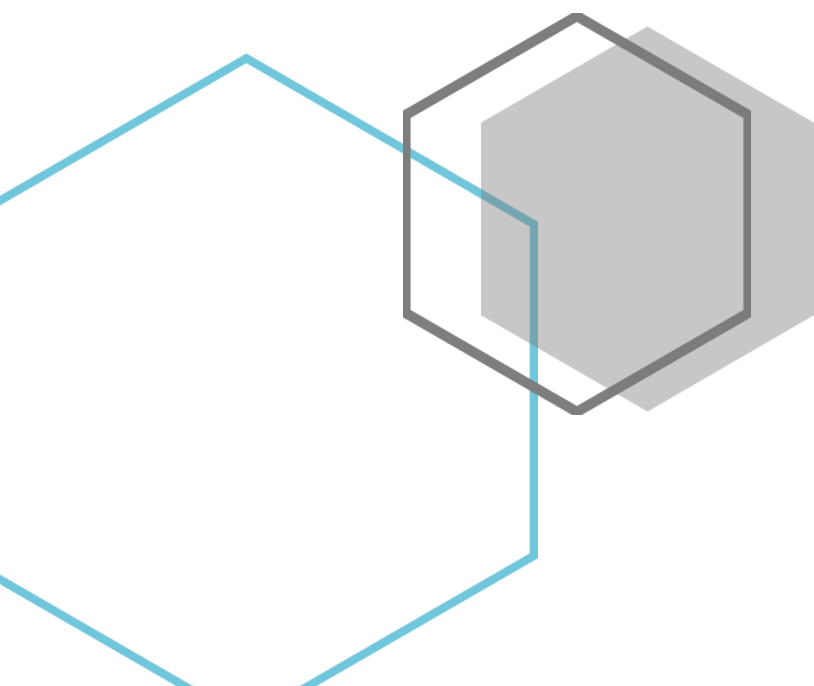
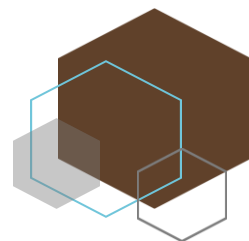


# Congrès des chimistes 2019

Par la promo Chimie 17

Ce document a été réalisé par les élèves du département de chimie, parti.e.s en stage pendant leur deuxième semestre de M1





9h30



## Synthesis of Manganese Complexes for Selective Electro-reduction of CO<sub>2</sub> to Formate, *Émile Escoudé*

*Carbon Dioxide Activation Center (CADIAC), Interdisciplinary Nanoscience Center, Department of Chemistry, Aarhus University, Denmark*



Manganese bipyridine and phenanthroline complexes have been synthesized and tested as catalysts for carbon dioxide electro-reduction into carbon monoxide and formate. It has been proved that the catalyst's selectivity could be tuned by an appropriate ligand designing. The effect of introducing aliphatic amines in the secondary coordination sphere of the manganese centre has been studied. A series of ligands have been synthesised and electrochemically tested in the electro-reduction of CO<sub>2</sub> to evaluate the effect of introducing a nitrogen lone pair of electron in the outer coordination sphere. New catalysts having a faradic efficiency of 71% for formate and a turn-over frequency of 2207s<sup>-1</sup> have been developed.

9h50

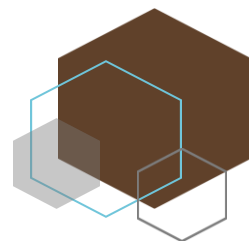


## Electrospraying of Self-Assembling Hexapeptides, *Lina El Hajji*

*Sous la supervision de Michael Reithofer, Institut de chimie inorganique, Université de Vienne, Autriche*



Electrospraying and electrospinning are widely used techniques for the fabrication of functional materials with tunable properties. Typically polymers are used for this process, but utilising peptides would offer access to new materials and applications. However, peptide-based electrospraying represents a significant challenge with only a few reports known today. In this work, polystyrene microfibres were fabricated as a starting point by electrospinning using a commercial electrospraying setting. In addition, peptide-based nanoparticles were synthesised by electrospraying using a self-assembling hexapeptide as a starting material, and the effect of processing parameters on particle morphology was investigated by scanning electron microscopy (SEM). Finally, encapsulation using electrospraying of an anti-inflammatory drug in a peptide shell was attempted.



