ParisTech AgroParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: **Energy, Processes**

Subfield: **Process Engineering**

Title: **Coupling and intensification of separation processes**

ParisTech School: **AgroParisTech**

Advisor(s) Name: **Irina IOANNOU**
Advisor(s) Email: **irina.ioannou@agroparistech.fr**
Research group/Lab: **URD ABI / Process engineering department (**

Lab location: **REIMS (40 min from Paris)**
(Lab/Advisor website): **https://chaire-abi-agroparistech.com/Home/**
Short description of possible research topics for a PhD:
The subject of this paper deals with the coupling of processes to improve the performance of extraction (liquid/solid) and functionalization processes. Two technologies will be mainly studied for intensification:
(i) membrane processes. Some results (Ioannou et al. (2020) have been obtained on improving the glycosylation yield of resveratrol by coupling the enzymatic reaction with a membrane process (Enzymatic Membrane Reactor). The objective will be to optimize functionalization reactions used in the chemistry department of our unit. The experiments will be carried out on a laboratory scale in small volumes (0.5 L) and then on a pilot scale (5 L).
(ii) membrane contactors. The coupling of the extraction processes with membrane contactor technology will be applied in order to increase the extraction yields but also to increase the extract purity. Extraction processes deal with vegetal biomass in order to valorize agro-industrial products.
Energy and material balances will be carried out to show the interest of the coupling of different technologies. The experiments will be carried out according to the DOE methodology (Design Of Experiments).

Required background of the student:
The student will have a background in process engineering and / or chemical engineering. Knowledge of membrane processes, extraction processes (L / L, S / L), analytical methods (HPLC, SM) and design of experiments will be required. A good level in English is obligatory.

A list of 5 (max.) representative publications of the group:

1. Ioannou *et al.* (2020) Implementation of an enzyme membrane reactor to intensify the enzymatic β-glycosylation of resveratrol. Submitted to Industrial & Engineering Chemistry Research.
2. Reungoat *et al.* (2020). Optimization of an ethanol-water based sinapine extraction from mustard bran using Response Surface Methodology. Food Bioprod. Process., 122, 322-331. https://doi.org/10.1016/j.fbp.2020.06.001
3. Chemarin *et al.* (2019) Recovery of 3-hydroxypropionic acid from organic phase after reactive extraction with amines in an alcohol-type solvent. Sep. Pur. Technol. DOI: 10.106/j.seppur.2019.02.026
4. Chemarin *et al.* (2018) Toward an in-situ product recovery of biobased 3-hydroxypropionic acid: influence of bioconversion broth components on membrane-assisted reactive extraction. J. Chem. Technol. Biotechnol. DOI: 10.1002/jctb.5845
5. Fayet *et al.* (2018) Detoxification of highly acidic hemicellulosic hydrolysate from wheat straw by diananofiltration with a focus on phenolic compounds. J.Membrane Sci. DOI: 10.1016/J.memsci.2018.08.045

ParisTech AgroParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Environment Science and Technology, Sustainable Development, Geosciences

Subfield: Biogeochemistry

Title: Soil microbial functioning in land surface models

ParisTech School: AgroParisTech

Advisor(s) Name: Matthias Cuntz, Delphine Derrien
Advisor(s) Email: *matthias.cuntz@inrae.fr*, *delphine.derrien@inrae.fr*
Research group/Lab: *UMR Silva*
Lab location: *INRAE Centre Grand-Est – Nancy, 54280 Champenoux*
(Lab/Advisor website): *https://www6.nancy.inrae.fr/silva*

Short description of possible research topics for a PhD:
Land Surface Models (LSM) are used for projections of future climate change such as in the reports of the Intergovernmental Panel on Climate Change (IPCC). Plant processes are described in great detail in LSMs while soil processes are represented only very coarsely. This project aims at an explicit vertical description of carbon (C) decomposition in soil, moving away from crude kinetically-defined soil organic matter (SOM) pools, but rather linking closer the C cycle with microbial activity, as well as water and energy distribution in soils. The LSM CABLE shall be extended with the SOM decomposition model DAMM, combining effects of temperature, soil water content, enzyme kinetics, and soluble substrate supply. This will give a framework to include new, detailed knowledge about aggregation and the influence of freezing and thawing on it, microbial population dynamics and functioning such as enzyme production.

Required background of the student: Natural sciences

A list of 5 (max.) representative publications of the group:
1. Balesdent *et al.* (2018) *Nature* 559, 599–602, doi: 10.1038/s41586-018-0328-3
2. Cuntz & Haverd (2018) *JAMES* 10, 54–77, doi: 10.1002/2017MS001100
3. Haverd & Cuntz (2010) *J Hydrolo* 388, 438–455, doi: 10.1016/j.jhydrol.2010.05.029
4. Haverd *et al.* (2016) *Geosci Model Develop* 9, 3111–3122, doi: 10.5194/gmd-9-3111-2016
5. Sainte-Marie *et al.* (in revision), *Nature comm* 11, https://go.nature.com/3ltNMOl

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Life Science and Engineering for Agriculture, Food and the Environment

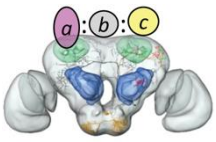
Subfield: Sensory Ecology

Title: Neural Processing of Pheromone Blend Ratio

ParisTech School: AgroParisTech

Advisor(s) Name: Abhishek CHATTERJEE, Philippe LUCAS
Advisor(s) Email: abhishekchttrj@gmail.com; philippe.lucas@inrae.fr
Research group/Lab: Neuroethology of Olfaction (NEO), iEES
Lab location: INRAe Versailles
(Lab/Advisor website):
https://ieesparis.ufr918.upmc.fr/spip.php?article244&lang=en
https://iees-paris.cnrs.fr/teams/neuroethology-of-olfaction/

Short description of possible research topics for a PhD: Moth sex pheromones are chemical cocktails produced by females to attract males for mating. Diverge moth species share subsets of the same compounds in their pheromone blend – but in different combinations, roles and/or concentration ratios. To evoke attraction of the males of *Agrotis ipsilon*, the three components of the pheromone blend must all be present, and crucially, be present in certain proportions. **Ratio coding** is a fascinating example of the moth's unique olfactory capability. While strengthening reproductive isolation, it also safeguards against large fluctuations in odor concentration that the moth faces during turbulent flight. We seek to identify how does the population-level network activity in the pheromone-processing centers of the moth brain compute the precise blend-ratio. We will employ behavioral, anatomical, electrophysiological and Ca^{2+} imaging-based methodologies to probe whether pheromone-evoked inter-glomerular synchronization play any part in ratio coding. In the end, results from this project will initiate the development of a network-level model of odor-integration which will be linked to organismal questions on adaptation.



Required background of the student: Neuroscience/ Biophysics/ Bioengineering/Biology

A list of 5 (max.) representative publications of the group:

1. A plant volatile alters the perception of sex pheromone blend ratios in a moth. Hoffmann A, Bourgeois T, Munoz A, Anton S, Gevar J, **Dacher M**, **Renou M**. *J Comp Physiol A Neuroethol Sens Neural Behav Physiol*. 2020 *Jul;206(4):553-570*.

2. Automatic tracking of free-flying insects using a cable-driven robot. Pannequin R, Jouaiti M, Boutayeb M, **Lucas P**, Martinez D. *Sci Robot*. 2020 *Jun 10;5(43):eabb2890*.

3. Reconfiguration of a Multi-oscillator Network by Light in the Drosophila Circadian Clock. **Chatterjee A**, Lamaze A, De J, Mena W, Chélot E, Martin B, Hardin P, Kadener S, Emery P, Rouyer F. *Curr Biol.* 2018 *Jul 9;28(13):2007-2017.e4*.

4. Firing and intrinsic properties of antennal lobe neurons in the Noctuid moth Agrotis ipsilon. Lavialle-Defaix C, Jacob V, Monsempès C, Anton S, **Rospars JP**, Martinez D, **Lucas P**. *Biosystems*. 2015 *Oct;136:46-58*.

5. Heterogeneity and convergence of olfactory first-order neurons account for the high speed and sensitivity of second-order neurons. **Rospars JP**, Grémiaux A, Jarriault D, Chaffiol A, Monsempes C, Deisig N, Anton S, **Lucas P**, Martinez D. *PLoS Comput Biol.* 2014 *Dec 4;10(12):e1003975*.

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Biology

Subfield: ecology – neurophysiology - evolution

Title: **Evolution of the detection and metabolism of ethanol in the olfactory system of drosophilids**

ParisTech School: AgroParisTech

Advisor(s) Name: **Maïbèche Martine / ChertempsThomas**
Advisor(s) Email: martine.maibeche@sorbonne-universite.fr
Research group/Lab: iEES PARIS – Ecosens department
Lab location: Paris
(Lab/Advisor website): https://ieesparis.ufr918.upmc.fr

Short description of possible research topics for a PhD:

Ethanol (EtOH) is a known psychoactive substance but its smell also drives various behaviors in animals. Surprisingly, the processes involved in EtOH detection and detoxification in the olfactory organs are still unknown. Fermenting fruit is the social hub for Drosophila melanogaster, this insect is thus remarkably adapted to detect EtOH and to resist to EtOH stress. Interestingly, closely related species of the Sophophora group display distinct EtOH tolerances and behavioral preferences. Using D. melanogaster and two sibling species, this project aims to discover the mechanisms underlying the olfactory detection of EtOH, to decipher the processes involved in the defense of the olfactory organ against this toxic compound, and to trace the evolution of EtOH adaptation in drosophilids, in light of their respective preferences and sensitivities. Molecular actors involved in EtOH detection identified could serve as new targets for the biocontrol of insect pests, such as D. suzukii.

