

ITI HiFunMat Master Internship Proposal

M 1

M 2

Exploration of novel pathway for the synthesis of trifluoromethyldiazirine derivatives for photoaffinity labelling in target- and binding-site identification

Internship supervisor

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Laboratory	LIMA
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Photoaffinity labelling is one of the methods used to study the interactions between low molecular weight biological substrate compounds with their biomolecular targets or receptors. The trifluoromethyldiazirine moiety is one of the most used and preferred photoactivatable crosslinking groups due to its favorable physicochemical properties, improved chemical and thermal stability in the dark, short UV irradiation time to generate the reactive carbene intermediate in high yields, predictable carbene insertion reactivity, and the ability to be activated at a wavelength benign for biomolecules.

Although various protocols have been developed to introduce trifluoromethyldiazirine functionality into organic compounds, these methods suffer from time consuming route, use of volatile, and toxic reagents and maintenance of low temperature for prolonged period.

In this internship, we will explore novel synthetic pathway based on photoinduced methods to introduce trifluoromethyldiazirine into complex bioactive molecules.

Proposition de stage de recherche à l'Institut Charles Sadron à Strasbourg

Description de l'offre

Équipe de recherche : IP2

Responsables : Doctorant Thomas Bugnand et Dr Michel Bouquey

Contexte : Soutien aux activités de recherche de Thomas Bugnand, doctorant travaillant sur un projet financé par l'ANR en partenariat avec une industrie.

Titre du stage : Synthèse de composites à base de polymères acryliques par polymérisation en plusieurs étapes

Sujet : Les systèmes acryliques sont couramment utilisés pour une multitude d'applications, que ce soit sous forme de matrice polymère seule ou de composite (mélange de particules solides avec la matrice polymère). Cependant, l'utilisation des acryliques présente certains inconvénients. La réaction de polymérisation génère beaucoup de chaleur et un retrait important. L'étude à mener porte sur la synthèse de polymères acryliques communs en plusieurs étapes afin de limiter ces phénomènes. Une des étapes de synthèse est en solution en présence de solvant (polymérisation par dispersion, par précipitation en présence ou non d'une charge). Les résultats seront à comparer avec une polymérisation en masse simple (en une étape).

Le travail consistera également à étudier les propriétés physico-chimiques des matrices obtenues (masse molaire, retrait, viscosité, détermination de la Tg, approche mécanique...), en se focalisant sur la synthèse de composites chargés.

Profil recherché : Nous recherchons un étudiant qui a un intérêt particulier pour la recherche, qui est à l'aise avec la synthèse en laboratoire et qui s'intéresse à la caractérisation des matériaux.

Pour postuler : Envoyer votre CV aux contacts.

Contacts :

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ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Modelising the pore growth in polyurethane matrices through a microfluidic setup

Internship supervisor

Name, first name	Wiebke Drenckhan-Andreatta & Luca Fiorucci
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Laboratory	Institut Charles Sadron (collaboration with BASF Polyurethanes)
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Wiebke Drenckhan-Andreatta

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	

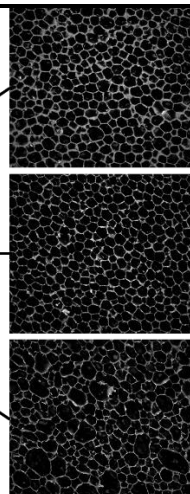
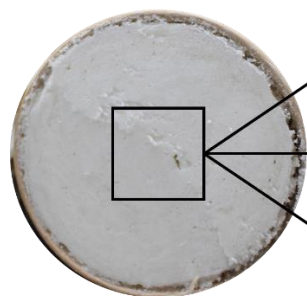
Internship description

Description

Over the last few decades, polyurethane foams have become the most widely used insulation material in the world and a key tool for achieving the climate goals of the Paris Agreement. The insulating properties of such materials depend largely on the morphology of their pores (e.g. size, connectivity). Although much effort has been made to understand the effect of different additives on the nucleation and to model the growth rate^{1,2}, a quantitative link between the used formulation, the nucleation rate and the growth rate of the pores is still lacking.

In the MIM (Mechanics of Interfaces and Multiphase Systems) team of the Institut Charles Sadron, and in collaboration with the multinational company BASF, we are therefore developing dedicated, microfluidic model experiments to elucidate the underlying processes.

As a first step, the internship student will optimise an existing microfluidic chip³ with respect to the chemical resistances of the chip and the architecture of the channels. He/she will then use this chip to quantitatively link and model the growth rate^{4,5} of gas bubbles in matrices of different compositions. The final aim of the internship will be to compare different additives in terms of their ability to nucleate, stabilise and grow pre-existing bubbles.



Cross-section of a polyurethane foam (left); Micrographs showing various foam morphologies after using different additives (right)

Requirements and application

We are looking for a highly motivated Masters 1 student with a background in physical chemistry, chemistry or material science and a strong interest in learning new techniques (CNC-milling, microfluidics, contact angle measurements, optical characterisation methods, etc.). The candidate should have a good level of English. French and German are an advantage. The intern will contribute on an international collaboration between the CNRS and our industrial partner BASF. He/she will work inside the ‘Mechanics of Interfaces and Multiphase Systems’ (MIM) team at the Charles Sadron Institute, an internationally renowned research unit of the CNRS, investigating various topics related to polymers and material science.

In case of interest, please submit your application (including CV and cover letter) to Dr. Wiebke Drenckhan-Andreatta (Wiebke.Drenckhan@ics-cnrs.unistra.fr) and Luca Fiorucci (Luca.Fiorucci@ics-cnrs.unistra.fr). The internship will take place at the Charles Sadron Institute which is located in a ZRR (zone à regime restrictif).

References

- (1) Pérez-Tamarit, S.; Solórzano, E.; Mokso, R.; Rodríguez-Pérez, M. A. In-Situ Understanding of Pore Nucleation and Growth in Polyurethane Foams by Using Real-Time Synchrotron X-Ray Tomography. *Polymer (Guildf)* 2019, 166, 50–54.
- (2) Blander, M.; Katz, J. L. Bubble Nucleation in Liquids. *AIChE Journal* 1975, 21 (5), 833–848.
- (3) Pivard, S.; Hourlier-Fargette, A.; Cotte-Carluer, G.; Chen, D.; Egele, A.; Lambour, C.; Schosseler, F.; Drenckhan-Andreatta, W. Bubbling up in a Lab-on-a-Chip: A Gravity-Driven Approach to the Formation of Polyelectrolyte Multilayer Capsules and Foams. *Colloids and Surfaces A* 2024.
- (4) Katz, J. L. Bubble Nucleation in Liquids.
- (5) Lubetkin, S. D. The Fundamentals of Bubble Evolution.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Biocompatible, in situ injectable, and curable foam for negative pressure therapy

Internship supervisor

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Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Context: The aims of wound healing by negative pressure therapy (TPN) systems are (i) to stimulate the mechanism that promote wound healing, (ii) to contract the wound edge, (iii) to improve local blood circulation, (iv) to stimulate the cell migration and proliferation, (v) to eliminate the exudates, (vi) to reduce the bacterial load. They are used for surgical wounds at high risk of complications, the non-saturable traumatic wounds, the wounds with extensive and/or deep loss of substance, with or without infection, and chronic wounds that do not heal in the first instance.

The limitations of the technique are the long process to apply the preformed foam that has to be cut to fit each wound, leading its administration can only be done by authorized nursing staff, which limits its use. This kind of foam have to be changed every 2 to 4 days (therapy lasts about 2 weeks), for the irregular wounds, the gauze is preferred and finally, the open-pores of the foam adheres to the wound tissue, causing pain to the patient and damage to the granulation tissue when changing foam is needed.¹

Goal of the project: Development of an injectable liquid foam form, in situ curable in deep wound for negative pressure therapy (TPN).

Methodology: prepolymer of the PU foams will be synthesized and the formulation of the foam will be optimized for the application.² The resulting foam will be characterized by rheology, microscopies (Numerical, Confocal, and SEM), tomograph, SAXS and WAXS. The foam will then be tested in mocked conditions with a TPN system.

References:

- (1) Lainé, P., La pression négative topique, *ACOPHRA*, Lyon, 2008; Lazaro, M. et Carre, E., La thérapie par pression négative, *ACOPHRA*, Lyon, 2018; Traitement des plaies par pression négative: des utilisations spécifiques et limitées, Haute autorité de santé, 2011.
- (2) Bonzani, I. C., *et al.*, *Biomaterials* 2007, 28, 423; medicaments.gouv.fr, (Ed.: santé, M. d. s. e. d. l.), base de données publique des médicaments, 2024; P. Bruin, J. Set al., *Biomaterials* 1990, 11, 291.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title : Natural Polymer Based Hydrogel for Supercapacitor Applications

Internship supervisor

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Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Supercapacitors have gained attention recently due to their high power density and their potential for numerous applications. [1] Nevertheless, the challenge is to increase their energy density, in order to compete with other energy storage materials. For this, a comprehension of the different supercapacitor components is crucial. One of the strategies is to develop hydrogel electrolytes that have better contact with the electrode material. The idea is to propose safe and easily-prepared hydrogel electrolytes with good mechanical and electrochemical properties for use in supercapacitor applications.

Hydrogel electrolytes present a potential alternative for conventionally used liquid electrolytes. [2] Their mechanical strength permits a limited degradation during ageing, and hence a longer lifetime prediction of the device. Moreover, their high water uptake enables a high ionic conductivity. The hydrogel electrolyte will be prepared using natural polymers such as gelatine or cellulose. Then, the preparation conditions will be adjusted to have the optimal self-standing hydrogels. The reticulation can be observed by IR spectroscopy while thermal stability can be assessed by TGA. The electrochemical performances will be tested using a two-electrode cell by cyclic voltammetry and galvanostatic charge discharge.

References:

- [1]: Simon, P., Gogotsi, Y. Materials for electrochemical capacitors. Nature Mater 7, 2008, 845–854.
[2]: Menzel, J., Frackowiak, E., Fic, K., Electrochimica Acta, volume 332, 2020, 135435.

Requirements:

We are looking for a motivated candidate willing to work in multidisciplinary environment, with a good background in materials science. Please address your application by e-mail.

receiving growing attention, but to the best of our knowledge layered oxides have not been explored yet for this purpose, contrarily to Layered Double Hydroxides or Metal Organic Frameworks,³² despite of the advantages they offer, such as great thermal and chemical stability. More specifically, in this project, while the inorganic hosts will consist in layered tantalate, layered niobate and layered titanates, the organic guest will be based on curcuminoid dye. Therefore, the guest molecules will be designed to favor persistent luminescence, and to be able to undergo insertion grafting reactions (*i.e.* being chemically stable in mild conditions and bearing an anchoring group).

- (1) Schaak, R. E.; Mallouk, T. E. Perovskites by Design: A Toolbox of Solid-State Reactions. *Chem. Mater.* **2002**, *14* (4), 1455–1471. <https://doi.org/10.1021/cm010689m>.
- (2) Sanjaya Ranmohotti, K. G.; Josepha, E.; Choi, J.; Zhang, J.; Wiley, J. B. Topochemical Manipulation of Perovskites: Low-Temperature Reaction Strategies for Directing Structure and Properties. *Adv. Mater.* **2011**, *23* (4), 442–460. <https://doi.org/10.1002/adma.201002274>.
- (3) Gopalakrishnan, J.; Sivakumar, T.; Ramesha, K.; Thangadurai, V.; Subbanna, G. N. Transformations of Ruddlesden–Popper Oxides to New Layered Perovskite Oxides by Metathesis Reactions. *J. Am. Chem. Soc.* **2000**, *122* (26), 6237–6241. <https://doi.org/10.1021/ja9914644>.
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- (6) Akbarian-Tefaghi, S.; Wiley, J. B. Microwave-Assisted Routes for Rapid and Efficient Modification of Layered Perovskites. *Dalton Trans.* **2018**, *47* (9), 2917–2924. <https://doi.org/10.1039/C7DT03865H>.
- (7) Wang, L.; Sasaki, T. Titanium Oxide Nanosheets: Graphene Analogues with Versatile Functionalities. *Chem. Rev.* **2014**, *114* (19), 9455–9486. <https://doi.org/10.1021/cr400627u>.
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- (10) Tahara, S.; Ichikawa, T.; Kajiwara, G.; Sugahara, Y. Reactivity of the Ruddlesden–Popper Phase H₂La₂Ti₃O₁₀ with Organic Compounds: Intercalation and Grafting Reactions. *Chem. Mater.* **2007**, *19* (9), 2352–2358. <https://doi.org/10.1021/cm0623662>.
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- (32) Gao, R.; Kodaimati, M. S.; Yan, D. Recent Advances in Persistent Luminescence Based on Molecular Hybrid Materials. *Chem. Soc. Rev.* **2021**, *50* (9), 5564–5589. <https://doi.org/10.1039/D0CS01463J>.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Plasma polymerization: investigation of physico-chemical properties of novel thin films

Internship supervisor

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Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

The research project:

Plasma polymer thin films are versatile coatings due to a broad range of factors. One important factor is the precursor used for the polymerization in the plasma reactor, as it influences the final chemical and physical properties of the thin film. The precursors are intrinsically linked to the formation and stability of the plasma film [1] as well as to the possible applications of the final coating [2]. The fact that the polymerization starts from species in the plasma state means that more varied chemical bonds can be created from the same precursors, when compared to other polymerization approaches. The tailoring of the polymer thin film properties can be performed by changing the operating parameters and the precursor chemistry. That makes plasma polymerization a flexible process, with potential applications from the textile to the pharmaceutical industries. In addition, plasma polymerization is performed in the absence of organic solvents, which appeals to its use as a greener process. The goal of the current offer is to **explore the plasma polymerization of original precursors and characterize the novel thin films**. The intern will have the opportunity to learn fundamental concepts of **surface functionalization and thin film characterization**, through the analysis of **physico-chemical and morphological properties** of the plasma polymers. The **3-month internship** will be carried in the **Institute of Materials Science of Mulhouse (IS2M, France)** and thus the intern will count with a set of available characterization techniques in the institute.