10h10



## Effect of kinetic energy on reactivity: an LA-ICP-MS/MS study, *Johanne Lebrun Thauront*

*Microgeochemistry group, Department of Earth Science, University of Gothenburg, Sweden*



UNIVERSITY OF GOTHENBURG

Plasma ion source mass spectrometers equipped with a reaction cell have been used in geology for quantitative trace element analysis and isotopic ratio determination for almost four decades. However, on commercial instruments, the conditions in the reaction cell are not specified. In particular the kinetic energy and kinetic energy distribution of the ions and their electronic state distribution is unknown. Kinetic and thermodynamic data available on ion-gas reactions are often determined in thermal conditions at 298 K. In order to use these data for method development, it is important to study the conditions in the reaction cell and to understand the effect of kinetic energy on ion-gas reactivity. I show that using the different lenses along the ion path in the spectrometer, it is possible to conduct such investigation and I draw conclusions for the use of kinetic data and kinetic energy in order to solve isobaric interferences.

10h30



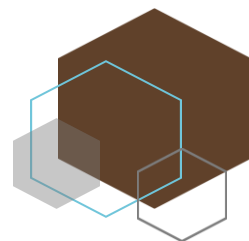
## Ab Initio Study of the Effect of Alkali Cations on Structural and Energetic Properties of Solvated Electrons in Liquid Ammonia, *Axel Gomez*

*Group of Pavel Jungwirth, Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic*



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Alkali metals dissolve in liquid ammonia into a blue electrolyte or a gold metallic solution at low and high concentrations, respectively. The solvation of the valence electron of the alkali metal is the source of this spectacular behaviour. By ab initio studies, the solvation of the excess electron can be investigated at electronic and atomic levels to support spectroscopy experiments. I studied isolated and implicitly solvated clusters of ammonia molecules with an alkali cation and a single solvated electron using density functional theory with a hybrid functional. We find the vertical detachment energy of the solvated electron to be comparable to the experimental value of 2.0 eV. We show that all alkali metals have approximately the same effect on the vertical detachment energy of the solvated electrons. Our work describes the behaviour of the solvated electron in a low concentration regime, being a necessary first step for further investigations at higher concentrations to get insight into the metallic nature of the golden solution.

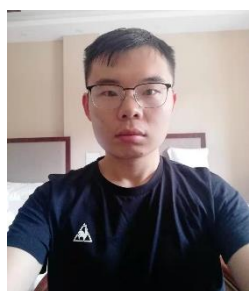

**11h10**


## Efficient synthesis and self assembly of the amphiphilic PEO-*b*-PEHOx-*b*-PEtOx towards asymmetric polymersomes, *Alexandra Fillion*

*Meier group, Department of chemistry,  
University of Basel, Switzerland*



Mimicking the asymmetry of the cell membrane is necessary for a direct insertion of transmembrane proteins into artificial vesicles like polymersomes. The self-assembly of amphiphilic ABC triblock copolymers is an interesting strategy to obtain asymmetric polymersomes. Here we report the efficient one-pot synthesis of a new biocompatible triblock ABC copolymer: Poly(ethyleneoxide)-*block*-poly(2-(3-ethylheptyl)-2-oxazoline)-*block*-poly(2-ethyl-2-oxazoline) (PEO-*b*-PEHOx-*b*-PEtOx) and its self-assembly into polymersomes. The self-assembly of the triblock copolymers was investigated using film rehydration and solvent switch. A combination of static and dynamic light-scattering and TEM analysis showed that monodisperse populations of polymersomes are obtained with film rehydration. A fluorescent dye attached by click-chemistry on the C-terminus the ABC triblock copolymers was detected by Fluorescence Correlation Spectroscopy (FCS) to probe the asymmetry of the polymersomes.

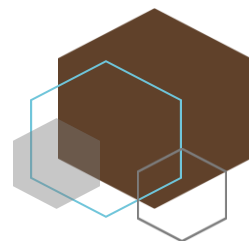
**11h30**


## Theoretical Studies on Electrified Aqueous Interfaces, *Yiwei Zhang*

*Supervised by Damien Laage, UMR 8640,  
ENS Paris*



Electrochemistry takes place at interfaces. Electrochemical interfaces are composed of electrodes and electrolytes. Electrodes bear accumulated net charges to create an electrostatic potential, leading to the responses from electrolytes. With different electrostatic potential applied, the alignment and dynamics of electrolyte molecules and ions shift due to changes in electrolyte-electrode interactions. This molecular-level process plays a decisive role in electrochemical processes including the transport and charge separation and thus calls for a molecular picture for detailed description. Here we provide a molecular picture of electrified water-graphene interfaces, including the alignment, reorientation and translation of water molecules at the interface and a prediction of vibrational sum-frequency generation of this interface. Details of the dynamical picture are provided by the molecular jump model. This detailed picture is going to promote the understanding of aqueous electrochemistry involving graphene electrodes at the molecular level.