Required background of the student: The Phd student must have a basic knowledge of molecular biology, genetics and neurophysiology, with sensitivity to evolutionary questions.

A list of 5 (max.) representative publications of the group

1. Chertemps T., *et al*. 2015. Front Physiol. 6:315.
2. Steiner C., *et al*. 2017. Sci Rep. 7(1):12629.
3. Younus F., *et al.* 2017. Sci Rep. 7:46188.
4. Younus F., *et al.* 2014. Insect Biochem Mol Biol. 2014 Oct;53:30-43.
5. Chertemps T., et al. 2015. BMC Biol. 2012 Jun 21;10:56.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Life and Health Science and Technology

Title: Design and development by continuous flow chemistry of new functionalized peptide nanoobjects for tumor diagnosis and therapy, with quantitative bioimaging monitoring

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: A. VARENNE / B.-T. DOAN
Advisor(s) Email: anne.varenne@chimieparistech.psl.eu /
bich-thuy.doan@chimieparistech.psl.eu
Research group/Lab: SEISAD team, iCLeHS (Chimie ParisTech PSL / CNRS 2027)
Lab location: Chimie ParisTech, 11 rue Pierre et Marie Curie, 75231 Paris Cedex 05
(Lab/Advisor website): https://iclehs.fr/research/seisad/

Short description of possible research topics for a PhD:

The development of new alternative therapeutic strategies to fight cancer by limiting the undesirable side effects of conventional chemotherapy is essential. Nanomedicine is an effective approach to meet these requirements because the coupling and encapsulation of antitumor molecules with nanovectors will allow reducing their toxicity while improving their circulation and *in vivo* targeting. The association with imaging probes will give rise to theranostic agents for image guided therapy.

The PhD proposal aims to explore the benefits and risks brought by the design and development of new self-assembled peptide-based nanoplatforms, breaking with the classical particulate nanovectors. The use of new synthesis processes in continuous flow and microflow will allow a stringent control of amino acid sequences and grafting for a fast identification of the most relevant candidates regarding structure and dynamics of self-assembly. Imaging methods will allow to control their biodistribution and evaluate their therapeutic efficacy for further applications in nanomedicine.

Required background of the student: organic synthesis, physico-chemistry, labelling, imaging

A list of 5 (max.) representative publications of the group:

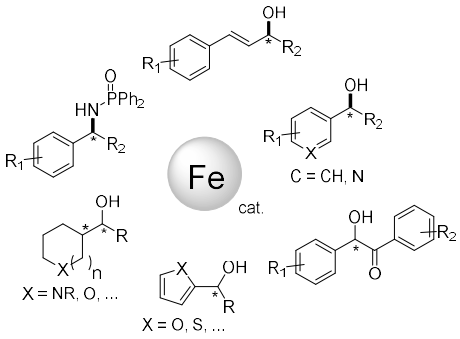
1. MOLECULAR IMAGING AND BIOLOGY, 2019, 21 : 269-278
2. ANALYTICAL BIOCHEMISTRY, 2016, 502 : 8-15
3. REACT. CHEM. ENG., 2020,**5** : 1981-1991
4. ACS APPLIED MATERIALS & INTERFACES, 2018, **10**: 17107-17116

Research Topic for the ParisTech/CSC PhD Program

Field : *Chemistry, Physical Chemistry and Chemical Engineering*
Subfield: *Organic Chemistry*
Title: *New iron complexes for enantioselective hydrogen transfer catalysis*
ParisTech School: *Chimie ParisTech*
Advisor(s) Name: *Virginie VIDAL and Guillaume LEFEVRE*
Advisor(s) Email:
virginie.vidal@chimieparistech.psl.eu; guillaume.lefevre@chimieparistech.psl.eu
Research group/Lab: *i-CLeHS – CSB2D, Chimie ParisTech*
(Lab/Advisor website): *Institute of Chemistry for Life and Health Sciences (i-CLeHS), CSB2D Team - https://www.chimie-paristech.fr/*

Short description of possible research topics for a PhD:

Asymmetric hydrogenation of unsaturated organic substrates is one of the most important synthetic tools used as an access to chiral scaffolds of pharmaceutical interest. The most powerful methods developed so far use noble metal catalysts (Ru, Rh, Ir, ...), which have a low natural abundance and are therefore expensive, and gaseous hydrogen. An important challenge is to develop new asymmetric hydrogenation methodologies which rely (i) on the use of non-noble transition metals as catalysts and (ii) on the use of liquid hydrogen vectors, which can be used as more easily-handled surrogates of H_2.



Iron appears as a good candidate for the development of new organometallic chiral catalysts, due to its low cost and toxicity. The goal of this project is to develop new chiral iron complexes which will be used in highly enantioselective hydrogenation and transfer hydrogenation of organic substrates, leading to a variety of targets of synthetic and pharmaceutical interest (Scheme 1). In order to ensure the robustness and the versatility of the system, various classic liquid hydrogen vectors will be used (e.g. formic acid, Hantzsch esters, cyclohexa-1,4-diene).

Required background of the student: experience in organic/organometallic synthesis.

A list of 5(max.) representative publications of the group:
(1) Review: Kyne, S.; Lefèvre, G.; Ollivier, C.; Petit, M.; Ramis-Cladera, V.-A.; Fensterbank, L. *Chem. Soc. Rev.*, **2020**. Iron and cobalt catalysis: new perspectives in synthetic radical chemistry, *accepted*.
(2) Rousseau, L.; Herrero, C.; Clémancey, M.; Imberdis, A.; Blondin, G.; Lefèvre, G. *Chem. Eur. J.* **2020**, *26*, 2417.
(3) Desaintjean, A.; Belrhomari, S.; Rousseau, L.; Lefèvre, G.; Knochel, P. *Org. Lett.* **2019**, *21*, 8694.
(4) Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Chem. Rec.* **2016**, *16*, 2750.
(5) Reviews : a) Echeverria, P.-G.; Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Synthesis* **2016**, *48*, 2523. b) R. Molina-Betancourt, Echeverria, P.-G.; Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Synthesis* **2020** (DOI: 10.1055/s-0040-1705918). Recent Progress and Applications of Transition-Metal-Catalyzed Asymmetric Hydrogenation and Transfer Hydrogenation of Ketones and Imines through Dynamic Kinetic Resolution.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Theoretical Chemistry

Title: DEVELOPMENT AND APPLICATION OF DENSITY BASED INDEXES FOR THE DIAGNOSTIC AND DESCRIPTION OF EXCITED STATES

ParisTech School: Chimie ParisTech | PSL
Advisor(s) Name: Ilaria Ciofini and Carlo Adamo
Advisor(s) Email: *ilaria.ciofini@chimieparistech.psl.eu and carlo.adamo@chimieparistech.psl.eu*
Research group/Lab: *CTM group; i-CLeHS*
Lab location: *Institute of Chemistry for Health and Life sciences (i-CLeHS) ChimieParisTech 11 rue P et M Curie, Paris*
Website: *https://www.quanthic.fr/* ***Twitter*** *https://twitter.com/group_ctm*

Short description of possible research topics for a PhD:
In the last years our group has developed several indexes enabling both the description of the excited states in terms of their nature (Locally Excited vs Charge Transfer) and the diagnostic of problematic cases to be treated at DFT level. These descriptors have allowed the investigation of excited state Potential Energy Surfaces of relevance to disclose the photophysical properties and the photoreactivity of molecular systems of interest in difference fields ranging from photovoltaics, to health sciences (ex. photodynamic therapy).
Within this doctoral work we aim at developing new indexes allowing to follow excited state evolution and to apply them to rationalize and predict the behavior of photo-active molecules. Homogeneous photo-catalytic reactions will be the target in terms of application.

Required background of the student: The student should have a strong background in physical and theoretical chemistry. Previous knowledge in ab-initio methods and Density Functional Theory as well programming experience will be greatly appreciated.

A list of 5 representative publications of the group in the field :
1. JCTC 7 (2011) 2498–2506
2. COORD. CHEM. REV. (2015) 304-305 166-178
3. JCTC 16 (2020) 4543–4553
4. JACS 142 (2020) 6578-6587
5. Nature Comm 11 (2020) 3262.