The missions of the intern:

The intern will carry out **plasma polymerization**. He/she will also perform **physico-chemical and morphological characterizations** of the surfaces using the available techniques at the IS2M (contact angle measurements, ellipsometry, infrared spectroscopy (FTIR), atomic force microscopy (AFM) ...).

Skills to be developed:

During the internship, the intern will develop disciplinary skills in materials chemistry, particularly in plasma treatments as well as in surface characterization. More generally, he/she will learn how to work within a research team, exploit data, use scientific databases, write a report and communicate on his/her results.

References:

- (1) Brioude, M. M. et al. Controlling the Morphogenesis of Needle-Like and Multibranched Structures in Maleic Anhydride Plasma Polymer Thin Films. *Plasma Process Polym* 2014, 11, 943–951.
- (2) Carneiro de Oliveira, J.; Meireles Brioude, M. de et al., Plasma polymerization in the design of new materials: looking through the lens of maleic anhydride plasma polymers. *Materials Today Chemistry* 2022, 23, 100646.

Candidate profile and application:

Master 1 student. Education in chemistry and/or materials science is required. The candidate is expected to show initiative and seriousness.

Applications including a CV and a cover letter should be sent electronically as soon as possible.

ITI HiFunMat Master Internship Proposal

M 1

M 2

MOFs as electrodes material for metal-ion batteries

Internship supervisor

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Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Derivatives of Alloxazines,¹ bio-inspired compounds, can be used for the formation of robust pillared coordination polymers, MOFs (Metal Organic Frameworks)². Allowing the presence of three stable redox states, the alloxazine motif, when appended with coordinating sites, can be a promising candidate for synthesizing new redox active MOFs, that can have application in energy storage devices.

We intend to extend the large library of pillared alloxazine MOFs (figure 1),³ that are then incorporated into an electrode of a metal-ion cell (Li or Na). The performances of the cells are studied through electrochemical studies. In order to tune the electrochemical properties, a special attention is paid on the structural changes observed during the charge/discharge processes of the battery.



Candidates motivated by inorganic synthesis, structural characterization, electrochemical studies, and the discovery of the synchrotron are highly encouraged to apply!

1 a) S. G. Mayhew, *The effects of pH and semiquinone formation on the oxidation-reduction potentials of flavin mononucleotide*, *Eur. J. Biochem.*, **1999**, 265, 698-702; b) F. Zarekarizi, M. Joharian, and A. Morsali, *Pillar-layered MOFs: functionality, interpenetration, flexibility and applications*, *J. Mat. Chem. A*, **2018**, 6, 19288.

2 H. Furukawa, K. E. Cordova, M. O'Keeffe, and O. M. Yaghi, *The Chemistry and Applications of Metal-Organic Frameworks*, *Science*, **2013**, 341, 6149.

3 J. Casas, D. Pianca, N. Le Breton, A. Jouaiti, C. Gourlaouen, M. Desage-El Murr, S. Le Vot, S. Choua, S. Ferlay, *Alloxazine based ligands appended with coordinating groups: synthesis, electrochemical studies and formation of Coordination Polymers*, *Inorg. Chem.*, **2024**, 63, 4802-4806. .

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Development of Ni@CrO_x electrocatalysts for the hydrogen evolution reaction

Internship supervisor

Name, first name	Asset Tristan; Guehl Julie
E-mail, Telephone	t.asset@unistra.fr ; julie.guehl@etu.unistra.fr, 0670410683
Laboratory	Institute for Chemistry and Processes for Energy, Environment and Health (ICPEES) Electrochemistry and energy conversion team
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Elena R. Savinova

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

This internship is a part of a project that aims to develop an alkaline membrane electrolyzer in which the catalytic materials exclude costly elements such as Pt, Ir, etc. Specifically, we focus on the design of the cathode's catalytic materials, where the reaction to reduce water to H₂ (*i.e.*, hydrogen evolution reaction – HER) takes place. Currently, Ni@NiO_x heterostructured materials are considered one of the most promising non-noble metal catalysts for said reaction¹: while metallic Ni has rather poor HER activity (Ni strongly adsorbing H), the presence of an optimal surface coverage in NiO_x substantially increase its activity. However, this NiO_x phase is not stable in the reducing HER conditions, leading to a gradual decrease of the electrocatalytic activity. This can be addressed by preparing an alloy made of NiCr (*e.g.* Ni/NiO-Cr₂O₃) materials. Indeed, Cr₂O₃ phase may act to stabilize the NiO_x during its operation, allowing the catalyst to retain the enhanced HER activity from synergistic Ni/NiO_x surface sites².

Considering this, the internship aims at the development of carbon-supported Ni@CrO_x composites, to (i) achieve high HER initial performance, owing to an optimized state of the electrode surface and (ii) maintain this high performance over extended periods of operation.

The student will develop alloys made of nickel and chrome via electrodeposition, first supported on a low-surface area glassy carbon electrode and then on a high surface area carbon black, and characterize their activity for the HER, as well as their stability during said reaction. The electrodeposition conditions will be optimized to finely tune the nanostructure shape and composition, using feedback from physicochemical (SEM, TEM, XPS, *etc.*) and electrochemical methods. The latter will include experimental determination of the HER kinetics (using voltammetry, impedance, *etc.*) and the effect of excursions at high/low potential on the surface chemistry, with a special attention to the stability of the surface oxides.

[1] A. G. Oshchepkov, et al. ACS Catal. 2019, 9, 9, 8520–8528

[2] M. K. Bates, et al. J. Phys. Chem. C 2015, 119, 10, 5467–5477

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title	Molecular Dynamics of Electrochemical systems
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Internship supervisor

Name, first name	Wolff, Jules; Asset, Tristan
E-mail, Telephone	juleswolff@unistra.fr , t.asset@unistra.fr
Laboratory	ICPEES – Equipe Electrochimie et Conversion d’Energie
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Elena R. Savinova

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	Fundamentals in coding

Internship description

- ◆ Whereas chemical reactions frequently occur in homogeneous environments, electrochemical reactions take place exclusively at the interface between an electrode and an electrolyte. Due to the localized nature of this reaction, understanding this interface is critical, as its properties can drastically affect the reaction kinetics. These properties are primarily influenced by the reorganization of the interface when a potential is applied to induce the reaction. Currently, the Guy-Chapman-Stern model is widely used to predict the distribution of charges as a function of distance from the electrode, within the first nanometers between the electrode and the core of the solution. This region is defined as the "electrochemical double layer" (EDL). However, this model has limitations. Firstly, it treats ions as point charges, *i.e.*, completely neglecting their volume and mass. Secondly, it does not account for neutral molecules (*e.g.*, water) that can nevertheless alter the electrolyte properties near the interface. In this context, the use of molecular dynamics allows for simulating a realistic representation of the reorganization of molecules in the solution when applying a potential while also accounting for uncharged molecules.
- ◆ Recently, a simulation tool called MetalWalls has been developed, offering the possibility to rigorously simulate electrodes and the applied potential (an illustration of an interface constructed through MetalWalls is presented in **Figure 1**, along with the cation distribution). In classical models, the electrode is approximated to a charged wall, but with MetalWalls, it is possible to dynamically represent the charge distribution in the electrode according to associated physical models. This feature of MetalWalls allowed our group to recently demonstrate/put in evidence that the dynamic of the charge is impacted by the cations size on Pt(100) surfaces. Hence, during this internship, the objective is to further investigate the effect of the cation nature (*e.g.*, Li^+) and of the Pt orientation (*e.g.*, Pt(110); Pt(111) – this on Na^+) on the organisation of the EDL as observed previously by MetalWalls. The selected candidate will study the impact of the cation/surface on the charge dynamic and identify solvent orientation trends based on simulation parameters. In this perspective, a solid knowledge of electrochemistry as well as a basic understanding of molecular dynamics and cheminformatics are necessary.

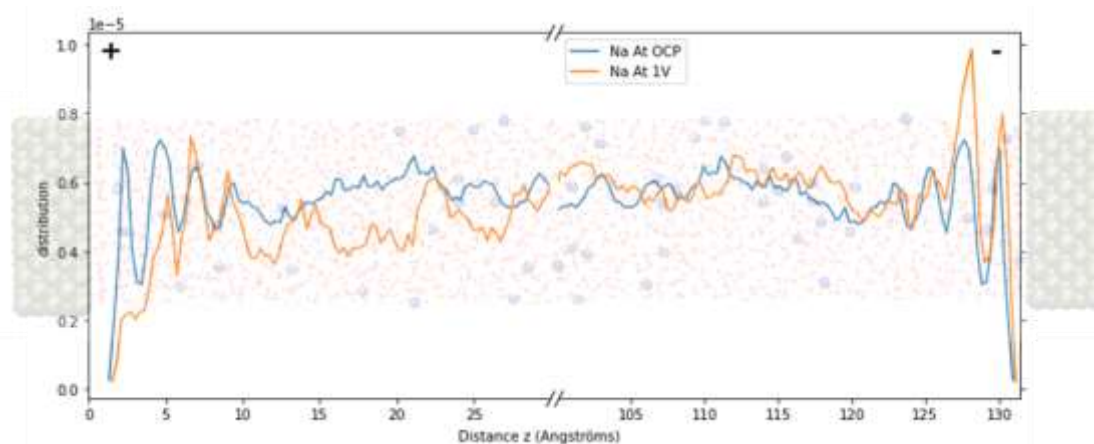


Figure 1. Distribution of the Na^+ cations in 1M NaOH near Pt(100) surfaces, in absence of an applied voltage (*i.e.*, at open circuit potential – OCP) and with a 1V voltage between the two electrodes stacked on a representation of the studied system

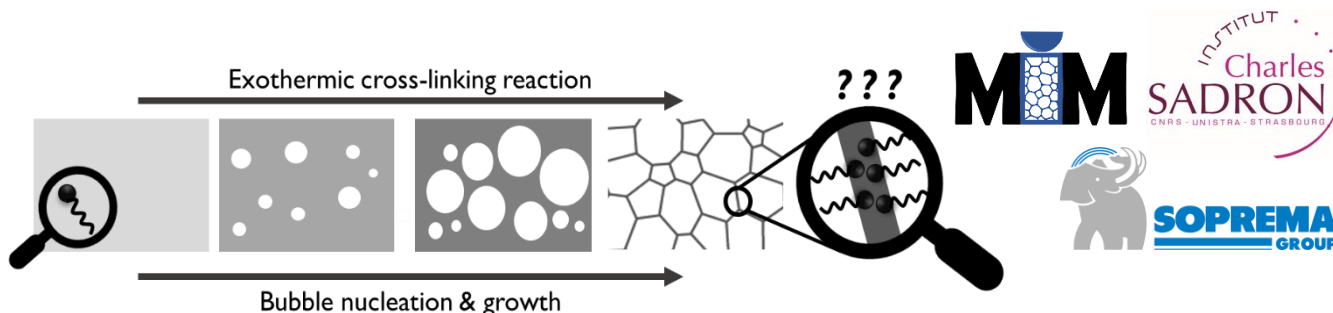
Research practical proposal in

“Towards sustainable polymer foams for thermal insulation” at the Charles Sadron Institute in Strasbourg

Description

Isocyanate-based polyurethane foams have been successfully optimized for thermal insulation for several generations, creating an annual production of billions of tons. However, increasing environmental concerns ask not only for even better insulation, but also for less harmful formulations.

Goal of this experimental project is therefore to participate in the activities of a collaboration between the MIM team at the ICS and the company SOPREMA to explore alternative, isocyanate-free formulations for the generation of new generations of thermally insulating polymer foams. We will focus on initially liquid systems containing physical blowing agents which evaporate into gas bubbles during an exothermic cross-linking reaction which eventually solidifies the foam. Of particular interest will be to establish the influence of the formulation on the final pore size and pore connectivity. We will also attempt to identify the relative importance of stabilizing agents with respect to the reaction kinetics. In order to establish the underlying mechanisms, we will combine foaming experiments with spectroscopic analysis, rheology and tomography.



Context

The internship will take place in the team “Mechanics of Interfaces and Multiphase Systems” (MIM) at the Institut Charles Sadron, an internationally renowned, interdisciplinary institute of the CNRS uniting chemists, physical chemists, physicists and engineers on a wide range of questions related to polymer science and materials. The internship student will interact closely with a postdoc working on this subject. The project is funded by a SOPREMA donation to the Strasbourg University Foundation and involves regular meetings with the company.

Possible techniques to be used

- Foaming techniques
- Interfacial tension measurements
- Rheology of reactive mixtures
- Mechanical, thermal and spectroscopic analysis of reactive blends and foams
- Computer tomography and scanning electron microscopy

Requirements & Application

We are looking for a motivated Masters student interested to work on an applied research problem. Good English skills are important for this internship.

Please address your application to drenckhan@unistra.fr and vipin.gopalakrishnan@ics-cnrs.unistra.fr.

