS Probe

BOUQUIAUX Charlotte, CHAMPAGNE Benoît

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Biological membranes are thin selectively permeable amphiphilic films that play a key and active role in the life of the cell. Those different functions are carried out by different lipids, explaining why eukaryotic cells invest substantial resources in generating thousands of different lipids. The huge diversity of lipids is due to the combination of various building blocks: *(i)* the fatty acids that vary in length, in the number and position of the unsaturation(s), and *(ii)* the diverse headgroup structures available that vary in size, polarity, charge, H-bond-donating, and -accepting capacities, which strongly impact interfacial structure and dynamics. Given all the possible combinations of headgroups and hydrocarbon chains, several thousand structurally distinct lipid molecules could theoretically exist, each potentially contributing to the properties of cellular membranes and the biological processes taking place within them. Therefore, having a tool to distinguish between membranes of various composition is helpful in the deeper understanding of lipid bilayers. In this work we investigate a collection of glycerophospholipid saturated bilayers varying only in their head group structure (namely PC, PE, DAG, PS, and PA, see Figure 1 for their definition and structure) via Molecular Dynamics simulations. Additionally, for PC, PE, and PS, lipids with unsaturated and/or longer fatty acids (R_1 and R_2) were also considered. The effect changing the head group structure or the fatty acid(s) on the properties of the bilayer are studied, namely the thickness, the area per lipid, the hydrocarbon parameter, the orientation of the diverse molecules within the membranes, and also the hydrogen bonds network. To complement the study, we also analyse the second-harmonic generation (SHG) nonlinear optical (NLO) response of a probe molecule, di-8-ANEPPS inserted into the membranes. This technique as the advantage to be specific to interfacial region, like lipid bilayer, and used in conjunction with an ANEPP-like molecule, allows us rapid acquisition at relatively low laser power. The structural analyses are then confronted to the molecular NLO response, b, computed at the TDDFT/M06-2X/6-311+G* level, and in particular the contribution to b parallel to the bilayer normal, b_{zzz}. This computational approach provides insights onto the link between the combination of head group structure and fatty acids and the diagonal component b_{zzz} of the first hyperpolarizability and so a first approach towards unravelling the changes due to the variation of both building blocks of lipid bilayers.

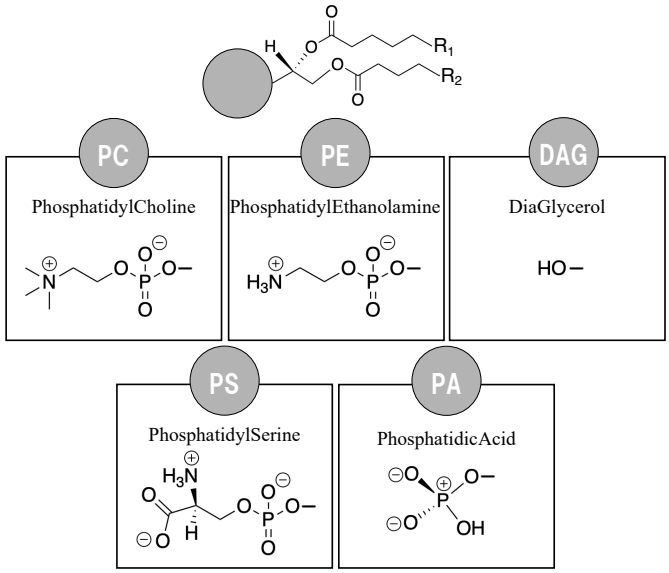

Figure 1:Glycerophospholipid backbone and headgroup structures.