ParisTech

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RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Chemistry
Title: Better understanding TiO_2 photocatalysis by Density Functional Theory approaches

ParisTech School: Chimie ParisTech
Advisor(s) Name: Frédéric Labat
Advisor(s) Email: *frederic.labat@chimieparistech.psl.eu*
Research group/Lab: Theoretical Chemistry and Modeling Group/i-CLeHS FRE 2027 CNRS
(Lab/Advisor website): www.quanthic.fr

Short description of possible research topics for a PhD:
Photocatalysis, where solar energy is used to drive chemical and energy processes, has received considerable attention since it is a potentially environmentally friendly energy technology, with various applications in different fields such as solar cells, water splitting and pollutant degradation. In particular, heterogeneous photocatalysis, in which the catalyst is in a different phase as the reactants, has seen considerable developments, not only to propose new photocatalysts but also to better understand and improve photocatalytic processes.
Among the different photocatalysts proposed, TiO_2 is particularly appealing since it is chemically stable, nontoxic and low-cost. Although TiO_2-based heterogeneous photocatalysis has been successful during the last years, a clear understanding of the various processes involved during a typical photocatalytic reaction in TiO_2-based photocatalysis is however still largely missing, preventing a more rational design of new photocatalysts or the detailed characterization of new photocatalytic processes.
The aim of this project is to better understand, from a modeling viewpoint, basic processes involved in TiO_2-based heterogeneous photocatalysis, and how these processes influence the whole photocatalytic reaction. Particular care will be devoted to the development of cost effective computational approaches enabling the description of both ground and excited state properties of complex interfaces using both periodic ab-initio approaches rooted on Density Functional Theory and finite cluster models in conjunction with embedding techniques and implicit solvation models to simulate the effect of the environment.
Required background of the student: Physical Chemistry, Chemical Physics and, if possible, theoretical chemistry and previous programming experience.
A list of 5(max.) representative publications of the group:
[1] F. Labat et al "Silver-decorated CeO2 (111) as a potential anodic electrocatalyst in fuel cells: a hybrid Density Functional Theory investigation", *J. Phys. Chem. C*, **123**, 25668-25679 (2019).
[2] F. Labat, et al "Improving the Heterointerface in Hybrid Organic-Inorganic Perovskite Solar Cells by Surface Engineering: Insights from Periodic Hybrid Density Functional Theory Calculations", *J. Comput. Chem.*, **41**, 1740-1747 (2020).
[3] F. Labat et al , "On the stability issues of TiO2-based composites in view of fuel cell application: a combined experimental and theoretical investigation", *J. Phys. Chem. C*, **123**, 12573–12582 (2019).
[4] F. Labat, et al, "First-principles modeling of dye-sensitized solar cells: Challenges and perspectives", *Acc. Chem. Res.*, **45**, 1268 (2012).

ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Chemistry

Title: 2D/3D Perovskites for Stable and High-Efficiency Solar Cells

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Thierry PAUPORTÉ
Advisor(s) Email: thierry.pauporte@chimieparistech.psl.eu
Research group/Lab: Institut de Rechreche de ChimieParis (UMR8247)
Lab location: 11 rue P. et M. Curie 75005 Paris
Website : www.pauportegroup.com

Short description of possible research topics for a PhD:

Recently, hybrid halogen perovskites (PVKs) have emerged as fascinating materials and highly versatile semiconductors. These compounds can be prepared as 2D (two-) and 3D (three-dimensional) materials, and their composition can be varied over a quite large extend. This ensures the possible fine tuning of their optoelectronic properties. Their superior properties make them especially attractive for an application to photovoltaic (PV) solar cells. If their PV power conversion efficiency is now reaching impressive values, these devices still suffer from a problem of stability.
The host group, which is leader in France on perovskite solar cells (PSCs) research, has discovered recently precursor solution chemistries that allow the preparation of highly stable 2D/3D perovskite layers. Moreover the power conversion efficiency achieved with these perovskites is very promising.
The aim of the PhD will be to get further insights into the preparation 2D/3D PVK with special stoichiometry and additive. The student will investigate the role of the additives and the effect of the composition on the layers morphological, structural, optical and electronic properties. PV cells based on these new materials will be prepared and characterized by various techniques (*J-V* curves, impedance spectroscopy, spectral response…). The objective will be to better understand the effect of chemistry and composition on the devices stability and high performances.

Required background of the student:
Material science, Chemistry, if possible: Physics of semiconductors, Photovoltaics.

A list of 5 representative publications of the group:
1- T. Zhu, D. Zheng, J. Liu, L. Coolen, Th. Pauporté, Electrical Response of High Efficiency and Stable Solar Cells Based on MACl Mediated Grown $FA_{0.94}MA_{0.06}PbI_3$ Perovskite. ACS Appl. Mater. Interfaces 12 (2020) 37197–37207.
2- T. Zhu, D. Zheng, M.-N. Rager, Th. Pauporté, Actual Organic Cations Composition Determination in Perovskite Thin Films. Application to Formamidinium Lead Iodide Stabilization for High Efficiency Solar Cell. Solar RRL 2020, 2000348.
3- T. Zhu, J. Su, F. Labat, I. Ciofini, Th. Pauporté, Interfacial Engineering through Chloride-Functionalized Self-Assembled Monolayer for High Efficiency Perovskite Solar Cells. ACS Appl. Mater Interfaces, 12 (2020) 744-752.
4- A. Leblanc, N. Mercier, M. Allain, J. Dittmer, T. Pauporté, V. Fernandez, F . Boucher, M. Kepenekian, C. Katan, Enhanced Stability and Band Gap Tuning of α-$[HC(NH_2)_2]PbI_3$ Hybrid Perovskite by Large Cation Integration. ACS Appl. Mater. Interfaces, 11 (2019) 20743-20751.
5- D. Pitarch-Tena, T.T. Ngo, M. Vallés-Pelarda, Th. Pauporté, I. Mora-Seró, Impedance Spectroscopy Measurements in Perovskite Solar Cells. Device Stability During the Measurement and Noise Reduction. ACS Energy Lett., 3 (2018) 1044–1048.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Chemistry

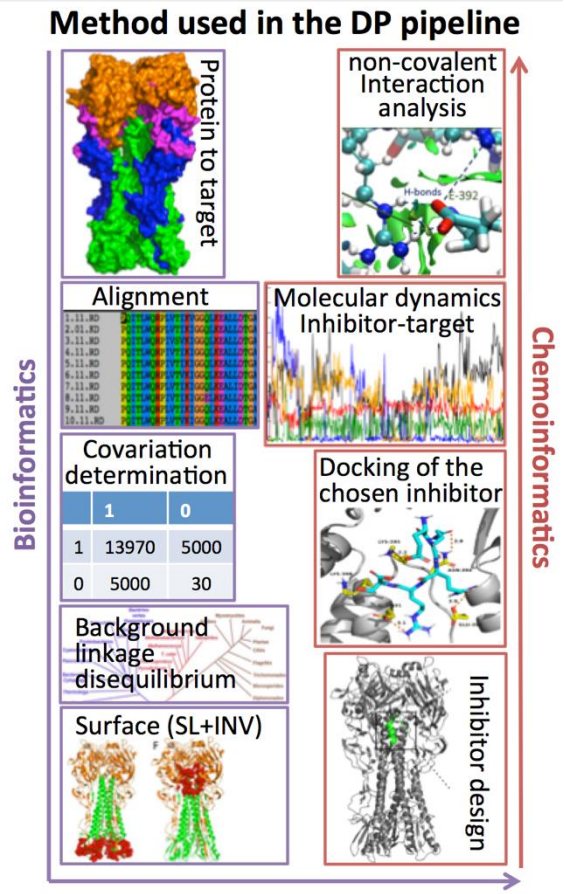
Title: In silico design of unescapable influenza therapies

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Dr. PERRIER Aurélie
Advisor(s) Email: aurelie.perrier@chimieparistech.psl.eu
Research group/Lab: *CTM / i-CLeHS*
Lab location: *Chimie Paris Tech, 11 rue Pierre et Marie Curie, F-75005 Paris*
Lab/Advisor website: *https://www.quanthic.fr/*

Short description of possible research topics for a PhD:

Influenza is a major Public Health threat. A single anti-influenza drug, oseltamivir, is available in Europe but resistance mutations against this drug can occur. Our goal is to develop anti-influenza drugs with little or no possibility of viral escape. For this purpose, *in silico* work allows us to describe new therapeutic targets that should reduce viral escape and to propose inhibitors potentially clinging to these targets. We have already defined a reusable data processing (DP) pipeline shown opposite.
During this project, the PhD student will participate to the (1) *in silico* design of antiviral targets and (2) drug design of potential inhibitors. Iterative cycles involving bioinformatics and chemoinformatics will allow us to refine both the targets (to consider the maximum of sub-types of influenza viruses) and the chemical structure of the inhibitors.



Required background of the student: Molecular modeling, computational chemistry or bioinformatics

Representative publications of the group:

1. Perrier, A. *et al.* J. Phys. Chem. B 2019,123, 582-592. DOI: 10.1021/acs.jpcb.8b10767.
2. Ozeel, V. *et al.* Symmetry 2019, 11(5), 662; DOI:10.3390/sym11050662.
3. Sharma, A. *et al.* Phys. Chem. Chem. Phys. 2016, 18, 30029-30039. DOI: 10.1039/C6CP05105G

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Chemistry

Title: Photocatalysis in Living Cells with Earth Abundant Metals for Cancer Therapy

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Gilles GASSER
Advisor(s) Email: gilles.gasser@chimieparistech.psl.eu
Research group/Lab: Institute of Chemistry for Life Sciences,
(Lab/Advisor website): www.gassergroup.com

Short description of possible research topics for a PhD: Photodynamic Therapy (PDT) is an approved medical technique to treat certain types of cancer. However, cancer cells have a lower amount of oxygen than healthy ones, limiting the success of PDT treatments since oxygen is one of the three required components with the presence of a photosensitizer and light. Recently, it was demonstrated that Ir(III) complexes could kill cancer cells upon light irradiation without the presence of oxygen.[1] *In this project, we aim at developing novel complexes based on biocompatible, earth-abundant metal complexes to kill cancer cells.*

Required background of the student: The applicant should have a sound knowledge (theoretical and practical) in both inorganic and organic chemistry and be proficient with analytical techniques such as NMR and MS. The applicant must be fluent in English since it is the language spoken in the Gasser group. Practical knowledge in biology would be an asset.