ITI HiFunMat Master Internship Proposal

X M 1

X M 2

Title:

How do Molecules Process Information : Conformational Spread in Giant Megamer Proteins

Internship supervisor

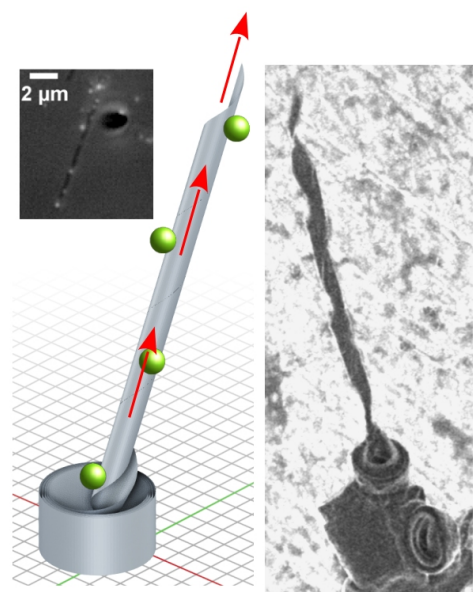
Name, first name	KULIC Igor & SCHMATKO Tatiana
E-mail, Telephone	tatiana.schmatko@ics-cnrs.unistra.fr , kulic@unistra.fr
Laboratory	Institut Charles Sadron, CNRS, Strasbourg
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes: I. KULIC , T. SCHMATKO, L. PIEUCHOT

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	

Internship description*

In Nature, we are surrounded by giant protein machines consisting of a large number of subunits that synergistically work together to achieve a common task. In our laboratory at ICS, CNRS in Strasbourg, we investigate the world's biggest synergistic protein network consisting of several millions of identical units. This supramolecular megastructure, called the "R body", once triggered by external stimuli cooperatively and rapidly switches its shape, from a compact scroll cylinder to a long tubular needle on sub-second timescales. Because of their enormous size, the shape transformations of R bodies can be followed in real time under the microscope, turning them into a unique model system for understanding the mystery of "conformational spread" – propagation of cooperative states in large multiprotein complexes.



In this combined theory/experiment M1 or M2 internship the student will learn how to quantitatively investigate and practically manipulate the conformational dynamics of R bodies and help us develop a computation model describing their collective lattice states. The internship will be in close collaboration with our partner Laurent Pieuchot (IS2M, CNRS, Mulhouse) and take place within a vibrant, growing environment of enthusiastic students and researches working together towards understanding the inner workings of this fascinating biomachine.

Requirements:

We are looking for a highly motivated, curious, analytical thinker from physics, cell physics, biophysics, polymer science and related fields with a taste for interdisciplinarity and learning new things. Experimental skills in (bio)polymers and Python programming are welcome but not mandatory.

The internship will take place at the Institut Charles Sadron, CNRS, Strasbourg with frequent meetings and some exchange visits to IS2M, CNRS, Mulhouse.

Contact: Applications to Tatiana SCHMATKO and Igor KULIĆ

tatiana.schmatko@ics-cnrs.unistra.fr , kulic@unistra.fr

** This internship may give rise to a Doctor thesis in continuation*

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Out of equilibrium dynamics of soft microparticles

Internship supervisor

Name, first name	Fabrice Thalmann
E-mail, Telephone	fabrice.thalmann@ics-cnrs.unistra.fr
Laboratory	Institut Charles Sadron UPR22, Strasbourg
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Stocco Antonio

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
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Internship description

At low Reynolds numbers, if a force is applied symmetrically in two opposite directions on the center of mass of a rigid object, at the end of the cycle the particle is expected to return to its initial state. More generally, the “scallop theorem” states that a rigid body showing some degrees of freedom cannot gain any net displacement after one cycle of reciprocal body motion when the surrounding fluid is purely viscous.¹ However, some differences are expected when the body is not rigid (and can undergo shape deformation) and when the fluid is not Newtonian. By tuning the frequency and amplitude of an external field in the cycle, an instability (e.g. buckling) or a non-linear effect (e.g. viscoelastic or viscoplastic effects) could be triggered. This may break the symmetry and results in a non-reciprocal body motion showing significant hysteresis. Hence, a shape deformation hysteresis of a soft particle may lead to swimming at low Reynolds numbers.¹

Self-propulsion under cycles of an external field has recently been reported for microbubbles coated with lipids. Pressure cycles induce asymmetric deformations due to buckling instabilities, which result in the microbubble propulsion at very high speeds, see Figure 1.²

In this internship we will study theoretically and experimentally the swimming of soft objects showing hysteresis. For experiments, giant vesicles able to be deformed under the effects of electric fields,³ ultrasounds⁴ and shear flows⁵ will be investigated.

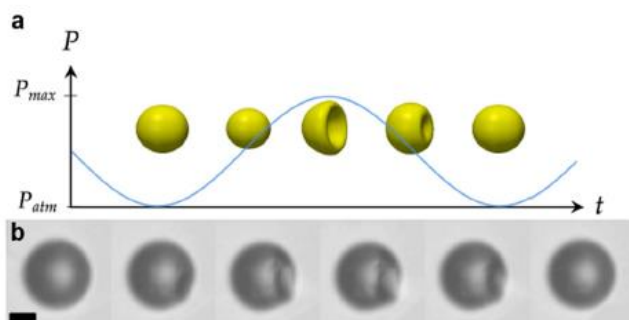


Figure 1. Reproduced from the literature: (a) Simulation results of the buckling of a spherical shell under a pressure cycle resulting in a non-reciprocal body motion. (b) Experimental observation of a buckling transition of a microbubble subjected to a pressure cycle.²

1. E. M. Purcell, Am. J. Phys., 1977 2. G. Chabouh et al., Commun. Eng, 2023. 3. M. Aleksanyan et al., Adv. Phys. X, 2023. 4. P. Marmottant et al., Proc. R. Soc. A Math. Phys. Eng. Sci., 2008. 5. M. Abkarian et al., Phys. Rev. Lett., 2002.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Synthesis of stimuli-responsive copolymers

Internship supervisor

Name, first name	VAUTHIER Madeline
E-mail, Telephone	madeline.vauthier@ics-cnrs.unistra.fr
Laboratory	Institut Charles Sadron
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	We are looking for a highly motivated Master 2 student interested in polymer chemistry and polymers' behavior in solution.

Internship description

Stimuli-responsive materials are undeniably attractive since they are able to adapt to their surrounding environment^{1,2} by creating reversible and specific interactions. This reversibility can be triggered by different environmental factors such as the pH, the light, a mechanical stress or temperature modifications for instance.

In this project, we are more precisely interested in the functionalization of copolymers to make them respond to a thermal stimulus. Thermally reversible materials fit in two categories: the ones based on reversible weak interactions³ and those based on reversible covalent bonds.⁴ The last ones are based on the reversible formation of covalent bonds according to the temperature of the system. Even though many studies report an effect of the temperature on the reversibility of a reaction, few reactions can be classified as thermoreversible reactions, in the sense that they lead to the formation of covalent bonds that are reversible only *via* a thermal stimulus. The Diels-Alder reaction⁵ is one of them and will be the topic of this internship. Since, in solution, copolymers tend to self-assemble to form micelles, cones or polymersomes.⁶ A look at the influence of temperature on the copolymers' aggregation behavior will also be investigated.

References

- 1) Theato, P. *et al. Chemical Society Reviews* **2013**, 42 (17), 7055–7056.
- 2) Alarcón, C. de las H. *et al. Chem. Soc. Rev.* **2005**, 34 (3), 276–285.
- 3) Amendola, V.; Meneghetti, M. *CRC Press*, **2011**.
- 4) Vauthier, M. *et al. Adv. Funct. Mat.* **2019**, 29 (10), 1806765.
- 5) Diels, O.; Alder, K. *Justus Liebigs Ann. Chem.*, **1928**, 460 (1), 98–122.
- 6) Discher, D. E. *et al. Progress in Polymer Science* **2007**, 32 (8), 838–857.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Synthesis of conjugated polymers for doped electronic applications

Internship supervisor

Name, first name	MERY, Stéphane
E-mail, Telephone	mery@ipcms.unistra.fr , 03 88 10 7165
Laboratory	IPCMS, Strasbourg
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : N. Leclerc, O. Bardagot (ICPEES) and M. Brinkmann (ICS)

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Since the Nobel Prize in Chemistry awarded to Heeger, MacDiarmid and Shirakawa on conducting polymers in 2000, conjugated polymers are today the focus of intense research for their application in organic electronics, and in particular the realization of lightweight, flexible and low-cost devices.

Good conduction properties arise from the self-assembly of π -conjugated polymers, achieved by microsegregation between conjugated polymer backbones and the presence of flexible side chains [1]. The addition of doping molecules to these polymers considerably amplifies the electrical conductivity of these systems [2]. However, the doping process and its mechanisms are still poorly understood. In particular, it is difficult to control the localization of dopants and avoid the destruction of self-assemblies.

The aim of the internship project is multidisciplinary and consists of synthesizing new high-performance π -conjugated polymers for doping. The molecular engineering work involves tailoring the side chains to (i) control the position of the dopant and (ii) stabilize the organization of the polymers in the solid state as thin films. Two applications in particular are targeted: electrochemical organic transistors [2] and thermoelectric devices [3,4].

In practice, the candidate will work essentially on the synthesis of organic conjugated systems and on polymerization. If interested, the candidate could also participate in the characterization of the physicochemical, electrical and charge transport properties in collaboration with other teams at the Cronenbourg Campus.

Selected publications by the host teams in the field: [1] N. Kamatham et al. *Adv. Funct. Mater.* **2021**, *31*, 2007734. [Link](#); [2] O. Bardagot et al., in Review in *Nature Materials*, **2023**. [Link](#); [3] P. Durand et al. *Adv. Energy Mater.* **2022**, *12*, 2103049. [Link](#); [4] V. Vijayakumar et al. *J. Mater. Chem. C* **2020**, *8*, 16470. [Link](#).

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Design of bimetallic nanostructures for plasmon-induced CO₂ recycling into methane

Internship supervisor

Name, first name	CAPS Valérie
E-mail, Telephone	caps@unistra.fr 06 21 33 29 06
Laboratory	ICPEES
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : CONSTANTIN Doru (ICS)

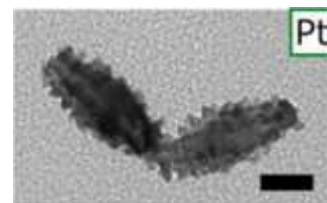
Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	

Internship description

Carbon dioxide is one of the major pollutants of our world. It is produced on a large scale, as an inevitable by-product of human activity, in particular of fossil fuel usage ($\text{CH}_4 + 2 \text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$). It is so far continuously released in the atmosphere, where it accumulates, with life-threatening consequences on climate change. What if CO₂ could be recycled and become the next generation, renewable and sustainable energy resource? At ICPEES, we have found that methane can be selectively and continuously produced from a CO₂/water mixture ($\text{CO}_2 + 2\text{H}_2\text{O} \rightarrow \text{CH}_4 + 2\text{O}_2$) using light as only energy source and plasmonic metal nanoparticles (M NPs) as catalyst. This appealing artificial photosynthesis process however critically depends on the composition of the M NPs. Segregated structures of bimetallic Au-Pt alloys in particular have appeared quite promising. So far, only Janus and core-shell NPs have been tested¹ and results suggest that structured NPs, with a large Au core covered by discrete smaller Pt NPs (rather than a full Pt shell, see Figure), could significantly boost the reaction rate.

This Master M2 internship will focus on the synthesis of such bimetallic nanostructures, according to previously established protocols,² on their purification, immobilization on relevant substrates and evaluation in the artificial photosynthesis of methane. The NPs will be characterized by scanning & transmission electron microscopy, X-ray photoelectron spectroscopy and UV-visible spectroscopy to correlate their photocatalytic performances, optical properties and nanostructures.



Work will take place in the Photocatalysis and Photoconversion (PHOTO) team of ICPEES. It will benefit from the experience of the team in artificial photosynthesis and from the experience of Doru Constantin in NPs synthesis and optical characterization. It will also benefit from the support of engineers and PhD researchers of the PHOTO team. The candidate is expected to be able to work both autonomously and in a team, with shared equipment and schedule.

This topic relates to both energy and environment.

¹ L. Hammoud, C. Strebler, J. Toufaily, T. Hamieh, V. Keller, V. Caps, Faraday Discuss. 242 (2023) 443.

² X. Li, J. Lyu, C. Goldmann, M. Kociak, D. Constantin, C. Hamon, J. Phys. Chem. Lett. 10 (2019) 7093.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title : Localized Photo-ElectroChemical measurements: Rapid optimization of photoelectrode materials for H₂ production

Internship supervisor

Name, first name	Cottineau Thomas
E-mail, Telephone	cottineau@unistra.fr / 03 68 85 28 14
Laboratory	ICPEES
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	

Internship description

The large amount of energy brought to Earth each year by sunlight, and its availability across the planet, makes it an attractive source of energy for future use. In addition to the conversion of photons into electricity in photovoltaic panels, new applications using semiconductor materials (SC) to convert light energy into chemical energy have emerged rapidly in recent times. These photoelectrochemical (PEC) approaches utilize thin-film electrodes to convert solar energy into storable chemical energy (solar fuel, e.g., H₂) or to degrade pollutants in air or water. While different research teams have obtained promising results, it appears that a single material cannot combine all the required properties in terms of light harvesting, charge carrier mobility (e⁻/h⁺ pairs), stability in water, and catalysis of redox reactions. It is therefore necessary to create composite electrodes combining different materials to ensure the various functions of the reaction. However, due to the complexity of these composite systems, optimization in terms of composition and morphology to achieve high performances requires a significant time investment.

Our team recently developed an original photoelectrochemical tool to accelerate the discovery of optimized structures of composite photoelectrodes. This method uses a small light spot as a probe to analyze the PEC efficiency of electrodes having variable properties along their surface (Fig. 1). This approach allows us to map the photoelectrode efficiency since the PEC reaction is only triggered under the illuminated area. Our team has already demonstrated promising results to optimize the light absorption in the case of TiO₂ nanotubes film with variable thickness (F. Gelb et al. *Sustain. Energy & Fuels*, 4, 2020, 1099). Furthermore, we demonstrate how this method can be used to determine some properties of the SC electrode *operando* in PEC conditions by modeling the numerous data obtained by mapping (S. Vergne et al. *Solar RRL*, 8, 2024, 2400156).