11h50



## Photo-control of embryonic morphogenesis with photocaged signaling molecules, *Chems Amari*

École Polytechnique Fédérale de  
Lausanne, Suisse

**EPFL**

The early stage of embryo development is a critical step in body organization for mammalian species: the first organization axis appears in the very first days following the implantation of the embryo. In order to study the mechanisms involved, one can replicate this event with *in vitro* stem cells aggregates. When stimulated with signaling molecules, those aggregates start to elongate and their cell differentiate, mimicking the development and gene expression of a real embryo.

In this study, we explore a new way of exposing to signaling molecules: we fix chemically a photolabile group on these molecules, leading to their inhibition. One can then expose aggregates to these photo-caged molecules and light the desired zone, allowing a photo-activation of the differentiation mechanism *in situ* with a fine-tuned spatial and temporal control of the exposition.

14h30

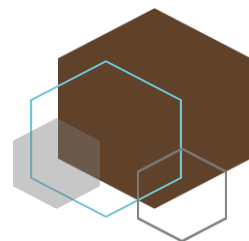


## The Influence of Additives on Pressure-induced and Humidity-induced Crystallization of Amorphous Calcium Carbonate (ACC), *Clémence Courrègelonge*

Soft Materials Laboratory (SMaL),  
Institute of Materials, EPFL, Suisse

**EPFL**

In nature, formation of CaCO<sub>3</sub>-based materials is well controlled such that these materials display excellent properties, for instance high toughness and strength. In biogenic condition, CaCO<sub>3</sub> usually crystallizes via an amorphous state, amorphous calcium carbonate (ACC), in presence of impurities such as Mg<sup>2+</sup> ions and acidic proteins. To synthesize CaCO<sub>3</sub>-based materials that mimic the structure and properties of natural counterparts, studying how ACC transforms into crystals in the presence of additives is required. Some crystallization processes of ACC that occur in humidity or under pressure remain poorly understood. We perform a systematic study to analyse the composition and structure of ACC particles at different stages of pressure-induced and humidity-induced crystallization and compare the influence of several additives on these two crystallization processes. Based on these studies, we underline the key role of water and additives during the transformation of ACC particles into crystalline particles.



14h50



## Atomistic Characterization of Amyloid Aggregation Inhibition by Alternating L/D, Peptides Using Advanced-Sampling Molecular Dynamics, *Sélène Forget*

*Princeton University, New Jersey, USA*



Amyloid proteins aggregation inhibition is one of the main issues in the fight against neurodegenerative diseases such as Alzheimer. In 2014, a novel peptide design was advanced as potential inhibitor. Composed of alternate L and D-amino acids, it has shown promising results by significantly decreasing aggregation experimentally. However, the reasons behind this efficiency remain unclear. In particular, the design was presented as an "α-sheet" structure, which is a very unusual protein conformation. Further investigations are needed to understand if this α-sheet structure is formed and how aggregation decrease can be explained. Our study uses Parallel Tempering Molecular Dynamics to investigate at an atomistic range the structures of Alzheimer's amyloid proteins Aβ42 and Aβ0, the L/D designed peptide and its full L equivalent. We show that the α-sheet structure rarely occurs. These characterizations will be taken as reference for a future double chain interaction investigation in order to propose an atomistic explanation of the aggregation inhibition.

15h10

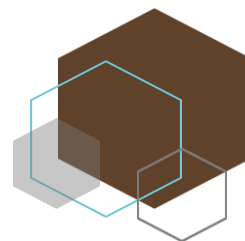


## Toward water soluble photoswitches based on dihydropyrene, *Léa Chocron*

*Humboldt Universität zu Berlin, Germany*



External control of a system by action of light is an efficient way to modulate its properties. It can be achieved by using photochromic molecules. Among all existing photochromes, the negative T-type photochromic dihydropyrene switch is really attractive because it allows quantitative conversion from a coloured form to a colourless one. However, its inherent hydrophobicity and the absence of functionality in the backbone limit the scope of its application, especially in biology. Here we describe the synthesis and characterisation of a new class of water-soluble photochromic derivatives based on aza-dihydropyrene. The thermal half-life of these compounds varies significantly between the protonated form (second scale) and the free base (day scale). Due to the modulation of electronic density of the nitrogen between the two isomers, these compounds are also promising candidates for photoswitchable base systems, allowing for light-induced protonation and deprotonation of the pyridine unit at constant pH.