A list of 5 (max.) representative publications of the group:

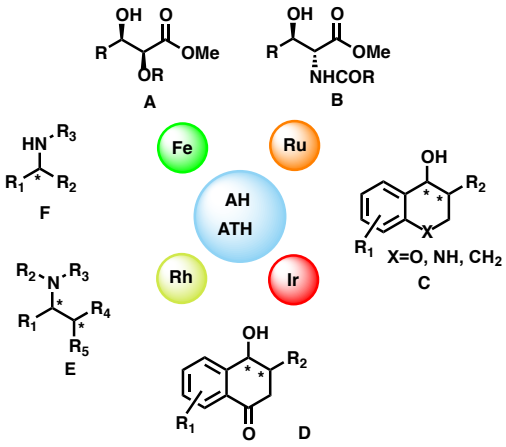
1. H. Huang, S. Banerjee, K. Qiu, P. Zhang, O. Blacque, T. Malcomson, M.J. Paterson, G.J. Clarkson, M. Staniforth, V.G. Stavros, **G. Gasser**,* H. Chao,* and P.J. Sadler,* *Nature Chem.*, **2019**, *11*, 1041-1048.
2. J. Karges, S. Kuang, F. Maschietto, O. Blacque, I. Ciofini, H. Chao,* and **G. Gasser**,* *Nature Commun.*, **2020**, *11*, 3262.
3. J. Karges, F. Heinemann, M. Jakubaszek, F. Maschietto, C. Subecz, M. Dotou, R. Vinck, O. Blacque, M. Tharaud, B. Goud, E. Viñuelas Zahínos, B. Spingler,* I. Ciofini,* and **G. Gasser,*** *J. Am. Chem. Soc.*, **2020**, *142*, 6578-6587.

Research Topic for the ParisTech/CSC PhD Program

Field : *Chemistry, Physical Chemistry and Chemical Engineering*
Subfield: *Organic Chemistry*
Title: *Asymmetric Catalysis toward BioRelevant Architecturally Novel Natural and Unnatural Products*
ParisTech School: *Chimie ParisTech*
Advisor(s) Name: *Virginie VIDAL*
Advisor(s) Email:
virginie.vidal@chimieparistech.psl.eu
Research group/Lab: *i-CLeHS – CSB2D, Chimie ParisTech*
(Lab/Advisor website): *Institute of Chemistry for Life and Health Sciences (i-CLeHS), CSB2D Team - https://www.chimie-paristech.fr/*

Short description of possible research topics for a PhD:

Our group develops new catalytic processes for the synthesis of natural products and targets of biological interest. We have been interested in the development of novel methods for synthetic efficiency and atom and step economical processes using transition metal-catalyzed reactions as they provide a direct and selective way toward the synthesis of highly valuable products. The research program will be dedicated to the development of asymmetric catalytic methods in a context of sustainable development for carbon-carbon and carbon-hydrogen bond forming reactions using asymmetric hydrogenation (AH) or asymmetric hydrogen transfer reactions (ATH) [1] through dynamic kinetic resolution (DKR)[2-4] to target scaffolds of biorelevant molecules of medicinal.[5] The PhD research program aims at developing new catalytic asymmetric approaches to address long-standing problems in the synthesis of chiral key intermediates such as A-F to access natural products and pharmaceutical drugs.



Required background of the student: experience in organic/organometallic synthesis.

A list of 5 (max.) representative publications of the group:
(1) Reviews : a) R. Molina-Betancourt, Echeverria, P.-G.; Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Synthesis* **2020** (DOI: 10.1055/s-0040-1705918; Recent Progress and Applications of Transition-Metal-Catalyzed Asymmetric Hydrogenation and Transfer Hydrogenation of Ketones and Imines through Dynamic Kinetic Resolution.
(2) He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org. Chem. Front.* **2020**, *7*, 975.
(3) He, B.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org Lett* **2020**, *21*, 3276.
(4) a) Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. *Org Lett* **2019**, *21*, 2998. b) Zheng, L.-S.; Férard, C.; Phansavath, P.; Ratovelomanana-Vidal, V. *Chem. Commun.* **2018**, *54*, 283.
(5) Ayad, T.; Phansavath, P.; Ratovelomanana-Vidal, V. *Chem. Rec.* **2016**, *16*, 2750.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Chemistry, Physical Chemistry and Chemical Engineering

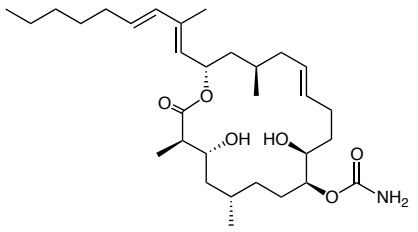
Subfield: Organic chemistry

Title: Total synthesis of tulearin A and analogues

ParisTech School: Chimie ParisTech

Advisor(s) Name: Phannarath Phansavath
Advisor(s) Email: phannarath.phansavath@chimieparistech.psl.eu
Research group/Lab: Institute of Chemistry for Life & Health Sciences (i-CLeHS), CSB2D team (Catalysis, synthesis of biomolecules and sustainable chemistry)
Lab location: i-CLeHS, Chimie ParisTech, Paris
(Lab/Advisor website): *https://www.chimieparistech.psl.eu/*

Short description of possible research topics for a PhD:



Tulearin A

Tulearins constitute a small family of macrolides isolated from a Madagascar sponge of the *Fascaplysinopsis* genus. The potent anti-proliferative activity of Tulearin A against two human leukemia cell lines made it an interesting target and two total synthesis of this compound have been reported. As part of our ongoing research directed toward the synthesis of biologically relevant compounds,[1-2] we propose in this PhD program to develop an efficient total synthesis of Tulearin A and of analogues of the natural product, using new catalytic systems to introduce the various stereogenic centers.[3-5]

Required background of the student:

Main field of study of the applicant before applying: organic chemistry.
Synthetic Organic Chemistry, Homogeneous Catalysis

A list of 5 (max.) representative publications of the group:

1. Echeverria, P.-G.; Prévost, S.; Cornil, J.; Férard, C.; Reymond, S.; Guérinot, A.; Cossy, J.; Ratovelomanana-Vidal, V.; Phansavath, P. *Org. Lett.* **2014**, *16*, 2390.
2. Perez, M.; Echeverria, P.-G.; Martinez-Arripe, E.; Ez Zoubir, M.; Touati, R.; Zhang, Z.; Genet, J.-P.; Phansavath, P.; Ayad, T.; Ratovelomanana-Vidal, V. *Eur. J. Org. Chem.* **2015**, 5949.
3. L.-S. Zheng, C. Férard, P. Phansavath, V. Ratovelomanana-Vidal *Chem. Commun.* **2018**, *54*, 283.
4. B. He, P. Phansavath, V. Ratovelomanana-Vidal *Org. Lett.* **2019**, *21*, 3276.
5. A. Westermeyer, G. Guillamot, P. Phansavath, V. Ratovelomanana-Vidal *Org. Lett.* **2020**, *22*, 3911.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: (Applied Physics, Chemistry, Mathematics, Mech. Eng.…)

Title: Synthesis of innovative nanomaterials for hydrogen production by water splitting process and the study of its efficiency by the rotating Ring Disk Electrode method.

ParisTech School: Chimie ParisTech | PSL
Advisor(s) Name: Abdelhafed Taleb
Advisor(s) Email: abdelhafed.taleb@chimieparistech.psl.eu
Research group/Lab: IRCP-UMR 8247
Lab location: Chimie Paris Tech
(Lab/Advisor website): https://www.ircp.cnrs.fr/
Short description of possible research topics for a PhD:Hydrogen energy is considered by the scientific community as one of the potential clean energy sources to replace the pollutant fossil energy. Therefore, the hydrogen production is becoming à hot topic in material science. The present PhD proposal will focus on the synthesis and electrochemical characterization of innovative semiconductor and transition metal materials (chalcogenide, oxide, mixed) for high efficiency of water splitting. The rotating Ring Disk Electrode (RRDE) method will be used to study the oxygen vs. chlorine evolution (OER vs. CER) in alkaline media. The objective of this study is to explore the efficiency of different materials for the competitiveness of both oxygen and chlorine evolution and the influence the transition metal catalysts. The optimized electrode materials will be integrated into new generation of electrolyzes for the electrochemical decomposition of water in the dark or under illumination which mimic the artificial photosynthesis (photoelectrochemical water splitting). This research aims to the development of low cost and active electrocatalysts for hydrogen fuel production efficiency. This work will be achieved in collaboration with Pr. Ahmed Ennaoui president of the scientific council of IRESEN (the Moroccan Research Institute for Solar Energy and New Energies)
Required background of the student: Solid State chemist, electrochemist, physical chemist
A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. A. Ennaoui, and H. Tributsch, Journal of Electroanalytical Chemistry 204 (1986) 185
2. A. Ennaoui, and H. Tributsch , Solar Energy Materials and Solar Cells, 29 (1993) 289-370
3. A. Taleb, F. Mesguich, X. Yanpeng, C. Colbeau-Justin P. Dubot, Solar Energy Materials and Solar Cells, 148, 52, (2016).
4. S. Mehraz, P. Konsong, A. Taleb, N. Dokhane, L. Sikong, Solar Energy Materials and Solar Cells, 189 (2019) 254-262.
5. H. Ennaceri, D. Erfurt, L. Wang, T. Köhler, A. Khaldoun, A. El Kenz, A. Benyoussef, A. Ennaoui, A. Taleb, Solar Energy Materials and Solar Cells, 201 (2019) 110058.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield:

Title: Design of new electrode materials based on nanoparticles for electrochemical nanosensing applications with environmental interest.