Based on these promising initial results, the main objective of the internship will be to utilize this approach for composite electrodes. The study will focus on the influence of the concentration of CoO nanoparticles, deposited on the surface of TiO₂, as a co-catalyst to accelerate the water-splitting reaction. The first task will be to synthesize photoelectrodes with a variable TiO₂ film thickness and a variable cocatalyst loading using methods developed in our laboratory. Subsequently, the local PEC properties will be investigated to determine the structure and composition providing the best PEC performance. The photocurrent mapping results will be fitted using a physical model of the reaction to determine the charge carrier transport properties and the efficiency of the charge transfer kinetic at the semiconductor/electrolyte interface.

This project is for a Master 2 student in the field of Chemistry, Physico-Chemistry or Material Science. It requires a strong motivation for experimental work and an ability to work on the multidisciplinary aspects of the project such as materials synthesis, electrochemistry, data treatment, optic, *etc.* The work will be done at the ICPEES on the campus of Cronenbourg (ZRR) and a PhD on the same topics can potentially follow this master's internship.

For more information and to apply please send a **CV and a motivation letter to Thomas Cottineau (cottineau@unistra.fr ; 03 68 85 28 14)**

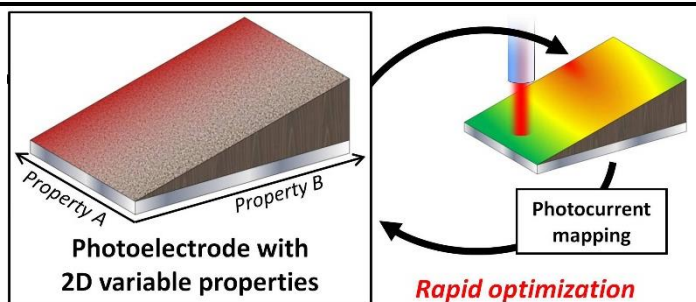


Figure 1: Schematic principle of the method for rapid measurement of functional properties of photoelectrode

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Synthesis and photophysical study of new potential photosensitizers for stimulative photodynamic therapy

Internship supervisor

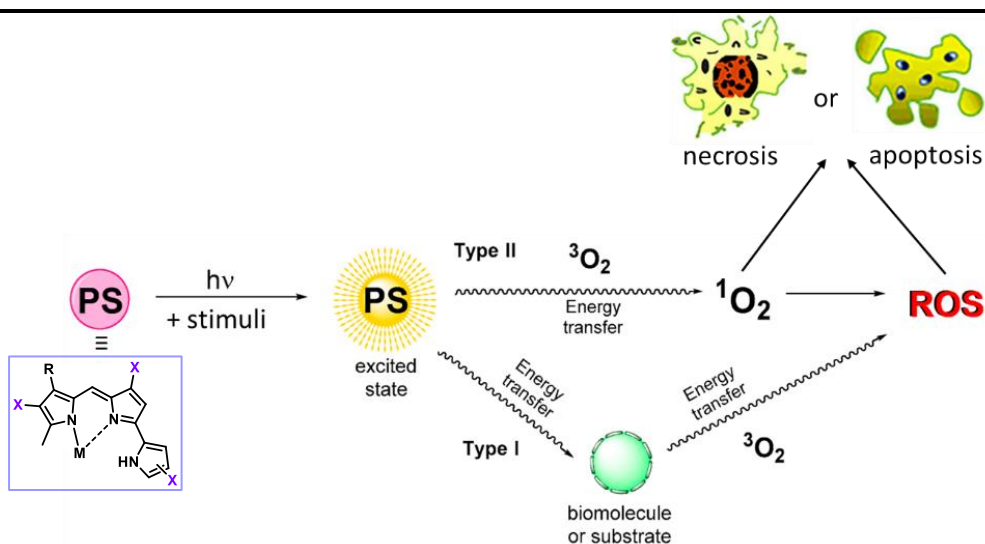
Name, first name	Figliola, Carlotta
E-mail, Telephone	figliola@unistra.fr
Laboratory	UMR 7515, Institut de Chimie et Procédés pour l'Environnement, l'Energie et la Santé (ICPEES)
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	Highly motivated candidate with good training in organic chemistry and willing to learn different spectroscopic and electrochemical techniques.

Internship description

Photodynamic therapy (PDT) is a photochemistry-based medical treatment combining two non-toxic components, *i.e.* the light at specific wavelength and a photosensitizer (PS). The absorption of the light by the PS produces the reactive oxygen species (ROS) and the singlet oxygen ($^1\text{O}_2$), both causing cell death followed by an inflammatory and immune response. PDT has been known for over 30 years as a promising anticancer and antimicrobial treatment, but it is still used as complement to other therapeutic solutions, such as radiotherapy, chemotherapy, and surgery. In case of head and neck cancers (HNC), PDT is an interesting and promising alternative with better outcomes than these treatments in terms of morbidity, mutilation, and other significant side effects affecting patients' compliance. Our laboratory proposes to evaluate the potential stimuli-activated PDT activity of new dyes, which are inspired to known and clinically approved PS. This internship will be dedicated to the synthesis of prodigiosin-inspired chromophores and their step-by-step functionalization. Each synthetic modification will be verified by photophysical studies, such as light absorption, fluorescence emission, $^1\text{O}_2$ production and electrochemical measurements. In case of promising candidates, the intern will also have the opportunity to perform the cytotoxic tests evaluating the *in vitro* photodynamic activity in the project partner laboratory, the Laboratory of Bioimaging and Pathologies (LBP, UMR 7021), on the Illkirch University campus.



Key words: Multi-step organic synthesis, fluorescence, singlet oxygen.

Application: please send CV, motivation letter and M1 final grades to Dr. Carlotta Figliola (figliola@unistra.fr).

ITI HiFunMat Master Internship Proposal

M 1

M 2

Solar light driven Fe-based heterogeneous catalysts for the degradation of biorecalcitrant antibiotics in water

Internship supervisor

Name, first name	KELLER, Nicolas
E-mail, Telephone	nkeller@unistra.fr – 03 68 85 28 11
Laboratory	ICPEES – Institut de Chimie et Procédés pour l’Energie, l’Environnement et la Santé, UMR 7515 CNRS/Université de Strasbourg, 25 rue Becquerel
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Water treatment is a priority health issue that scientists must address. In particular, in hospitals and the care sector, wastewater is polluted by medical products (antibiotics, anti-cancerous, anti-inflammatory or contraceptive drugs). Impact on the world’s population health is dramatic at short- and long-term, with eg. higher cancer risks and reduction of the human reproductive capacity, as treatments in place to date are not efficient enough.

In this field of research of prime importance, solar light driven Advanced Oxidation Processes (AOPs) are promising sustainable cost-effective and efficient water treatment technologies. They generate highly active HO_x[°] radicals at ambient temperature, that react with the pollutants and further with the reaction intermediates to yield full mineralization of pollutants. Along this line, ICPEES lab developed a leadership in the design of (low energy input) solar light driven Fe-based heterogeneous catalysts able to act simultaneously as Fenton-type catalysts and photocatalysts [1].

- **Fe-based Fenton-type catalysts are able to decompose under solar light hydrogen peroxide (H₂O₂), a green oxidant that forms H₂O and O₂ as byproducts.**
- **Photocatalysts are materials able to drive catalytic transformations of molecules using the redox properties developed at the surface of a semiconductor material under solar light for conducting reduction and oxidation reactions.**

Combination of both catalytic functions in one single body is a highly promising way to enhance reaction rates and photonic efficiencies in water treatment. So, the internship will aim at investigating new solar-light driven Fe-based heterogeneous catalysts combining both functions and able to degrade fastly contaminants of emerging concern such as antibiotics in water. The work will concentrate on the design of innovative heterogeneous solar-light driven catalysts and their physico-chemical characterizations, as well as on the evaluation of their catalytic behaviors under solar light.

The internship will be part of ANR- and IdEX-funded projects. It will benefit from the scientific, technical and human resource environment provided by the ‘Photocatalysis and Photoconversion’ team, and fully equipped with the necessary tools to conduct the research.

1. Appl. Catal. B: Environ. 262 (2020) 118310 ; ACS Appl. Mater. Interfaces, 12(51) (2020) 57025.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Solar light driven synthesis of H₂O₂ from H₂O and O₂ on 2D-layered g-C₃N₄ based catalysts

Internship supervisor

Name, first name	KELLER Nicolas
E-mail, Telephone	nkeller@unistra.fr – 03 68 85 28 11 – 06 74 87 52 95
Laboratory	ICPEES UMR 7515 CNRS-Université de Strasbourg
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Hydrogen peroxide (H₂O₂) is an efficient and environmentally friendly oxidant due to its large active oxygen content (47 wt.%), relatively high oxidation potential (E°=1.763 V vs. NHE at pH 0), easy-handling and non-toxic oxidation by-products (water and oxygen). These properties make H₂O₂ suitable for varied applications like wastewater treatment (eg., Fenton processes and disinfection), chemical manufacturing or pulp bleaching, with an annual worldwide production over 5 Mt. Moreover, H₂O₂ is also a promising energy-carrier alternative to hydrogen, since it can be used as fuel in single-compartment cells and can be conveniently transported and stored.

Currently, H₂O₂ is produced industrially by the well-known high E-factor and low atom efficiency multi-step anthraquinone process, which requires high energy input and generates large amounts of wastes (eg. organics-containing wastewater, solid waste). Thus, it is worth to develop cost-effective and sustainable approaches for H₂O₂ production. In this context, solar light-driven photocatalysis has emerged as it utilizes H₂O and molecular O₂ as raw materials, and solar light as energy supply. Photocatalysis is also a worth strategy for the safe and cost-efficient implementation of decentralized small-scale production units as well as for the *in-situ* synthesis of H₂O₂ for use as oxidant in high-efficiency chemical reactions.

2D-layered graphitic carbon nitride (g-C₃N₄) is a prominent candidate for H₂O₂ synthesis because of its relatively narrow band gap (*ca.* 2.7 eV), suitable electronic structure for O₂ reduction and a high chemical stability [1]. g-C₃N₄ benefits also from easy, low-cost preparation methods, as well as from its metal-free and non-toxic nature.

The internship will study to which extent the photonic efficiency and the production rate of H₂O₂ from H₂O and O₂ under solar light can be significantly enhanced by implementing synthetic strategies based on molecular and electronic modifications of g-C₃N₄ photocatalysts. The work will focus on designing innovative heterogeneous solar-light driven catalysts and their characterizations, as well as on the evaluation of their catalytic behaviors under solar light.

The internship will benefit from the scientific, technical and human resource environment provided by the 'Photocatalysis and Photoconversion' team at ICPEES.

- Ru*-modified graphitic carbon nitride for the solar light-driven photocatalytic H₂O₂ synthesis, L. Valenzuela, [...], N. Keller **Catal. Today** 441 (2024) 114881 ; *Photocatalysis synthesis of hydrogen peroxide from molecular oxygen and water*. P. Garcia-Munoz, [...] N. Keller, **Top. Curr. Chem.** 381(4) (2023) 15

ITI HiFunMat Master Internship Proposal

M 1

M 2

Solar light driven photocatalysis for the synthesis of H₂ solar fuel by reforming of plastics

Internship supervisor

Name, first name	KELLER, Nicolas
E-mail, Telephone	nkeller@unistra.fr – 03 68 85 28 11
Laboratory	ICPEES – Institut de Chimie et Procédés pour l’Energie, l’Environnement et la Santé, UMR 7515 CNRS/Université de Strasbourg, 25 rue Becquerel
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

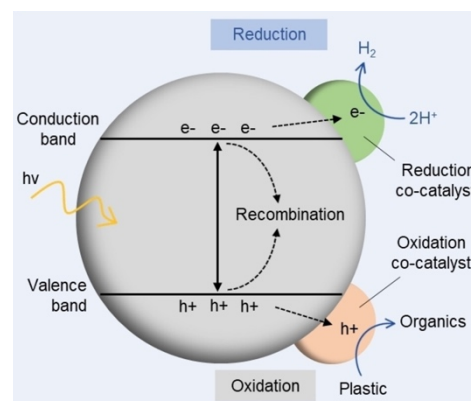
Internship description

Plastics, as one of the most influential invention of the 20th century, has been widely applied in our daily life. Currently, about 360 million tonnes are produced each year. However, only a small portion of the produced plastics is recycled after use, and around 80% of all plastics is directly incinerated, thereby contributing extensively to the CO₂ release and global warming, or discarded as wastes in landfills or in the natural environment, with high negative environmental impacts. Additionally, solar hydrogen (H₂) is a versatile energy carrier and a promising source of (sunlight-derived) clean energy to tackle vital energy challenges stemming from the combustion of fossil fuels.

The internship will aim at studying **the ability of the photocatalysis technology to produce H₂ as solar fuel from plastic wastes at ambient temperature using simulated solar light as sole energy input**. Indeed, heterogeneous photocatalysis is a low energy-input technology able to drive catalytic transformations of molecules at ambient temperature, that uses the redox properties developed at the surface of a semiconductor material under solar light for conducting reduction and oxidation reactions.

The work will concentrate on the design of innovative heterogeneous photocatalysts associating different semiconductor materials (TiO₂, g-C₃N₄, etc.) and decorated with metal nanoparticles as co-catalyst. It will be focused on both synthetic and physico-chemical characterization aspects, as well as on the evaluation of the photocatalytic behavior of the materials synthesized.

Depending on the progress of the work, the ability of solar light photocatalysis to produce high added-value organic chemicals as side-products of the hydrogen generated will also be studied by means of several analytical techniques.