15h50



## Exploratory copper phosphonate MOF synthesis using high-throughput methods, *Ramiro Zapata*

*Christian Albrechts Universität zu Kiel, Institut für Anorganische Chemie, Kiel, Germany*



Kiel University  
Christian-Albrechts-Universität zu Kiel

Through the use of high-throughput methods, an exploratory investigation of Metal Organic Frameworks (MOFs) built of tetrakisphosphonate linker molecules and  $\text{Cu}^{2+}$  salts was performed. Two main phases were observed, for which different characterizations were carried out including powder X-ray and electron diffraction measurements, water sorption measurements, as well as elemental, thermogravimetric and energy dispersive X-ray analysis. Using different copper salts, different phases were obtained, and a trend was recognized for two of these phases, in which the obtained phase transitioned from one to another depending on the number of equivalents of  $\text{Cu}^{2+}$  added to the reaction mixture. Different modifications to reaction conditions were also explored, with the aim of obtaining products with higher crystallinity and single crystals. These involve varying the concentrations of reactants used, changing the reaction solvent, and the use of a modulator. The use of high-throughput methodology allowed for the acquisition of large amounts of information in a short amount of time.

16h10



## Meteorite Dating by the U-Pb Methode, *Célia Bresson*

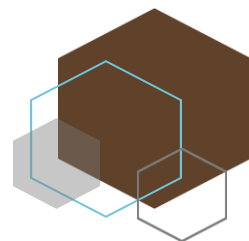
*Centre for Star and Planet Formation (STARPLAN), Natural History Museum of Denmark, Copenhagen, Denmark*

NATURAL  
HISTORY MUSEUM  
OF DENMARK

UNIVERSITY OF  
COPENHAGEN



The U-Pb method is the only long-lived available method that resolves the age of meteorites with a precision of  $\pm 200\,000$  years. These are indeed critical data used to better understand the processes that led to the Solar System formation. In this study, we attempted to date a chondrule by using the stepwise Pb-Pb dissolution method. We describe the protocol used for its cleaning, dissolution and lead extraction. We also want to evaluate a recently proposed limitation of the U-Pb method in general, namely  $^{222}\text{Rn}$  loss. This effect has been proposed to explain the observation that the age obtained with the U-Pb method is older than the age obtained by the  $^{26}\text{Al}$ - $^{26}\text{Mg}$  method. In this hypothesis, discordance is attributed to the loss of one isotope in the uranium decay chain,  $^{222}\text{Rn}$ , which is volatile and escapes the sample, leading to erroneously high Pb/Pb ratios. To test this theory, we dated a large fraction of zircons from a terrestrial granite, by the stepwise dissolution method



16h30



## Total synthesis of an advanced intermediate of Alstolactine A, *Clémence Topart (M1)*

*Laboratoire de synthèse et produits naturels, EPFL, Lausanne, Suisse*

**EPFL**

Alstolactine A belongs to the akuammiline alkaloid family that has been widely studied for decades. This family is characterized by a hindered cage-like structure and a large range of biological activities. Herein we report a 12-step synthesis of an advanced intermediate of this natural product from commercially available starting materials. Our approach features following key steps: a) creation of a quaternary stereocenter at an early stage; b) titanium trichloride mediated reductive cyclization to obtain an indolenine scaffold and c) rapid building-up of the  $\gamma$ -lactone.

## Development and use of a high throughput chemistry for C-N couplings, *Clémence Topart (césure)*

*Glaxosmithkline, Stevenage, UK*



High-throughput chemistry is an extremely valuable tool that has had a growing part in the pharmaceutical industry over the past decades. Herein we report the use and development of tools to accelerate the drug discovery process in GlaxoSmithKline (GSK). Array chemistry is particularly emphasized, and the following C-N reactions were carried in parallel: amide coupling, reductive amination,  $S_NAr$ , Buchwald coupling and Ullmann coupling. Buchwald and Ullmann couplings are very challenging reactions in an array format and further screening were performed. Side projects on novel photochemistry and ligand synthesis also emerged from those C-N coupling issues and aim at extending the medicinal chemist's tool box.