ParisTech School: Chimie ParisTech | PSL
Advisor(s) Name: Abdelhafed Taleb
Advisor(s) Email: abdelhafed.taleb@chimieparistech.psl.eu
Research group/Lab: IRCP-UMR 8247
Lab location: Chimie Paris Tech
(Lab/Advisor website): https://www.ircp.cnrs.fr/

Short description of possible research topics for a PhD: In the field of material science, one of the main question is, does it make sense to define desired properties first and then design the material with the architecture that match these properties. The actual research topic of our group is within this concern, and it consist of new material design developments that emerge new properties and functions. Actually, one of the main research topics we are developing is dealing with the enhancement of detection limit and selectivity of sensing, based on nanostructure through a new design of metallic nanoparticles modified electrode. Our design strategies combine nanomaterials and different deposition methods to prepare desired material structure of required properties.
Over the years, our group has acquired expertise in nanoparticle synthesis, surface modification and deposition of thin film based on nanoparticles. Our goal in this PhD proposal is to develop hierarchical electrode material based on metallic nanoparticles. We expect that our results could be helpful in understanding the electrochemical properties of hierarchical electrode and may have potential applications in sensing. Additional, the performance of prepared electrode will be optimized.

Required background of the student: Electrochemistry, ideally with some knowledge of surface modification and/or nanomaterial synthesis.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. A. Taleb, X. Yanpeng, P. Dubot, J. Electroanal. Chem. 693 (2013) 60.
2. A. Taleb**,** X. Yanpeng, P. Dubot, Applied surface science, 420 (2017) 110-117.
3. Sana Falah, Xue Yanpeng, Abdelhafed Taleb, Mohamed Beji, Electrochemica Acta, 292(1) (2018) 594-601.
4. Z. Ait-Touchente, S. Falah, E. Scavetta, M. M. Chehimi, R. Touzani, D. Tonelli, A. Taleb, Molecules 25 (2020) 3903.

ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering, Life Science and Engineering for Agriculture, Food and the Environment

Subfield: Electrochemistry, Bio analytical chemistry

Title: Hydrogel Matrix Grafted electrochemical Aptasensors for the Detection of emerging pollutants

ParisTech School: Chimie ParisTech

***Advisors Name*:** Cyrine Slim, Sophie Griveau, Fethi Bedioui
Advisors Email: Cyrine.slim@chimieparistech.psl.eu/sophie.griveau@chimieparistech.psl.eu
Research group/Lab: Institute of Chemistry for Life and Health Sciences, i-CLeHS
Lab location : ENSCP Chimie Paristech
11, rue Pierre et Marie Curie 75231 Paris Cedex 05, France
Lab website: https://iclehs.fr/research/seisad/

Short description of possible research topics for a PhD:

Driven by the growing concern about the release of the untreated emerging pollutants and the urgent demand of determining low level of these pollutants present in environment, novel biosensors dedicated to molecular recognition will be developed. The objective of the project is to design biosensors using a novel class of grafted polymers, surface-attached hydrogel thin films on conductive transducer as biocompatible matrix for biomolecule immobilization. From biomolecules, aptamers constitute an attractive alternative to antibodies due to their high affinity and their excellent specificity for a target or a family of selected targets. It is also possible to functionalize them with specific chemical functions and/or with tag to label the aptamers, for their further immobilization and/or for their analysis. The immobilization of the aptamer onto surface-attached hydrogel thin films by covalent attachment provides a biodegradable shelter, providing the aptamer excellent environments to preserve its active and functional structure while allowing the detection of pollutants. For improved sensitivity and higher stability of the sensor, a high density of immobilized aptamer is enabled. Within a constant miniaturization effort, we will tend towards the transposition of this work, towards microfluidic electrochemical biosensors on real samples due to their miniature, portable and low-cost systems as well as high through put and automation. The integration of electrochemical sensors into microfluidic formats with the incorporation of unique materials for detection will be explored in this project. The development of these systems would lead to significant advantages compared to the current analytic systems, in terms of simplicity, speediness, cost, and automation.

***Required background of the student*:** Physical chemistry, ideally background in basic electrochemistry

A list of representative publications of the group:

1- Kassahun, G.; Griveau, S.; Juillard, S.; Champavert, J.; Ringuedé, A.; Bresson, B.; Tran, Y.; Bedioui, F.; Slim, C. Poly(acrylic acid) hydrogel matrix based impedimetric aptasensor for the detection of diclofenac. Langmuir 36 (2020) 827–836.
2- Quinton, D., Girard, A., Thi Kim, L. T., Raimbault, V., Griscom, L., Razan, F., Bedioui, F. (2011). On-chip multi-electrochemical sensor array platform for simultaneous screening of nitric oxide and peroxynitrite. Lab on a Chip, 11(7), 1342–1350
3- Griveau, S., & Bedioui, F. (2013). Electroanalytical methodologies for the detection of S-nitrosothiols in biological fluids. The Analyst, 138(18), 5173–81
4- Ramirez-Garcia, G., Martinez-Alfaro, M., Gutierrez-Granados, S., Alatorre-Ordaz, A., Griveau, S., & Bedioui, F. (2015). Electrochemical assessment of possible melatonin effect on nitric oxide production from kidneys of sub-acute lead treated rats. Electrochimica Acta, 166, 88–92
5- Slim, C., Ratajovà, E., Griveau, S., Kanoufi, F., Ferraro, D., Perréard, C., Bedioui, F. (2015). Two-step local functionalization of fluoropolymer Dyneon THV microfluidic materials by scanning electrochemical microscopy combined to click reaction. Electrochemistry Communications, 60, 5–8

ParisTech

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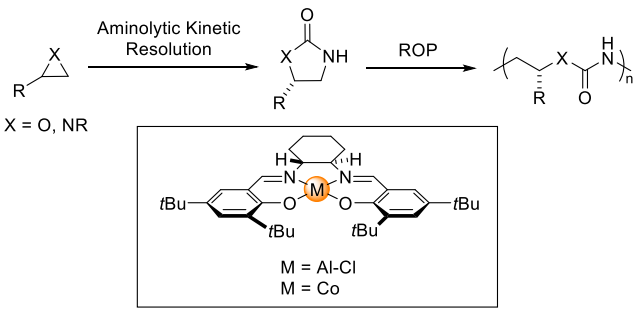
RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Chemistry and Materials Science
Title: Synthesis of Biobased Polyurethanes from Renewable Resources: A New Tandem Approach to Polypeptide Analogues

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Prof. Christophe Thomas
Advisor(s) Email: christophe.thomas@chimieparistech.psl.eu
Research group/Lab: Organometallic Chemistry and Polymerization Catalysis
Lab location: 11 rue Pierre et Marie, 75005 Paris
(Lab/Advisor website): http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/

Short description of possible research topics for a PhD:



Tandem catalysis is one of the strategies used by Nature for building macromolecules.[1] However, these biological processes rely on highly complex biocatalysts thus limiting their industrial applications. In the same biomimetic spirit, we want to initiate a research effort to synthesize **biodegradable** polymers[2] via tandem **catalytic transformations**, where "activated" monomers are synthesized from raw materials (in one or more steps) and subsequently (co)polymerized. The objectives for this are clear: not only can a reduction in workload, waste and energy consumption be achieved, but also the synthesis of complex products that are otherwise difficult to obtain (*e.g.*, because of thermodynamic hurdles) comes within reach. In other words, the combination of chemistries may allow the direct synthesis of macromolecules with high structural complexity. Therefore, we want to direct investigative efforts toward the synthesis of new **renewable monomers** and the subsequent catalytic conversion of these monomers into their corresponding polymers.[3] The general idea is to use a tandem procedure of combining synthesis of new biomass derived monomers with subsequent polymerization by well-defined metal-based catalysts, aiming at novel polymeric materials.

Required background of the student: Polymer Chemistry, Catalysis

A list of 5 (max.) representative publications of the group:
1. *Nature Comm.*, **2011**, *2*, 586.
2. *J. Am. Chem. Soc.* **2017**, *139*, 6217.
3. *Angew. Chem. Int. Ed.* **2019**, *58*, 12585.