Reforming of plastics into H₂ and organic by solar light-driven photocatalysis

nanostructures through seed-mediated growth of zinc oxide nanorods covered by metal and metal oxide nanoparticles in a similar way as we reported (Azeredo et al. *J. Mater. Chem. C*, 6, **2018**, 10502). The characterization of such nanostructures will require a wide panel of techniques (X-ray diffraction, infrared and UV-visible spectroscopies, electron microscopies, XPS, granulometry ...). The photoelectrochemical properties will be investigated at ICPEES. This research work will also give opportunities to interact with numerous researchers in Strasbourg. This project is for a Master 2 student in the field of Chemistry, Physico-Chemistry or Material Science. It requires a strong motivation for experimental work and an ability to work on the multidisciplinary aspects of the project such as materials synthesis and characterization, photoelectrochemistry, *etc.*

For more information and to apply please send a **CV and a motivation letter to Benoit Pichon (pichon@ipcms.unistra.fr) and Thomas Cottineau (cottineau@unistra.fr)**

This project is for a master 2 student in the field of Chemistry, Physico-Chemistry or Material Science. It requires a strong motivation for experimental work and an ability to understand the multidisciplinary aspects of the project such as electrochemistry, optic, materials synthesis *etc.* For more information and to apply please contact **Thomas Cottineau** (cottineau@unistra.fr) or **Olivier Bardagot** (bardagot@unistra.fr) ICPEES (campus Cronenbourg ZRR).

Daily work will include:

- Bibliographic study of the bilirubin/TiO₂ interactions
- Processing of (semi)conducting polymers in solution (mainly PEDOT:PSS)
- Synthesizing TiO₂-Nanotubes gate electrodes
- Molecule grafting on TiO₂ (physico-chemistry of interfaces)
- Scanning electron microscopy (SEM) to visualize the resulting gate electrodes
- OPECT manufacture
- Electrical characterization of OPECT (transfer, output)
- Time-resolved Vis/NIR absorbance spectroscopy during OPECT operation
- Data analysis using Python (computing)
- Calibration and use in 'test' and 'applicative' conditions of novel biosensors
- English writing and oral presentation

Hard skills which will be learnt:

- Bibliographic search
- Database management
-
- Electrochemical synthesis
- Surface chemistry
- Polymer processing
- Vis-NIR absorbance spectroscopy
- Electrochemistry
- Computing (Python for heavy data analysis and graph plotting, LabVIEW if interested)

Soft, transferable, skills which will be learnt:

- Collaboration, teamwork
- Effective communication
- Scientific data presentation (oral and written in English)
- Project management (time management, supply management, etc)
- Progress reporting
- Creativity/independency (depending on the will of the student)

References:

1. **High-performance OECT manufacture:** O. Bardagot*, P. Durand, S. Guchait, G. Rebetez, P. Cavassin, J. Réhault, M. Brinkmann, N. Leclerc, N. Banerji, *In Review - Nature Materials*, **2023**, 10.21203/rs.3.rs-3221543/v1
2. **OECT doping kinetics:** B. T. DiTullio, L. R. Savagian, O. Bardagot, M. De Keersmaecker, A. M. Österholm, N. Banerji, J. R. Reynolds, *J. Am. Chem. Soc.* **2023**, *145*, 122–134.
3. **TiO₂ Nanotube synthesis:** F. Gelb, Y.-C. Chueh, N. Sojic, V. Keller, D. Zigah, T. Cottineau*, *Sustainable Energy Fuels* **2020**, *4*, 1099–1104.
4. **TiO₂-based sensors:** D. Spitzer, T. Cottineau, N. Piazzon, S. Josset, F. Schnell, S. N. Pronkin, E. R. Savinova, V. Keller, *Angewandte Chemie International Edition* **2012**, *22*, 5334–5338.
5. **TiO₂-gated OECT:** M.-J. Lu, F.-Z. Chen, J. Hu, H. Zhou, G. Chen, X.-D. Yu, R. Ban, P. Lin, W.-W. Zhao, *Small Structures* **2021**, *2*, 2100087.

Required skills

- Background in materials science
- Rigorous experimental work
- Curious and proactive.
- Ability to work in a team and communicate results

Skills to develop during the M2 internship

- Electrospinning
- Structural characterization of electrospun membranes: SEM, porometry...
- Fluorescence spectroscopy
- Mass transfer

Références

- [1] D. Mailley, A. Hébraud, G. Schlatter, A Review on the Impact of Humidity during Electrospinning: From the Nanofiber Structure Engineering to the Applications, *Macromolecular Materials and Engineering* 306 (2021) 2100115. <https://doi.org/10.1002/mame.202100115>.
- [2] B. Gross, G. Schlatter, P. Hébraud, F. Mouillard, L. Chehma, A. Hébraud, E. Lobry, Green Electrospinning of Highly Concentrated Polyurethane Suspensions in Water: From the Rheology to the Fiber Morphology, *Macromolecular Materials and Engineering* 2400157. <https://doi.org/10.1002/mame.202400157>.
- [3] J. Magisson, A. Sassi, A. Kobalyan, C.-T. Burcez, R. Bouaoun, M. Vix, N. Jeandidier, S. Sigrist, A fully implantable device for diffuse insulin delivery at extraperitoneal site for physiological treatment of type 1 diabetes, *Journal of Controlled Release* 320 (2020) 431–441. <https://doi.org/10.1016/j.jconrel.2020.01.055>.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Study of the electrospun nanofibers morphology obtained from liquid-liquid dispersions containing fluorophore-labelled polymers for biomedical applications

Internship supervisor

Name, first name	LOBRY Emeline and FIGLIOLA Carlotta
E-mail, Telephone	elobry@unistra.fr and figliola@unistra.fr
Laboratory	ICPEES
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Contexts and missions

The work will be carried out at the Institute of Chemistry and Processes for Energy, Environment and Health (ICPEES UMR7515) as part of a collaborative project between the COMBO (<https://icpees.unistra.fr/chimie-moleculaire-et-analytique/mari/themes-de-recherche/>) and the POLYFUN team (<https://icpees.unistra.fr/en/polymer-engineering/electrospinning/>).

Electrospinning can be used to produce polymer nanofibrous materials. The architecture of both the mat and the fibre can be controlled to be used for a variety of applications (air filtration, biomedical, energy, etc.). Traditionally, nanofibres are obtained by solubilising the polymer in a mixture of organic solvents that are often toxic to health and the environment. In addition, the polymers used are sometimes not very soluble and the production of nanofibres is limited by the rheological properties of the solutions, making it difficult to obtain average submicron diameters. To overcome these limitations, this project involves formulating liquid-liquid dispersions, in which each phase will be labelled with a fluorophore to characterise the nanofibers.

The project will be divided in three tasks:

- 1) The synthesis of biocompatible polymers covalently functionalized by a fluorophore. These polymers will be then electrospun to form fluorescent fibrous mats whose photophysical properties will be studied for further studying specific cell development.
- 2) the study the photophysical properties of model liquid-liquid dispersions and their electrospinning. The aim here is to identify the operating conditions (droplet size, dispersed phase concentration, nature

of the phase solvents) that will enable the structuring of the fibres (morphology, distribution of the different phases within the fibre) to be controlled.

3) the combination of the previous two points to prepare nanostructured materials for biomedical applications (drug delivery, anti-cancer treatment, etc.).

Required skills

- Strong background in organic synthesis
- An interest in polymer science and photochemistry
- Rigorous experimental work
- Curious and proactive.
- Ability to work in a team and communicate results

Skills to develop during the M2 internship

- Synthesis of fluorophores
- Polymer functionalization by covalent grafting of fluorophores
- Formulation
- Electrospinning
- Characterisation techniques (SEM, NMR spectroscopy, UV/Visible spectroscopy, confocal fluorescence microscopy)

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Elaboration of mesoporous conducting polymer layers for ammonia sensor

Internship supervisor

Name, first name	Binieck, Laure
E-mail, Telephone	Laure.binieck@ics-cnrs.unistra.fr , 03.88.41.41.78 https://www.ics-cnrs.unistra.fr/member-346-Binieck%20Laure.html
Laboratory	Institut Charles Sadron* – Campus de Cronenbourg - Strasbourg
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Nicolas Leclerc, Olivier Bardagot, Patrick Lévêque

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

With the expansion of the myriad applications for ammonia, the development of reliable, low-cost detectors has become a socio-economic necessity. However, there are still many advances to be made to ensure high sensitivity, selectivity and stability of the sensors.

Our project is focusing on three main innovations which, combined, should enable the selective detection of low concentrations of NH₃ using organic field effect organic transistors. [1]

(i) New n-type air-stable conducting polymers based on PNDI-2T, highly sensitive to NH₃ (ii) Mesoporous thin films of these polymers in order to increase sensitivity; (iii) A new method for processing data measured by OFETs to increase selectivity.

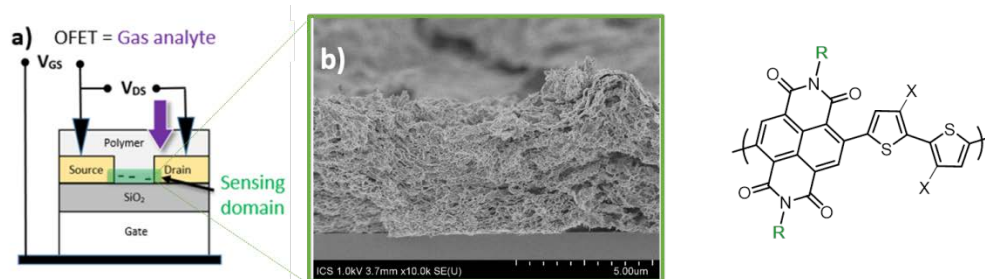


Figure: Field effect transistor schematic which sensing domain is composed of n-type porous conducting polymer.

The aim of this internship is to develop new processing methods to promote the self-assembly of polymer chains in solution. This will play an important role in the charge transport properties in the solid state. Then, porosity will be introduced using the freeze-drying method. [2]. The effect of

freezing conditions (solvent, freezing rate, freezing temperature) will be modulated to control the porosity of the films. The structure of the films will be characterized by scanning electron microscopy. The final aim is to fabricate field effect transistors (with porous conducting channels) and characterize the charge transport properties under ammonia exposure.

References:

- [1] O. Bardagot, P. Lévêque et al. J. Mater. Chem. C **11** (2023) 14108.
- [2] Q. Weinbach, L. Biniek et al, J. Mater. Chem.C (2023), 11, 7802-7816

Requirements & Application

We are looking for motivated and creative team-worker master student interested in organic electronics and willing to learn about polymers processing, scanning electron microscopy, and charge transport properties. The candidate is expected to be at ease with physical-chemistry of polymers and not afraid of multidisciplinary field.

Please address your application including a CV, a motivation letter and Master transcript of records to Laure Biniek, SYCOMMOR Team, Institut Charles Sadron.

Possible starting date : Jan -February 2025

***Note that the lab is within a ZRR (Zone à Régime Restrictive)**

Requirements & Application

We are looking for motivated and creative team-worker master student interested in supercapacitors and willing to learn about polymer science, scanning electron microscopy, and electrical and electrochemical properties. The candidate is expected to be at ease with physical-chemistry of polymers and not afraid of multidisciplinary field.

Please address your application including a CV, a motivation letter and Master transcript of records to Laure Biniek and Sirine Zallouz, Institut Charles Sadron.

Possible starting date : Jan -February 2025

***Note that the lab is within a ZRR (Zone à Régime Restrictive)**

Anisotropic n-type Thermoelectric Polymers ***prepared by polarity switching***

Supervisor: Martin Brinkmann , directeur de recherche

Laboratory : Institute Charles Sadron, 23 rue du loess, 67034 Strasbourg (ZRR)

Description. Plastic electronics has become a major field of both fundamental research and innovative applications in industry. Organic Light Emitting Diodes (OLEDs) are now integrated in a routine way in new electronic items such as smartphones and TVs. New applications are now currently attracting researchers in plastic electronics, in particular in the field of thermoelectricity. Thermoelectric materials have the capability to convert a temperature gradient in electric current or vice versa. They can be used in numerous places such as industry, cars or intelligent textiles where lost heat could be recovered and converted to electricity. Efficient TE materials are usually semi-conductors or conductors and must show high electric conductivity, high Seebeck coefficients ($S=\Delta V/\Delta T$) and low thermal conductivity. So far, inorganic materials were dominating the field of TE, but, in the last decade, it has been demonstrated that polymeric systems such as PEDOT-Tos show remarkable TE properties.¹

In this internship, we propose to investigate a simple method to fabricate stable and effective n-type thermoelectric polymer films. Therefore, we combine orientation of polymer chains in thin films using the method of high temperature rubbing developed at ICS and the mechanism of polarity switching that allows to turn a doped p-type material into an n-type one.^{2,3} We will use a new doping strategy to achieve this objective by combining redox dopants and Lewis acids. In this work, we will investigate under which conditions the polarity switching p→n can be observed. In a second step, we will investigate the stability of the new n-like materials in inert atmosphere and ambient.

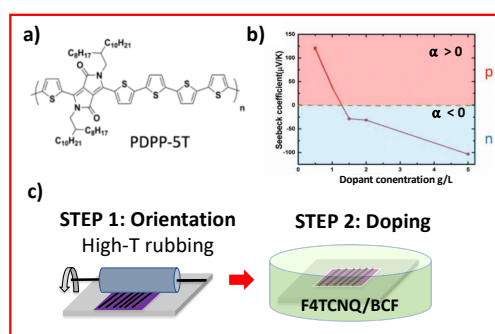


Figure 1. (a) Molecular structure of the donor-acceptor polymer. (b) Typical polarity inversion of the Seebeck coefficient upon heavy p doping of PDPP-ST. (c) Preparation method of aligned polymer films by rubbing (step 1) and sequential doping in solution of a dopant mixture F4TCNQ/BCF (step 2).