INVITED TALK 2

Rationalization and tuning of doublet emission in organic radicals

Claire Tonnelé,[a,*] David Casanova[a,b]

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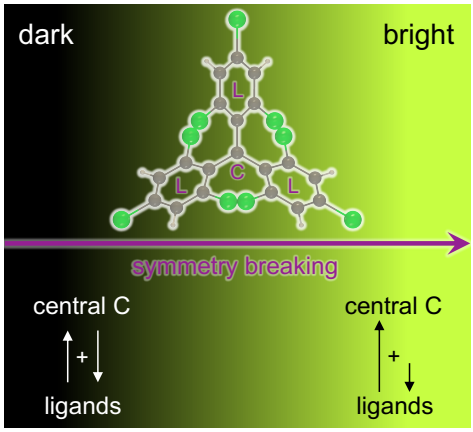
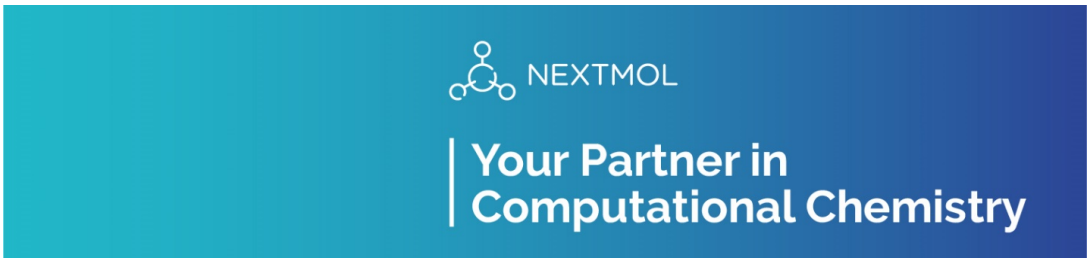
[b]*Ikerbasque Foundation for Science, 48009 Bilbao, Euskadi, Spain*

Neutral organic radical emitters have emerged as a promising new route for efficient OLEDs. Using conventional closed-shell materials, electroluminescence efficiency of OLEDs is limited to 25%, as spin statistics dictates that charge recombination leads to 25% singlets and 75% triplets, the latter being intrinsically dark. While several strategies have been proposed to brighten those triplets (inclusion of heavy metal atom, thermally activated delayed fluorescence, etc), the use of radical emitters with spin-allowed doublet emission is a conceptually superior solution to elegantly circumvent the spin statistics limited efficiency issue[1]. These organic radicals were originally considered to be dark and efficient luminescence quencher until a seminal study reporting a bright substituted TTM radical, a paradigmatic doublet emitter.[2] In this work, we present a detailed physical interpretation of the origin of the intrinsic poor emissive properties of TTM from a computational perspective. The weak emission is rationalized on the basis of the mixing of intramolecular charge transfer excitations between the radical center and the ligands whose transition dipole moments significantly cancel, giving rise to a vanishing oscillator strength. We demonstrate how the modulation of their relative contributions to the composition of the lowest excited doublet state via donor substitution can brighten the organic radical. This is further illustrated through the study of a series of TTM derivatives.



[1]J. M. Hudson, T. J. H. Hele and E. W. Evans, *J. Appl. Phys.*, 2021, **129**, 18091.
[2]V. Gamero et al., *Tetrahedron Lett.*, 2006, **47**, 2305-2309.

INVITED TALK 3



Molecular Modelling and Machine Learning for the Chemical Industry

PETUYA Rémi[A], ALSINA COWIE Marc,[A] and MOHR Stephan[A]

A) Nextmol (Bytelab Solutions SL), Carrer de Roc Boronat, 117, 08018 Barcelona, Spain

Nextmol is a start-up specialized in computational chemistry, which develops advanced molecular modelling and artificial intelligence tools to accelerate R&D in the chemical industry. Its mission is to help chemical companies in adopting computational techniques in their R&D for a more efficient development of better and more sustainable chemicals. Nextmol's activities cover a variety of research fields such as surfactants for flow assurance, lubricant additives or polymers.