ParisTech

Chimie Paris ParisTech | PSL

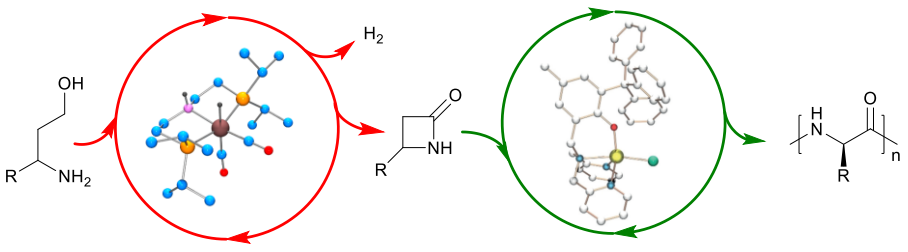
RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Chemistry
Title: Smart multi-catalytic systems for the production of biocompatible polymers

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Dr. Régis Gauvin, Prof. Christophe Thomas
Advisor(s) Email: regis.gauvin@chimieparistech.psl.eu; christophe.thomas@chimieparistech.psl.eu
Research group/Lab: Organometallic Chemistry and Polymerization Catalysis
Lab location: 11 rue Pierre et Marie, 75005 Paris
(Lab/Advisor website): http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/

Short description of possible research topics for a PhD:
Biocompatible materials such as polyesters and polyamides hold a prominent position in the portfolio of specialty and commodity polymers. Controlling their structural features such as chain size and microstructure is key in establishing specific properties. In this context, **organometallic catalysis** is instrumental, thanks to its outstanding ability to achieve both high degree of stereoselectivity and mass control. Smart approaches such as **tandem catalysis** can be game changers: Combining several complementary systems is a unique opportunity to perform series of chemical reactions with higher efficiency. In this project, **hydrogen borrowing**, a clean, atom-economical technology, will be harnessed in a first step to synthesize lactones or lactames monomers from biosourced raw materials. These will then be polymerized via **stereoselective ring opening polymerization**, affording novel polyesters or polyamides. A strong emphasis will be put on the design of novel organometallic catalysts based on **Earth-abundant metals**, as well as on establishing catalysts structure and polymers' physicochemical properties relationships.



Required background of the student: organic and polymer synthesis.

A list of 5 (max.) representative publications of the group:
1. *Nature Comm.*, **2011**, *2*, 586.
2. *J. Am. Chem. Soc.* **2017**, *139*, 6217.
3. *ACS Catal.*, **2017**, *7*, 2022.
4. *Angew. Chem. Int. Ed.* **2019**, *58*, 12585.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

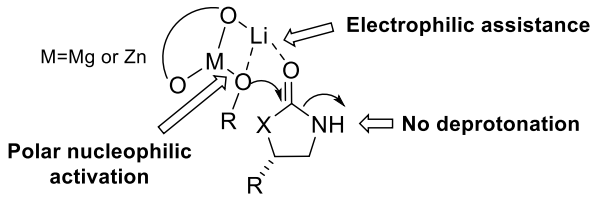
Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Chemistry and Materials Science
Title: Synthesis of Biodegradable Polymers from Renewable Resources

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Dr. Régis Gauvin, Prof. Christophe Thomas
Advisor(s) Email: regis.gauvin@chimieparistech.psl.eu; christophe.thomas@chimie-paristech.psl.eu
Research group/Lab: Organometallic Chemistry and Polymerization Catalysis
Lab location: 11 rue Pierre et Marie, 75005 Paris
(Lab/Advisor website): http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/

Short description of possible research topics for a PhD:

The ring opening polymerization (ROP) of *N*-carboxyanhydrides (NCA) can yield homopolymers and block-copolymers with well-controlled structures where the repeat units are natural amino acids.[1] Similarly to proteins, these synthetic polypeptides possess well-defined secondary structures (α-helix and β-sheets), whereas synthetic polymers generally present a disordered coil structure. Therefore, these biomimetic polymers produce sophisticated superstructures with new material properties. Our aim will be to develop an efficient route from readily available reactants to synthesize new polypeptide analogues with a conserved ability to form well-defined secondary structures.



In this regard, there is growing evidence that magnesium or zinc derivatives can be effective catalysts for homogeneous polymerization. Their low toxicity, low cost, and accessibility make them attractive candidates for the development of affordable, sustainable and green catalysts. Bimetallic reagents are ideal candidates for this purpose since the polar organometallic moiety will act as a strong nucleophile with a concomitant electrophilic assistance created through the coordination of carbonyl oxygen of urea by the lithium cation. Therefore we want to use these bimetallic systems to synthesize aliphatic polyureas and polyurethanes via an auto-tandem catalytic transformation[2] where cyclic urethanes or ureas are synthesized from respectively epoxides or aziridines and subsequently polymerized by ROP.[3]

Required background of the student: Organic & Polymer Chemistry, Catalysis

A list of 5 (max.) representative publications of the group:

1. *Chem. Commun.*, **2014**, *50*, 13773.
2. *Nature Comm.*, **2011**, *2*, 586.
3. *Chem. Soc. Rev.*, **2013**, *42*, 9392.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

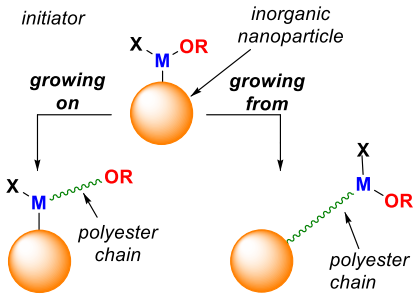
Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Chemistry and Materials Science
Title: Vectorizing nanoparticles using biocompatible and biodegradable polymer coating mediated by surface organometallic chemistry

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Dr. Régis Gauvin, Prof. Christophe Thomas
Advisor(s) Email: regis.gauvin@chimieparistech.psl.eu; christophe.thomas@chimie-paristech.psl.eu
Research group/Lab: Organometallic Chemistry and Polymerization Catalysis
Lab location: 11 rue Pierre et Marie, 75005 Paris
(Lab/Advisor website): http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/

Short description of possible research topics for a PhD:

The design of efficient vectorizing agents is at the cornerstone of modern pharmaceutical agents. In this view, the tailoring of specific (molecular) objects by covalent bonding with polymer chains is of major interest, to confer them significant compatibility with physiological environments.[1]



In this view, biocompatible and biodegradable polymers are ideal candidates as components within such advanced formulations. These can be most efficiently prepared using ring opening polymerization (ROP) of lactones or lactides into polyesters or polylactic acid mediated by organometallic initiators.[2] On the top of that, immobilization of organometallics on inorganic surfaces via surface was demonstrated to boost stereoselectivity of these considered polymerization processes.[3] In this project, we propose to combine surface organometallic chemistry and ROP of polar monomers to design specific nanoobjects by "*growing from*" or "*growing on*" approaches, where chain growth is mediated by specifically designed supported organometallic entities. The ultimate goal will be the development of biopolymer-coated nanoparticles for future implementation into delivery systems.

Required background of the student: Organic Chemistry, Polymer Chemistry, Catalysis

A list of 5 (max.) representative publications of the group:

1. *Chem. Sci.*, **2020**, *11*, 2657.
2. *Angew. Chem. Int. Ed.* **2019**, *58*, 12585.
3. *Chem. Commun.* **2010**, *46*, 1032.

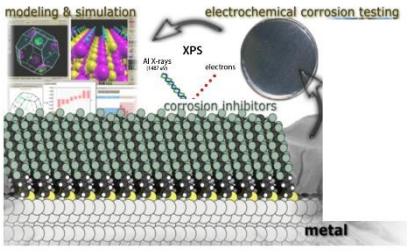
ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Chemistry, Physical Chemistry and Chemical Engineering
Subfield: Surface Science, Molecular Modeling
Title: **Organic molecules for the corrosion inhibition of Al alloys: theoretical and experimental model approach**
ParisTech School: Chimie ParisTech | PSL
Advisor(s) Name: Dominique COSTA (Dimitri Mercier, Sandrine Zanna, Philippe Marcus co-advisors)
Advisor(s) Email: *dominique.costa@chimieparistech.psl.eu*
Research group/Lab: *PSC/IRCP*
Lab location: *11 rue P et M Curie 75005 Paris*
(Lab/Advisor website): *https://www.ircp.cnrs.fr/en/la-recherche/equipe-pcs/pcs-group/*

Short description of possible research topics for a PhD:



The corrosion of metals is a universal phenomenon with significant economic and societal impacts and their protection has become a major issue. This thesis subject aims to target new organic coatings allowing an improvement in the corrosion resistance of Al alloys as well as a reduction of the environmental load compared to existing coatings. We propose to develop a rationalized search for organic inhibitors based on a combined theoretical / experimental approach aimed at understanding i) molecule / surface interactions at the atomic scale, ii) the 2D and 3D self-organization in dense layers of organic molecules on metal surfaces and iii) the corrosion resistance of the metal surfaces thus functionalized. This approach, coupling modeling by DFT, advanced characterization of surfaces (XPS, ToF-SIMS, AFM) and electrochemical measurements will be applied to Al alloys and to specific organic anchoring molecules (silanes, phosphonates), which are known to be effective in Al corrosion inhibition.