The student will have the opportunity to work in a dedicated environment for plastic electronics i.e. perform all processing under controlled atmosphere. The student will perform the characterization of the devices from a structural point of view (transmission electron microscopy) and from the electronic point of view (conductivity and Seebeck coefficient) so as to draw structure-property correlations. Polarized UV-vis-NIR and FTIR spectroscopies will also be used to follow the doping processes.⁴ The student will be integrated in an international team working on two collaborative projects on n-type TE materials (ITN Horates and ANR Thermopolys) as well as other projects (ANR TRIPODE and SMOOTH). The successful applicant will be invited to pursue for a PhD that is funded by the ANR TRIPODE.

(1) O. Bubnova et al., *Nat. Mat.* **2011**, 10, 429.

(2) H. Zeng, M. et al. *Advanced Electronic Materials* **2021**, 7, 2000880.

(3) S. Guchait, Y. Zhong, M. Brinkmann, *Macromolecules* **2023**, 56, 6733.

(4) S. Guchait, et al. *Advanced Functional Materials n/a*, 2404411.

Contact: Martin Brinkmann; e-mail: martin.brinkmann@ics-cnrs.unistra.fr

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Catalytic localism in layer-by-layer composite films for light-driven water treatment

Internship supervisor

Name, first name	FELIX Olivier
E-mail, Telephone	olivier.felix@ics-cnrs.unistra.fr , 03.88.41.40.67
Laboratory	CNRS – Institut Charles Sadron
Collaboration with a HiFunMat member <i>(please indicate their name)</i>	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : KELLER Nicolas, PLOUX Lydie

Student profile looked for

Master program <i>(more than one box can be ticked)</i>	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Water treatment is a priority health issue that scientists must address. In particular, in hospitals and the care sector, wastewater is polluted by medical products (antibiotics, anti-cancerous, anti-inflammatory or contraceptive drugs). Impact on the world's population health is dramatic at short- and long-term, with eg. higher cancer risks and reduction of the human reproductive capacity, as treatments in place to date are not efficient enough.¹ The development of novel sustainable cost-effective water treatment technologies is thus necessary.² In this context, H₂O₂-driven photo-Catalytic Wet Peroxide Oxidation (CWPO) catalysis is a high-prospect advanced oxidation process operating under solar light for mineralizing those refractory compounds in water at room-temperature. Albeit very active, and although H₂O₂ is a green oxidant, producing only H₂O and O₂ as end-products, this catalysis still faces a limited perspective for technological deployment, that results from the use of costly and non-sustainably produced H₂O₂ instead of O₂ as oxidant.

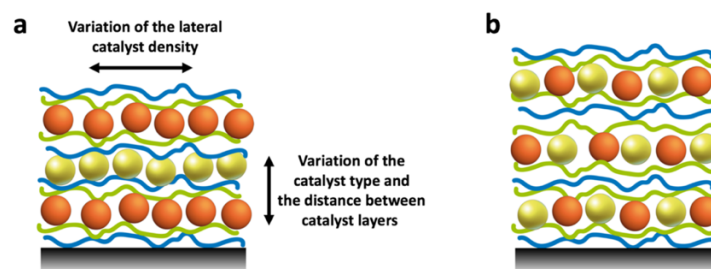


Figure. Schematic representation of idealized catalyst-based LbL-assemblies.

The aim of this master work, which is part of the CATLOC HiFunMat project, is to contribute to the development of a novel multi-functional catalysts for solar light-driven water treatment, by applying a strategy of catalytic (chemical) localism. This new concept proposes to combine two catalysts working

in synergy under solar-light, the first one producing H₂O₂ from molecular water and O₂, and the second one using H₂O₂ for degrading the pollutants. To do so, we will rely on the bottom-up layer-by-layer self-assembly³ to precisely control the spatial positioning of both catalysts and the resulting properties of the multilayer catalysts.⁴ The novelty here relies on the replacement of organic polyelectrolytes by inorganic polyelectrolytes, namely polyoxometalates, to improve the stability of films against self-oxidation issues, induced by the production of highly active oxidative radicals within the layers. The use of different building blocks (catalysts, polyelectrolytes), deposition methods and deposition conditions will allow exploring various assembly structures and determining those leading to the most relevant properties for our application. This work will be carried out in collaboration with ICPEES and BIOMAT labs.

References:

- [1] C. Baines *et al. Environ. Int.* **2021**, *149*, 106391.
- [2] D. B. Miklos *et al. Water Res.* **2018**, *139*, 118.
- [3] G. Decher *Science* 1997, *277*, 1232; Multilayer Thin Films: Sequential Assembly of Nanocomposite Materials, 2nd Edition (Eds: Decher, G. and Schlenoff, J. B.), Wiley-VCH: Weinheim, 2012.
- [4] D. Dontsova *et al. Macromol. Rapid Commun* **2011**, *32*, 1145 ; L. Truong-Phuoc *et al. ACS Appl. Mater. Interfaces* **2016**, *8*, 34438 ; M. Motay *et al. ACS Appl. Mater. Interfaces* **2020**, *12*, 55766.

Requirements & Application:

We are looking for a highly motivated master student having a formation in chemistry, physical chemistry, materials science, nanoscience and preferably with skills and/or interests in the following areas: materials, physical chemistry, thin layers, catalysis and surfaces.

Please address your application (CV, motivation letter, copy of recent grades) to Olivier Félix [olivier.felix@ics-cnrs.unistra.fr].

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Constructing complex multilayer stacks from sustainable materials with anisotropic properties

Internship supervisor

Name, first name	FELIX Olivier
E-mail, Telephone	olivier.felix@ics-cnrs.unistra.fr , 03.88.41.40.67
Laboratory	CNRS – Institut Charles Sadron
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : ROLAND Thierry

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Nature has developed composite materials (*e.g.* plant cell walls and Arthropod exoskeleton) with complex and hierarchical organization from the nano- to the macro-scale via molecular assembly. Such materials often possess remarkable optical and/or mechanical properties by simply assembling hard and soft elements. The outstanding properties of these materials have prompted the fabrication of bio-inspired composites.

Among all methods available for the preparation of multifunctional nanostructured composite materials, Layer-by-Layer (LbL) assembly,[1] is currently one of the most simple and versatile nanofabrication method.[2] Recently, we have assembled isotropic and anisotropic transparent wood-inspired nanocomposite materials with mechanical properties challenging even medium quality steel (Figure 1, middle).[2][3] The combination of LbL assembly with grazing incidence spraying (GIS)[4-6] has permitted us to extend our approach toward the preparation of complex (*e.g.* helical) multilayer films (Figure 1, right) in which the composition and orientation of anisotropic nano-objects like nanocelluloses can be controlled independently in each layer (Figure 1, left).

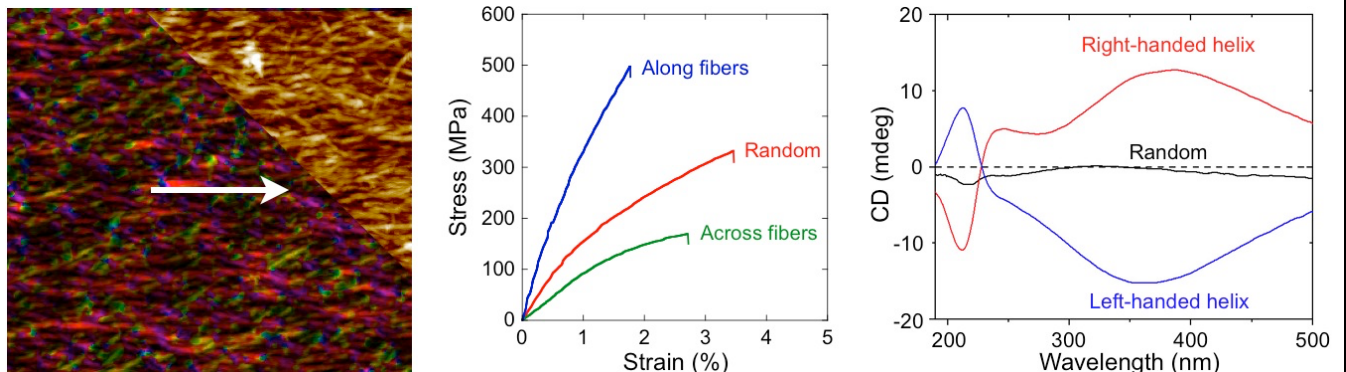


Figure. (left) In-plane alignment of cellulose nanofibers deposited by GIS. (middle) Mechanical properties of random and oriented nanocomposite films. (right) CD spectra of random and helical films with opposite handedness.

The goal of this internship is to study the preparation of nanocellulose-based composite materials using different deposition methods (dipping, spray-assisted, GIS, ...) and various surface analysis techniques (ellipsometry, UV-vis spectroscopy, ...) and their optical and mechanical properties. The performance of these materials will be determined by advanced mechanical and optical characterization tools as a function of their composition and structure, the orientation of reinforcing agents, and the experimental conditions. This work will involve the PECMAT and MIM teams at Institut Charles Sadron (Strasbourg, France) and a collaboration with the CERMAV (Grenoble, France) and LCP-A2MC (Metz, France).

- [1] G. Decher *Science* **1997**, *277*, 1232.
- [2] R. Merindol, S. Diabang, O. Felix, T. Roland, C. Gauthier, G. Decher *ACS Nano* **2015**, *9*, 1127.
- [3] R. Merindol *et al.* *ACS Nano* **2020**, *14*, 16525.
- [4] R. Blell, X. Lin, T. Lindström, M. Ankerfors, M. Pauly, O. Felix, G. Decher, *ACS Nano* **2017**, *11*, 84.
- [5] R. Mujica *et al.* *Compos. Sci. Technol.* **2023**, *233*, 109889.
- [6] R. Mujica *et al.* *Adv. Mater.* **2024**, *36*, 2401742.

Requirements & Application:

We are looking for a highly motivated master student having a formation in physical chemistry, chemical engineering or materials science and preferably with skills and/or interests in the following areas: materials, physical chemistry, thin layers, polymers and surfaces.

Please address your application (CV, motivation letter, copy of recent grades) to Olivier Félix (olivier.felix@ics-cnrs.unistra.fr).

ITI HiFunMat Master Internship Proposal

M 1

M 2

Novel Recyclable Multifunctional Biporous Materials Based on Poly(Ionic Liquid)s

Internship supervisor

Name, first name	Grande Daniel
E-mail, Telephone	daniel.grande@ics-cnrs.unistra.fr , 03 88 41 40 16
Laboratory	Institut Charles Sadron (ICS)
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

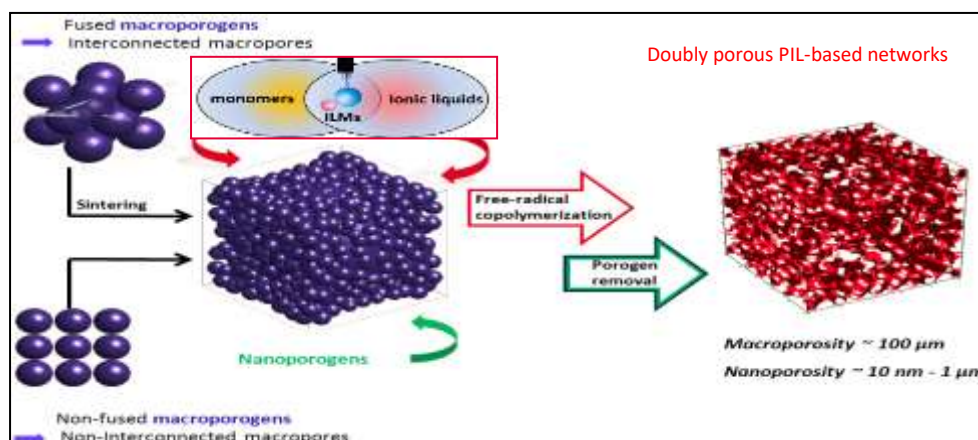
Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

This Master 2 internship aims at developing novel recyclable multifunctional biporous materials based on poly(ionic liquid)s (PILs) meant for important environmental issues. First, the double porogen templating approach will be exploited to elaborate biporous PIL networks with controlled pore surface functionality and morphology. Then, such ionic polymer materials will be investigated in CO₂ adsorption and subsequent conversion into fine chemicals, along with their recyclability. Removal of heavy metals or per- and polyfluoroalkyl substances (PFAS) in contaminated water is another potential application of major interest for the tailor-made PIL networks.

The Master student will benefit from unique expertise (molecular chemistry, macromolecular engineering, polymer processing) and state-of-the-art platforms (physico-chemical characterization, electron microscopy, X-ray tomography) available at ICS.



The ICS is an interdisciplinary Institute dedicated to soft matter science, and more particularly self-assembled systems and polymeric materials, at the interface of chemistry, physical chemistry and physics. It is located on the CNRS Cronenbourg campus in Strasbourg. As it is a ZRR (restricted regime zone) laboratory from CNRS, an authorization is required prior to any access to the Institute.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title Optical probes for the measurement of viscosity in complex coacervates

Internship supervisor

Name, first name	Monreal Santiago, Guillermo and Vahdati, Mehdi
E-mail, Telephone	monrealsantiago@unistra.fr; mehdi.vahdati@ics-cnrs.unistra.fr
Laboratory	Coacervates and Systems Chemistry, Équipe SFAM, UMR7140
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Mehdi Vahdati

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	An open-minded, curious, and interactive student ready to work as part of a multidisciplinary research team. Interest in polymer physical chemistry, microscopy, and or rheology is a plus. Fluent communication in English is a requirement. No previous experience in confocal microscopy, rheology, or chemical synthesis is required.