The formation of natural gas hydrates, ice-like solids made of natural gas molecules trapped inside cages of hydrogen-bonded water molecules, is a major problem in flow assurance for the oil and gas (O&G) industry.[1] Indeed, as oilfields mature, they produce increasing quantities of water,[2] and hydrate nucleation, growth and agglomeration can cause pipeline blockage in deep water subsea flow lines as illustrated in Figure 1. Natural gas hydrates are thus the predominant problem to overcome in transporting oil, gas and water mixtures.[3]

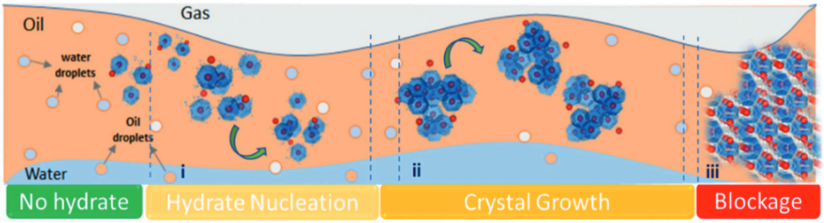


Figure 1: Schematic diagram of the drivers of hydrate crystals formation and aggregation in hydrocarbon transportation pipelines and three-step process of (i) hydrate nucleation, (ii) crystal growth, and (iii) blockage. Reproduction from Hassanpouryouzband et al. [1]

For reasons of efficiency and cost, rather than trying to entirely prevent the formation of hydrates, industry has turned to hydrate management: allowing the formation of small hydrate particles but preventing their agglomeration via the addition of a specific type of low-dosage hydrate inhibitors (LDHIs) called anti-agglomerants (AA). AA are surfactant molecules (short for "surface active agent") made of a polar hydrophilic head and of a lipophilic (and thus hydrophobic) tail.

The deployment of a series of molecular dynamics simulation protocols, validated via comparison with experiments,[4] permits the *in-silico* characterization of the surfactant ability to inhibit the agglomeration of sII hydrate particles. Two main physico-chemical descriptors of the surfactant performance have been identified: i) the surfactant affinity for the hydrate surface and ii) the energy barrier that a pre-adsorbed layer of surfactants opposes to the coalescence process between a hydrate slab and a water droplet. After the computationally intensive study of a series of candidates, provided by our industrial partner, we have trained supervised machine learning models to predict the inhibitor performance of surfactants. These models provided an impressive acceleration of the screening of publicly available databases and of newly generated candidates, and open new perspectives for the design of hydrates anti-agglomerant.

[1] A. Hassanpouryouzband et al., Chem Soc Rev, 2020, 49, 5225-5309.
[2] M. A. Kelland, Production Chemicals for the Oil and Gas Industry, Taylor & Francis Group, 2nd Edition, 2014
[3] M. A. Kelland, IOP Conf. Ser. Mater. Sci. Eng., 2019, 700, 012057
[4] S. Mohr et al., J. Phys Chem. B, 125 (2020), 1487-1502

INVITED TALK 4

My personal experience at Procter & Gamble and a career opportunity for you too

Coralie Naudin
Research manager P&G, Bruxelles

This will share the work experience of a PhD graduated from University of Bordeaux within the private sector and the career opportunities that a company like P&G can offer.

INVITED TALK 5

Magnetic materials for photonic applications: Borontungstate and rare earth ions glasses

Leonardo Vieira Albino

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The vitreous state offers new application possibilities by adapting its chemical composition. In recent decades, the development of glasses with magnetic properties has aroused great interest. Indeed, new highly paramagnetic compositions have been developed which open new technological perspectives for the development of integrated photonic systems combining optical properties and magnetism (MO). Possible applications include data storage, healthcare, lasers, and information technology.

New compositions of tungsten borate glasses or glass-ceramics developed in the project have a high solubility of rare-earth ions and thus offer the ability to introduce a large percentage of paramagnetic species. The scientific challenges to be met in this work focus mainly on the synthesis and the study of the physical and structural properties of new materials. Particular attention is also paid to the shaping of these glasses in the form of optical fibers for their future integration within photonic systems.