Required background of the student:

The applicant should have a solid physico-chemical (material sciences) background together with a formation in theoretical chemistry.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Cornette, P.; Zanna, S.; Seyeux, A.; Costa, D.; Marcus, P. The Native Oxide Film on a Model Aluminium-Copper Alloy Studied by XPS and ToF-SIMS. *Corros. Sci.* **2020**, *174*, 108837
2. Poberžnik, M.; Chiter, F.; Milošev, I.; Marcus, P.; Costa, D.; Kokalj, A. DFT Study of N-Alkyl Carboxylic Acids on Oxidized Aluminum Surfaces: From Standalone Molecules to Self-Assembled-Monolayers. *Appl. Surf. Sci.* **2020**, *525*, 146156.
3. Vernack, E.; Costa, D.; Tingaut, P.; Marcus, P. DFT Studies of 2-Mercaptobenzothiazole and 2-Mercaptobenzimidazole as Corrosion Inhibitors for Copper. *Corros. Sci.* **2020**, *174*, 108840.
4. I. Milošev, T. Bakarič, S. Zanna, A. Seyeux, P. Rodič, M. Poberžnik, F. Chiter, P. Cornette, D. Costa, A. Kokalj, P. Marcus - Electrochemical, Surface-Analytical, and Computational DFT Study of Alkaline Etched Aluminum Modified by Carboxylic Acids for Corrosion Protection and Hydrophobicity – J. Electrochem. Soc., **2019**,166 (11), C3131-C3146.
5. A Kokalj, D Costa, Molecular Modeling of Corrosion Inhibitors **2018** Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry Chapter: 13444, 332-345, Elsevier Inc.

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Chemistry

Title: Development of new iodine(III) compounds for antibiotic applications

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: Kevin Cariou
Advisor(s) Email: kevin.cariou@chimieparistech.psl.eu
Research group/Lab: Institute of Chemistry for Life Sciences
(Lab/Advisor website): www.gassergroup.com

Short description of possible research topics for a PhD:

Resistant bacteria are becoming a worldwide threat and, unless solutions are found, global projections for 2050 lead to an estimate of 10 million deaths per year that would be attributable to antimicrobial resistance. This situation dictates the development of new antibiotics that can overcome the resistances associated with all existing treatments. *To explore uncharted chemical space in the area of antibiotics, this project aims at designing and synthesizing hypervalent iodine(III) compounds as antibacterial or anti-resistance compounds.*

Required background of the student:

The applicant should have strong theoretical and practical background in organic chemistry. Mastery of purification and analysis (NMR, MS, IR, etc.) techniques is mandatory as well as excellent written and oral communication skills and the ability to work as part of a team. The applicant must be fluent in English since it is the language spoken in the Gasser group. Practical knowledge in biochemistry would be an asset.

A list of 5 (max.) representative publications of the group:

Hypervalent iodine:
1. Habert, L.; **Cariou, K.*** *Angew. Chem. Int. Ed.*, **2020**, *just accepted*, https://doi.org/10.1002/anie.202009175;
2. Peilleron, L.; Retailleau, P.; **Cariou, K.*** *Adv. Synth. Cat.* **2019***; 361*, 1753–1769
Antibiotic compounds:
3. Romero, E.; Oueslati, S.; Benchekroun, M.; D'Hollander, A. C. A.; Ventre S.; Vijayakumar, K.; Minard, C.; Exilie, C.; Tlili, L.; Retailleau, P.; Zavala, A.. Eliséee, E.; Selwa, E.. Nguyen, L. Pruvost, A.; Naas, T.;* Iorga, B.;* Dodd, R. H.; **Cariou, K.*** **2020**, *preprint: DOI: 10.26434/chemrxiv.11897157*

ParisTech

Chimie Paris ParisTech | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Chemistry, Physical Chemistry and Chemical Engineering

Subfield: Analytical and Physical Chemistry, Materials

Title: *In situ analytical approaches to understand environmental stability of materials for energy*.

ParisTech School: Chimie ParisTech | PSL

Advisor(s) Name: VOLOVITCH Polina
Advisor(s) Email: *polina.volovitch@chimieparistech.psl.eu*
Research group/Lab: *IRCP or IPVF (https://ipvf.fr/) or both depending on candidate*
Lab location: *Paris region (1 h travel by public transport between IRCP and IPVF)*
(Lab/Advisor website): *https://sites.google.com/site/volovitchp/home*

Short description of possible research topics for a PhD:

Weight reduction of materials and devices in mobile applications can lead to more than 25 % decrease in total CO_2 emissions. The development of stable lightweight structural materials is hence one of the up to date occupations of material science. Another big challenge for mobile devices lays in a way to produce sustainable energy, including thin layer photovoltaic cells and new rechargeable lightweight batteries. Finally, an important characteristic of the new energy devices relays on a guarantee that their efficiency is stable in time and will not decline in service by material degradation or spontaneous discharge … The stability of new materials and assemblies is strongly affected by the service conditions, in particular by the presence of electrolytes or humid films and environmental pollutants. The interactions of materials with their environment are composed complex and the environment evolves by itself. A combined multi-disciplinary, multi-scale approach able to describe the evolution of chemical, electrochemical and mechanical state of new materials/ assemblies as a function of time in presence of evolving environments with good time and spatial resolution is necessary, requiring continuous improvement of existing and development of new analytical methodologies. The research in my team is centered around the development of such analytical approaches. The type of the application (structural materials, battery materials or photovoltaic materials) chosen for the PhD will depend on the profile of the candidate.

Required background of the student: Strong background and interest in chemistry (analytical/physical) is necessary. Deep knowledge of material science, electrochemistry and/or instrumentation is a plus but not mandatory.

A list of 5 (max.) representative publications of the group: *see website*

ParisTech

École des Ponts ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Environment Science and Technology, Sustainable Development, Geosciences

Subfield: Applied Physics

Title: Spatio-temporal variability of rainfall drop size distribution across scales: retrieval, characterization and uses

ParisTech School: Ecole des Ponts ParisTech

***Advisor(s) Name*:** August Gires /Ioulia Tchiguirinskaia
Advisor(s) Email: August.Gires@enpc.fr /ioulia.tchiguirinskaia@enpc.fr
Research group/Lab: *Hydrology Meteorology and complexity, ENPC*
Lab location: *École des Ponts ParisTec, 6 et 8 avenue Blaise- Pascal – Cité Descartes – Champs-sur-Marne – 77455 Marne- la- Vallée cedex 2*
(Lab/Advisor website): *https://hmco.enpc.fr/*

Short description of possible research topics for a PhD

Rainfall is a geophysical field extremely variable over wide range of spatio-temporal scales which makes it complex to analyse and even to measure. Weather radars are currently the only devices providing a spatio-temporal insight into this field. Radars basically analyse the signal backscattered by the hydrometeors of the atmosphere and derive rainfall maps from it. These conversion algorithms rely on assumed features of the rain Drop Size Distribution (DSD), and notably its homogeneity within a radar gate. DSD is also directly measured with the help of disdrometers.

The student will review and implement techniques to generate DSD maps from radar data. After, he/she develop an appropriate theoretical framework based on Universal Multifractal to explore and quantify the spatio-temporal variability of DSD. This will enable the development and validation of innovative algorithms for rain rate retrieval with weather radars which will account for the variability DSD from large scale to sub-radar gate scale.

Required background of the student: geophysics, statistics

A list of 5 (max.) representative publications of the group:

1. Brandes, E.A., G. Zhang, and J. Vivekanandan, 2004: Comparison of Polarimetric Radar Drop Size Distribution Retrieval Algorithms. J. Atmos. Oceanic Technol., 21, 584–598, https://doi.org/10.1175/1520-0426(2004)021<0584:COPRDS>2.0.CO;2
2. Gires, A., Tchiguirinskaia, I., and Schertzer, D.: Multifractal comparison of the outputs of two optical disdrometers, Hydro. Sci. J., 6, 1641–1651, https://doi.org/10.1080/02626667.2015.1055270, 2015.
3. Schertzer, D. and Lovejoy, S., 2011. Multifractals, generalized scale invariance and complexity in geophysics. International Journal of Bifurcation and Chaos, 21 (12), 3417–3456. doi:10.1142/S0218127411030647

ParisTech

École des Ponts ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Mathematics and their applications

Subfield: Applied Physics, Geosciences, Data Science, Environment Science

Title: Multiscale short-term forecasts of geophysical fields based on remotely-sensed big data

ParisTech School: Ecole des Ponts ParisTech

Advisor(s) Name: Daniel SCHERTZER, Ioulia TCHIGUIRINSKAIA

Advisor(s) Email: Daniel.Schertzer@enpc.fr, ioulia.tchiguirinskaia@enpc.fr

Research group/Lab: Hydrology Meteorology and Complexity lab (HM&Co)

Lab location: École des Ponts ParisTech, 6 et 8 avenue Blaise Pascal – Champs-sur-Marne – 77455 Marne- la-Vallée cedex 2, France

(Lab/Advisor website): *https://hmco.enpc.fr/*

Short description of possible research topics for a PhD:
We are witnessing a rapid deployment, in particular around large cities, of various recent remote sensing technologies, such as lidars and polarimetric radars, which provide more and more data (wind, precipitation, pollutants) with increasing resolutions. To take full advantage of these technologies and data, qualitatively new short-term forecasts ("nowcasts") must be developed.
It is proposed to develop stochastic nowcasts based on cascading multifractal processes which are much faster than classical deterministic forecasting methods while being closer to the multiscale and nonlinear physics of the processes involved, as well as their intrinsic limit of predictability. The 2024 Olympic Games (Paris) will be an important case of experimentation.