Internship description

Context

Biomolecular condensates are micrometer-sized droplets that form in the cytosol due to the interactions between different biomolecules, in a process called liquid-liquid phase separation (LLPS). They are involved in a broad range of cellular processes, from RNA transcription to the formation of amyloid plaques during the development of neurological diseases [1]. It has been hypothesized that their mechanical properties (such as their viscosity) are connected to their function. However, condensates are normally not mechanically characterized – since not many techniques can measure the mechanical properties of liquids at such a small scale [2].

Fluorescent probes show great promise to study the mechanical properties of small volumes of liquid. For example, the viscosity of a medium can be calculated from the speed at which fluorescent molecules diffuse through it, or by the speed at which part of a fluorescent rotor can spin around a single bond [3]. Optical techniques such as these can be performed non-invasively in a confocal microscope, on very small amounts of sample, and in their native environment. However, calculating viscosity values from them requires several assumptions and simplifications. To continue using these techniques to characterize biomolecular condensates, they must be verified and calibrated against standard, bulk methods.

Objectives

In this project, the intern will work with complex coacervates as models for biomolecular condensates. Complex coacervates are droplets formed via LLPS due to the interactions between charged polyelectrolytes [4]. Unlike biomolecular condensates, complex coacervates can be easily prepared at a large scale and studied with standard techniques for materials. The intern will first prepare a series of complex coacervates, and characterize their mechanical properties using bulk techniques such as oscillatory and rotational rheology. Once that the mechanical properties of the different coacervates are well known, the intern will use fluorescent probes to calculate the viscosity of the same systems from confocal microscopy measurements. Comparing the outcome of both types of techniques will determine if the optical methods can be validated for this purpose, or if other factors also need to be taken into consideration.

References

[1] Banani, et. al. *Nature Reviews Molecular Cell Biology* 2017, 18 (5), 285–298; [2] Jawerth, et. al. *Physical Review Letters* 2018, 121 (25), 258101; [3] Paez-Perez, Kuimova, *Angewandte Chemie Int Ed* 2023, e202311233; [4] Vahdati, et. al. *Progress in Polymer Science* 2023, 139, 101649.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title Coupling of Nanoindentation and Microsphere-Assisted Microscopy for the Characterization of Polymer Surfaces

Internship supervisor

Name, first name	Pecora Marina, Gauthier Christian
E-mail, Telephone	marina.pecora@ics-cnrs.unistra.fr , 03 88 41 40 11 christian.gauthier@ics-cnrs.unistra.fr
Laboratory	
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Sylvain Lecler , IPP / Icube

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	

Internship description

Context and Background

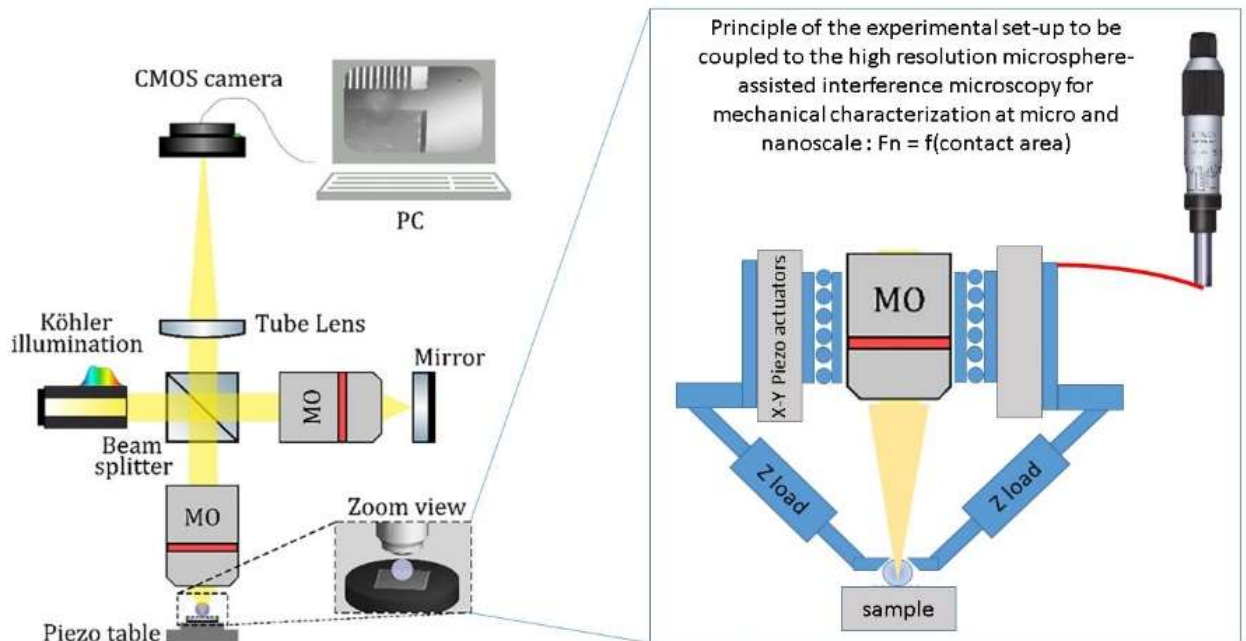
The instrumented indentation test is one of the few experimental techniques that allows for the local characterization of materials with heterogeneities, property gradients, or confinement in small regions, such as thin layers, coatings, and adhesives. Traditional indentation tests involve pressing a rigid indenter tip into the surface of a material and measuring the tip's displacement as a function of the applied force. The analysis of the force-displacement curve, often using the Oliver and Pharr method [1], enables the determination of key mechanical properties such as the elastic modulus and hardness. However, this method is less effective for polymers due to their viscoelastic and time-dependent behavior, complicating the analysis and interpretation of indentation data.

A recent collaborative project between two research teams—the Mechanics of Interfaces and Multiphase Systems team (MIM) at the Charles Sadron Institute (ICS) and the Photonics Instrumentation and Processes team (IPP) at the ICube laboratory—led to the development of a new instrumented indentation setup (see figure below). This device integrates microsphere-assisted microscopy [2] for in-situ observation of polymer surfaces during contact. It allows for the observation of non-transparent polymers with sub-micron resolution, overcoming the limitations of existing methods [3], such as low resolution and the restriction to transparent materials.

Objectives of the Internship

The newly developed device requires initial validation through testing on standard materials and comparison with results from commercial devices. The student will then focus on optimizing the optical setup and analyzing high-resolution images of the contact areas captured during indentation.

Once the setup is validated, the student will study time-dependent behaviors by performing a series of indentation experiments on various polymer substrates. These experiments will include creep tests, relaxation tests, recovery tests, and cyclic loading tests. The analysis and interpretation of the results will require a thorough literature review on instrumented indentation of polymer surfaces [4-6].



From A. Leong-Hoi et al. *Phys. Status Solidi A*, 215(6) : 1700858

Figure. Microsphere-assisted microscopy device [2] (left) and working principle of the new experimental set-up coupling microsphere-assisted microscopy and nanoindentation (right)

Skills and Profile

The ideal candidate should have a background in materials science, mechanical engineering, or physics, with a focus on polymer characterization, and a strong interest in experimental work.

Interested candidates can send their application (CV, motivation letter and recent grades) to Marina Pecora (marina.pecora@ics-cnrs.unistra.fr) and Christian Gauthier (christian.gauthier@ics-cnrs.unistra.fr)

[1] W.C. Oliver and G.M. Pharr. *J Mater Res*, 7(6):1564–1583, 1992.

[2] A. Leong-Hoi et al. *Phys. Status Solidi A*, 215(6) : 1700858.

[3] T. Chatel et al. *J Phys D Appl Phys*, 44 :1–10, 2011.

[4] M. Hardiman et al. *Polym Test*, 52:157–166, 2016.

[5] O. Smerdova et al. *J Mater Res*, 34(21): 3688-3689, 2019.

[6] S. Yang et al. *J Appl Phys*, 95(7):3655–3666, 2004.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Exploration of the link between structure and properties of Elastin-like peptides

Internship supervisor

Name, first name	Rodon-Fores, Jennifer
E-mail, Telephone	jennifer.rodon-fores@ics-cnrs.unistra.fr
Laboratory	Institut Charles sadron
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Context: Supramolecular materials arise from non-covalent interactions between molecular building blocks that self-assemble in a bottom-up approach into well-organized functional structures. Forming a network of fibers with a branched appearance, elastin provides elasticity to tissues, such as skin and arteries, ensuring that they remain in their original state after the application of an external force.¹ The elastic property of elastin is due to its high content of hydrophobic amino acids, which hide from the aqueous medium, leading to partially stretched conformations.² Studies carried out on tropoelastin have revealed the existence of a repeating sequence of amino acids, valine – proline – glycine – valine – glycine (VPGVG) pentapeptide. This sequence forms β -turn structures leading to the formation of a β -spiral, important for the elastic properties.³

The goal of the project: The amino acids and their order have tremendous importance on peptide/protein properties. The objective of the project is to deliver a library of elastin-like peptides and dig into the relationship between the peptide sequence (the order of the amino acids) and the secondary structure and rheological properties of the obtained hydrogels. To this aim, modified Fmoc-VPGpY peptides will be synthesized by combinatorial chemistry by changing the order of amino acids and their structural and rheological properties will be characterized.

Methodology: A combinatorial peptide library will be synthesized, and the selection assay will be optimized to obtain self-assembling peptides. Then, the best conditions of gelation will be determined as well as the robustness of the system. The gel characterization will be done by inverted tube test, rheology, fluorometry, fluorescent microscopy, UV-Vis spectrophotometry and infra-red spectroscopy.

References

- (1) Wang, K., et al., Elastin Structure, Synthesis, Regulatory Mechanism and Relationship with Cardiovascular Diseases. *Front Cell Dev Biol*, 2021, 9, 596702.
- (2) Alberts B., et al., *Molecular Biology of the Cell*. Garland Science. New York 2002.
- (3) Chaffey, N., et al., *Molecular biology of the cell*. 4th edn. Annals of Botany, 2003, 91, 401.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Effect of unsaturation position within phospholipids on oxidation of simple model of cell membranes

Internship supervisor

Name, first name	Schmatko tatiana, Muller Pierre
E-mail, Telephone	Tatiana.schmatko@ics-cnrs.unistra.fr
Laboratory	Institut Charles Sadron
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Oxidation plays a central role in the lifecycle of eukaryotic cells, as it can influence the levels of biological self-assembly embodied by intracellular and plasma membranes. Oxidation is a natural metabolic outcome. It is a direct consequence of many processes such as mitochondrial respiration, inflammation, virus phagocytosis, ultraviolet and ionic irradiation, to name only a few. Lipid constituents of membranes are highly prone to oxidation, mainly on unsaturations of their alkyl chains. Previous studies of the physical effects of lipid oxidation have shown that it may lead to modifications in the membrane properties such as permeability, headgroup hydration, fluidity, thickness, and packing order. However, the most prominent physicochemical effect of lipid oxidation is the membrane area increase [1]. In this internship, the student will use a previously developed experimental protocol and analysis method, developed in the team [2], to measure the membrane area increase as a function of the position of the lipid unsaturation within the aliphatic tail. Giant Unilamellar vesicles (GUVs), which are closed membrane capsules, will be grown using a gel assisted template technique [3], with different unsaturated phospholipids. Glass surfaces will be modified to allow controlled adhesion of the GUV to the surface. Combined epifluorescence and RICM (Reflection Interference Contrast Microscopy) experiments will be performed to measure precisely the increase of total membrane area. Oxidation will be induced by photosensitizers irradiated with intensive light, leading to a well-controlled hydroperoxidation reaction. The reorganization of the hydroperoxidized molecule within the membrane is expected to depend heavily on the distance between the unsaturation and the lipid head group, which is the key aspect of interest for this internship.

[1] Weber G., Charitat T., Baptista M. S., Uschoa A. F., *et al.* Soft Matter (2014), Vol 10 p 4241

[2] Aoki P. H. B., Schroder A. P., Constantino C. J. L., and Marques C. M. Soft Matter (2015) Vol 11 p 5995

[3] Weinberger A., Tsai F. C., Koenderink G. H., Schmidt T., *et al* Biophys. J. (2013) Vol 105 p 154

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title Biosourced Complex Coacervates for the Development of Tissue Adhesives

Internship supervisor

Name, first name	Vahdati, Mehdi and Precheur, Maxime
E-mail, Telephone	mehdi.vahdati@ics-cnrs.unistra.fr maxine.precheur@ics-cnrs.unistra.fr
Laboratory	CNRS, Institut Charles Sadron
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	Candidates with a profile in in the physical chemistry of (bio-sourced) polymers and biomedical applications. Experience and or good marks in polymer physical chemistry is a plus.

Internship description

Context

Replacing invasive wound closure procedures such as sutures and staples with minimally invasive adhesives and sealants is a well-established need in the field of medical devices. Most current surgical adhesives and sealants rely on the in-situ polymerization and or cross-linking of a liquid-like precursor to form strong bonds to tissues [1]. Several natural organisms, such as mussels and sandcastle worms, have developed robust underwater adhesives based on complex coacervates of charged biomacromolecules [2]. Polyelectrolytes complex coacervates are obtained via associative phase separation of a polycation (positively charged polymer) and a polyanion (negatively charged polymer) in aqueous medium. The polymer-rich materials obtained have good wetting properties (important for bonding to substrates) and widely tuneable viscoelastic properties. Model and bio-inspired complex coacervates have shown great potential for the development of soft tissue adhesives [3]. Our group recently highlighted the potential of bio-sourced complex coacervates in this context [4].

Objectives

The internship subject aims to study the phase behavior and mechanical properties of bio-sourced complex coacervates for potential biomedical applications. The intern will investigate different combinations of polysaccharides as bio-sourced polymers to develop a library of complex coacervates. The parameters of the study include the chemistry, molecular weight, and concentration of the polymers as well as the salt concentration. The composition of the complex coacervates will be studied via thermogravimetric analysis and the mechanical properties will be characterized using a rheometer.

References

[1] Ge, Chen, *Polymers*, 2020, 12; [2] Hofman, et al. *Adv. Mater.* 2018, 30; [3] Vahdati, et al. *Prog. Polym. Sci.* 2023, 1392; [4] Galland, et al. *JCIS*, 2024, 661.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title **Physics and mechanics of polymer solutions and gels in novel green solvents**

Internship supervisor

Name, first name	Vahdati, Mehdi and Lescure, Mathilde
E-mail, Telephone	mehdi.vahdati@ics-cnrs.unistra.fr mathilde.lescur@ics-cnrs.unistra.fr
Laboratory	CNRS, Institut Charles Sadron
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	Candidates with a profile in polymer physical chemistry, polymer physics, and soft matter mechanics are encouraged to apply. Experience in polymer physical chemistry is a plus; no experience in polymer chemistry is required.

Internship description

Context

Organic- Soft polymers networks swollen in water, known as hydrogels, are promising for many applications from biomedical devices to soft robotics. The use of hydrogels is limited by their low fracture resistance and their short-term environmental stability. Current strategies to reinforce the fracture resistance of hydrogels consist in providing the polymer network with energy dissipation mechanisms [1], for instance, by introducing a first sacrificial network into double-network hydrogels [2].

In this context, little attention has been paid to potential effects of the solvent. Deep Eutectic Solvents (DES) are an emerging class of green solvents formed due to hydrogen bonding interactions between hydrogen bond donors and acceptors at specific compositions. These typically viscous liquids are particularly interesting due to their widely tunable physico-chemical properties, dense network of hydrogen bonding, and extremely low volatility [3]. Preliminary results from our group show that single-network gels prepared in a model DES have enhanced nonlinear mechanical properties compared to their hydrogel counterparts.

Objectives

The goal of the internship is to investigate DES as polymerization medium and its effects on the network structure and mechanical properties of polymer networks. The role of the solvent viscosity and hydrogen bonding network will be studied for a library of polymer solutions and gels synthesized in different solvents. The solutions will be characterized via size exclusion chromatography and rheology. In the case of the gels, the swelling degree, gel content, and mechanical properties (in compression) will be determined.

References

[1] Creton, C. *Macromolecules*, 50 8297–8316 (2017); [2] Gong, J. P. *Advanced Materials*, 1155–1158 (2003); [3] Hansen, B. *Chemical Reviews*, 121 1232–1285 (2021).

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title Tuning the thermomechanical properties of novel sustainable polymeric materials

Internship supervisor

Name, first name	Vahdati, Mehdi and Cedano, Francisco
E-mail, Telephone	mehdi.vahdati@ics-cnrs.unistra.fr francisco.cedano@saint-gobain.com
Laboratory	CNRS, Institut Charles Sadron in collaboration with Saint-Gobain Recherche Aubervilliers
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	Candidates with a profile in polymer physical chemistry, polymer physics, and materials science are encouraged to apply. Experience in polymer physics and/or thermomechanical characterization techniques will be a plus.

Internship description

Context

Organic-based binders widely used in the construction chemicals sector allowed to build low-cost, long lasting and high-performance structures. To reach carbon neutrality by 2050, this industrial sector requires new products that can be recycled, reuse or deconstructed easily, while being low cost, water based, versatile in different environments, and performing as conventional products. Lately, Saint-Gobain has developed new bio-inspired materials based on complex coacervation to meet these industrial challenges. These coacervates have many potential applications in various fields, including coatings, binders, and adhesives.

In collaboration with Institut Charles Sadron (ICS), Saint-Gobain Research Paris (SGR P) has developed coacervate-based formulations that cure when sprayed with water reducing work time for the users. However, controlling the mechanical properties, and in particular the flexibility, of the final materials (i.e. once dry) is a challenge.

The main objective of this internship is to formulate at ICS novel coacervates in close collaboration with SGR P and to study different parameters on the composition and the mechanical properties of coacervates before and after application. In particular, the goal is to explore various polymers of different molecular weights to develop a library of coacervates with wide-ranging mechanical properties.

Objectives

1. Formulate coacervates using different polymers by adjusting salt concentration and or pH
2. Determine the composition the coacervates using thermogravimetric analysis (TGA)
3. Mechanical characterization of the coacervates via linear rheology
4. Determine the thermomechanical properties of dry coacervates
5. Transfer of formulations and technical meetings between ICS and SGR P

ITI HiFunMat Master Internship Proposal

M 1

M 2

Encapsulation of fragrance molecules in polymeric particles

Internship supervisor

Name, first name	VAUTHIER Madeline
E-mail, Telephone	Madeline.vauthier@ics-cnrs.unistra.fr
Laboratory	Institut Charles Sadron
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : SERRA Christophe

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

Micro- and nano-technologies are fast-growing fields, with a wide range of potential applications such as diagnosis and treatment of diseases, cosmetics, electronics, paints, etc.^{1,2} However, the laborious processes of manufacturing particles and the highly transdisciplinary nature of this area, still remain obstacles to a fast development of these technologies in the perfume industry.

In this project, we're looking at polymer particles capable of encapsulating different types of (highly volatile) fragrances thanks to a microfluidic version of a homemade, extremely efficient emulsification device.³⁻⁵ The quantity and chemistry of the encapsulated molecule as well as those of the polymer, and the process operating variables are all parameters influencing the encapsulation and release of those molecules of interest.

During this internship you will learn how to combine physical chemistry, microfluidic processes and polymer science to elaborate fragrance-loaded (nano)particles with controlled release profiles, and more.

References

- 1) Prasad, R. *Fungal Nanotechnology - Springer*. **2017**, 55–75, ISBN: 978-3-319-68424-6.
- 2) Sozer, N. *et coll. Trends in Biotechnology*. **2009**, 27 (2), 82-89.
- 3) Yu, W. *et al. Macromol. React. Eng.* **2017**, 11 (1), 1600024.
- 4) Chang, Z. *et al. Lab on a Chip* **2009**, 9, 3007-3011.
- 5) Abdurahim, J. *et al. J. Drug Del. Sci. Tech.* **2022**, 71, 103358.

ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Sustainable Solvents For High-Performance Organic Solar Cells By Reverse Engineering

Internship supervisor

Name, first name	Heiser Thomas
E-mail, Telephone	thomas.heiser@unistra.fr
Laboratory	ICUBE
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input type="checkbox"/> No <input checked="" type="checkbox"/> Yes : Patrick Lévêque, Yaochen Lin

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input type="checkbox"/> Chemistry <input checked="" type="checkbox"/> Physics
Other indications if necessary	

Internship description

Scientific Context

For a sustainable scale-up of solution-processed organic photovoltaic modules, the replacement of toxic solvents by alternative “green” solvents, which minimize the environmental impact and pose no risk to human health, is a critical issue. Yet, because of the complex relationship between the solvent properties and the device performances, the selection of alternative solvents most often relies on time-consuming and costly trial-and-error approaches. A more efficient and less empirical method to identify green solvents, based on a reverse engineering approach, has recently been proposed by our project consortium.^{1,2} The method starts by specifying the requested physico-chemical properties of the target solvent and utilizes a genetic algorithm, combined with the modeling of critical molecular properties, to identify potentially new solvents. The candidate solvents are ranked as a function of a global performance factor, which specifies how the estimated properties compare to the target values. The initial application of this method to select alternative solvents for the fabrication of organic solar cells has produced promising results. However, the molecular property estimation tool was originally based on a group contribution method, which limits result accuracy. Recently, a more advanced modeling approach, COSMO-RS (COnductor-like Screening MOdel for Real Solvents), was implemented, significantly enhancing the relevance of the solvent performance factor.

The objective of this internship is to experimentally evaluate the performance of alternative solvents identified using the enhanced reverse engineering method. This project will be conducted in close collaboration with Professor Ivonne Rodriguez's team (Laboratoire de Chimie Agro-Industrielle at INP Toulouse), where the reverse engineering technique is applied. The focus will be on depositing and characterizing thin films of cutting-edge organic photovoltaic blends formulated with the new eco-friendly solvents. The top-performing solution will then be used to fabricate and analyze organic solar cells.

References:

[1] *J. Wang et al, Mol. Syst. Des. Eng., 2022, 7, 182*

[2] *Projet ANR/DFG GreenPhotoSolv, ANR-21-CE05-0031*

Requirements & Application

We are seeking a motivated master's student with a strong interest in organic photovoltaics, eager to learn about wet thin film deposition of organic semiconductors, as well as fabrication and characterization (optical and electrical) of organic devices.

Please address your application including a CV, a motivation letter and Master transcript of records to Thomas HEISER and Yaochen LIN, Laboratoire ICUBE.

Possible starting date : Jan- February 2025

***Note that the lab is within a ZRR (Zone à Régime Restrictive)**

- [1]: Sandanayaka, A. S. D.; Matsushima, T.; Bencheikh, F.; Terakawa, S.; Potscavage, W. J.; Qin, C.; Fujihara, T.; Goushi, K.; Ribierre, J.-C.; Adachi, C.: Indication of current-injection lasing from an organic semiconductor. *Applied Physics Express* 2019, 12, 061010
- [2]: Kim, D.-H.; D'Aléo, A.; Chen, X.-K.; Sandanayaka, A. D. S.; Yao, D.; Zhao, L.; Komino, T.; Zaborova, E.; Canard, G.; Tsuchiya, Y.; Choi, E.; Wu, J. W.; Fages, F.; Brédas, J.-L.; Ribierre, J.-C.; Adachi, C.: High-efficiency electroluminescence and amplified spontaneous emission from a thermally activated delayed fluorescent near-infrared emitter. *Nature Photonics* 2018, 12, 98-104.
- [3]: Ye, H.; Kim, D. H.; Chen, X.; Sandanayaka, A. S. D.; Kim, J. U.; Zaborova, E.; Canard, G.; Tsuchiya, Y.; Choi, E. Y.; Wu, J. W.; Fages, F.; Bredas, J.-L.; D'Aléo, A.; Ribierre, J.-C.; Adachi, C.: Near-Infrared Electroluminescence and Low Threshold Amplified Spontaneous Emission above 800 nm from a Thermally Activated Delayed Fluorescent Emitter. *Chemistry of Materials* 2018, 30, 6702-6710.
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ITI HiFunMat Master Internship Proposal

M 1

M 2

Title: Plasma polymerization: novel thin films, their properties and possible impact of light on their formation

Internship supervisor

Name, first name	Carneiro de Oliveira, Jamerson
E-mail, Telephone	jamerson.carneiro-de-oliveira@uha.fr , 03 89 60 88 30
Laboratory	Institute of Materials Science of Mulhouse
Collaboration with a HiFunMat member (<i>please indicate their name</i>)	<input checked="" type="checkbox"/> No <input type="checkbox"/> Yes :

Student profile looked for

Master program (<i>more than one box can be ticked</i>)	<input checked="" type="checkbox"/> Material science and engineering <input checked="" type="checkbox"/> Chemistry <input type="checkbox"/> Physics
Other indications if necessary	

Internship description

The research project:

Plasma polymers are commonly defined as thin films (nm to μm thickness) generated through the deposition of organic species from a plasma phase. Their formation process depends on several factors, such as: the precursor nature, the plasma operating conditions and the physico-chemical properties of the surface over which they are deposited [1]. The precursors are intrinsically linked to the formation and stability of the plasma film as well as to the possible applications of the final coating [2]. The fact that the polymerization starts from species in the plasma state means that more varied chemical bonds can be created from the same precursors, when compared to other polymerization approaches. The tailoring of the polymer thin film properties can be performed by changing the operating parameters and the precursor chemistry. That makes plasma polymerization a flexible process, with potential applications from the textile to the pharmaceutical industries. In addition, plasma polymerization is performed in the absence of organic solvents, which appeals to its use as a greener process. The goal of the current offer is to explore **plasma polymerization of original precursors** and gather initial data about the **chemistry of the plasma phase**. The intern will further **characterize the novel plasma polymers**. The intern will thus have the opportunity to learn fundamental concepts of **plasma diagnostics, surface functionalization and thin film characterization**, through the analysis of physico-chemical and morphological properties of the plasma and of plasma polymers. The preparation of the surface exposed to the plasma will allow the intern to obtain an extra set of competences in **wet chemistry functionalization procedures**. The **6-month internship** will be carried in the **Institute of Materials Science of Mulhouse (IS2M, Mulhouse, France)** and thus the intern will count with a set of available characterization techniques in the institute.

The missions of the intern:

The intern will carry out **plasma polymerization** and perform **chemical, physico-chemical and morphological characterizations** of the **plasma** and/or **plasma polymers** using the available techniques at the IS2M (contact angle measurements, ellipsometry, infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM) ...).

Skills to be developed:

Thanks to this internship, the intern will develop disciplinary skills in **materials chemistry**, particularly in **surface functionalization** as well as in **plasma treatments**. More generally, she/he will learn how to work within a research team, exploit data, use scientific databases, write a report and communicate on her/his results.

References:

- (1) Brioude, M. M. et al. Controlling the Morphogenesis of Needle-Like and Multibranched Structures in Maleic Anhydride Plasma Polymer Thin Films. *Plasma Process Polym* 2014, 11, 943–951.
- (2) Carneiro de Oliveira, J.; Meireles Brioude, M. de et al., Plasma polymerization in the design of new materials: looking through the lens of maleic anhydride plasma polymers. *Materials Today Chemistry* 2022, 23, 100646.

Candidate profile and application:

Master 2 student or student in last year of engineering school. Education in chemistry and/or materials science is required. The candidate is expected to show initiative and seriousness.

Applications including a CV, a cover letter and a copy of grades (last 2 years) should be sent electronically as soon as possible.