Required background of the student:
Stochastic processes; data science; informatics. A first part of the thesis will be devoted to update knowledge in those domains.

A list of 5 (max.) representative publications of the group:

1. Lovejoy, S. and Schertzer, D. (2013), The Weather and Climate: Emergent Laws and Multifractal Cascades. Cambridge U.K.: Cambridge University Press. pp. 491
2. Marsan, D., Schertzer, D. & Lovejoy, S. (1996), Causal space-time multifractal processes: Predictability and forecasting of rain fields. *J. Geophys. Res.* 101, 26,333-26,346
3. Paz, I., Tchiguirinskaia, I & Schertzer, D. (2020), Rain gauge networks' limitations and the implications to hydrological modelling highlighted with a X-band radar. Journal of Hydrology, 583, 124615
4. Schertzer, D. & Tchiguirinskaia, I. (2017), An Introduction to Multifractals and Scale Symmetry Groups, in Fractals: Concepts and Applications in Geosciences. Ghanbarian, B. and Hunt, A. (eds) CRC Press, 1-28
5. Schertzer, D. & Tchiguirinskaia, I. (2020), A century of turbulent cascades and the emergence of multifractal operators. *Earth Sp. Sci.* 7, e2019EA000608

ParisTech

École des Ponts ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Environment Science and Technology, Sustainable Development, Geosciences
Subfield: Hydrology

Title: Optimal implementation of Nature-Based Solutions to mitigate Urban Heat Islands

ParisTech School: Ecole des Ponts ParisTech

Advisor(s) Name: Pierre-Antoine VERSINI
Advisor(s) Email: *pierre-antoine.versini@enpc.fr*
Research group/Lab: *HM&Co*
Lab location: *Champs-sur-Marne*
(Lab/Advisor website): *https://hmco.enpc.fr/*

Short description of possible research topics for a PhD:

Urban Heat Island (UHI) is a microclimatic phenomenon occurring in urbanized spaces that tend to have higher temperatures than their surrounding countryside. In a context of climate change, the increase of heat waves, in terms of frequency and intensity, has placed the mitigation of UHI as a priority in many cities. Nature Based Solutions (NBS) as rain garden, green roofs, and parks represent some relevant infrastructures to address this challenge and make cities more resilient. As urban environments are complex and very heterogeneous in space, the implementation of NBS regarding the most vulnerable (hot) areas represents a difficult task. The objective of this PhD subject is therefore to develop a methodology, which helps to optimize NBS implementation with regard to UHI. First, temperature fields and their space-time variability will be analysed at the urban scale. For this purpose, every available data will be used, that they are produced by observation devices (satellite, public and private sensors networks) or models (simulations). A particular effort will be made to valorize crowdsourced and remote sensing data. Second, existing NBS spatial distribution will be studied. Finally, based on both fields' properties, some prospective (urban and climate) scenarios will be proposed to optimize NBS cooling effect.

Required background of the student:

Have skills in the modelling of mechanics (graduated in fluid mechanics or environmental physics), capabilities in computer simulations, and be of interest to urban geophysics.

A list of 5 (max.) representative publications of the group:

1. Versini, P.-A., Kotelnikova, N., Poulhes, A., Tchiguirinskaia, I., Schertzer, D. and Leurent, F., 2018. A distributed modelling approach to assess the use of Blue and Green Infrastructures to fulfil stormwater management requirements. Landscape and Urban Planning, 173: 60-63
2. Versini, P.-A., Gires, A., Schertzer, D. and Tchiguirinskaia, I., 2020. Fractal analysis of green roof spatial implementation in European cities. Urban Forestry & Urban Greening, 49, 126629

ParisTech

École des Ponts ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Environment Science and Technology, Sustainable Development, Geosciences

***Title*:** Develop an innovative framework to assess the environmental performances of a new train station over time

ParisTech School: Ecole des Ponts ParisTech

Advisor(s) Name: Pierre-Antoine VERSINI
Advisor(s) Email: *pierre-antoine.versini@enpc.fr*
Research group/Lab: *HM&Co*
Lab location: *Champs-sur-Marne*
(Lab/Advisor website): *https://hmco.enpc.fr/*

Short description of possible research topics for a PhD:
Train stations appear as complex infrastructures as they can no longer be considered just as some transit points, but rather as systems advocating multimodality and multi-functionality. This complexity should also be considered when studying their environmental impacts. In this context, this PhD subject aims to study, through the example of a particular station of the Greater Paris (Grand Paris Express under construction), the necessary consideration of the interactions between the different geophysical fields (temperature, precipitation), urban form (transport network, planning and green spaces) and human flows, as well as their space-time variability. Coupling literature review, measured observations, and distributed model simulations (New tools should also be developed if necessary) will led to identify and assess the main environmental issues concerning the station. They will aim to capture the space-time variability of the involved processes and variables, but also their interactions. This work should illustrate the necessity to adopt a complex system and multi-scale approach to well understand the interaction of an infrastructure with its surrounding urban environment.

Required background of the student:
Have skills in the modelling of mechanics (graduated in fluid mechanics or environmental physics), capabilities in computer simulations, and be of interest to urban geophysics.

A list of 5 (max.) representative publications of the group:
1. Versini, P.-A., Kotelnikova, N., Poulhes, A., Tchiguirinskaia, I., Schertzer, D. and Leurent, F., 2018. A distributed modelling approach to assess the use of Blue and Green Infrastructures to fulfil stormwater management requirements. Landscape and Urban Planning, 173: 60-63
2. Versini, P.-A., Gires, A., Schertzer, D. and Tchiguirinskaia, I., 2020. Fractal analysis of green roof spatial implementation in European cities. Urban Forestry & Urban Greening, 49, 126629

ParisTech

École des Ponts ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: [redacted]

Subfield: Applied mathematics (scientific computing), Computational mechanics (hydraulics)

Title: Modelling and simulating complex flows for engineering puposes

ParisTech School: [redacted]

Advisor(s) Name: BOYAVAL Sébastien
Advisor(s) Email: *sebastien.boyaval@enpc.fr*
Research group/Lab: *Laboratoire d'Hydraulique Saint-Venant (LHSV)*
Lab location: *Chatou (78400)*
Website: *https://www.saint-venant-lab.fr/membres/boyaval_s%C3%A9bastien*

Short description of possible research topics for a PhD:

Continuum mechanics has provided engineers with models that are useful for numerous quantitative predictions. Navier-Stokes or Saint-Venant equations e.g. provide one with realistic numerical simulations of *fluid* flows in various practical situations. But real flows are complex, even water : in river floods for instance. And engineers are mostly interested by particular *real* situations, with specific features that are well observed but not easily predicted yet using generic models like Navier-Stokes or Saint-Venant : heat fluxes, the mixing of chemical species, the rheology of non-Newtonian fluids, the fluctuations in turbulent flows etc. That is why one keeps developing new flow models, on adding complexities to standard models.

At LHSV, given recent improved measurements of real fluid flows (see [5] and Illustration 1. below for an example regarding floods), we aim at validated new flow models, with a better quantitative description than standard models in specific engineering situations. Numerical simulations are verified first, and a sound mathematical framework is required to that aim.

Possible research topics are the construction of new models for complex flows with Partial Differential Equations (PDEs) [2,4], the construction of numerical schemes [1] (for mathematically inclined students) and the numerical simulation of new models [3] (for computer inclined students).

Required background of the student:

PDEs applied to field theories in physics (mechanics preferably), discretization methods (Finite-Volume/Finite-Element), numerical analysis, scientific computing (with Python/C++)

A list of 5 (max.) representative publications of the group:

1. John Barrett, Sébastien Boyaval, Finite element approximation of the FENE-P model, *IMA Journal of Numerical Analysis* (OUP), 2017
2. Sébastien Boyaval, Viscoelastic flows of Maxwell fluids with conservation laws, working preprint https://hal-enpc.archives-ouvertes.fr/hal-02908379 , 2020
3. Sébastien Boyaval, Alexandre Caboussat, Arwa Mrad, Marco Picasso, Gilles Steiner, A semi-Lagrangian splitting method for the numerical simulation of sediment transport with free surface flows, *Computers and Fluids, 2018 172*
4. François Bouchut, Sébastien Boyaval, Unified derivation of thin-layer reduced models for shallow free-surface gravity flows of viscous fluids, *European Journal of Mechanics - B/Fluids*, 2016
5. Sébastien Proust, Céline Berni, Martin Boudou, Antoine Chiaverini, Victor Dupuis, et al.. Predicting the flow in the floodplains with evolving land occupations during extreme flood events (FlowResANR project) 3rd European Conference on Flood Risk Management, Oct 2016, Lyon, France. Hal-01585278

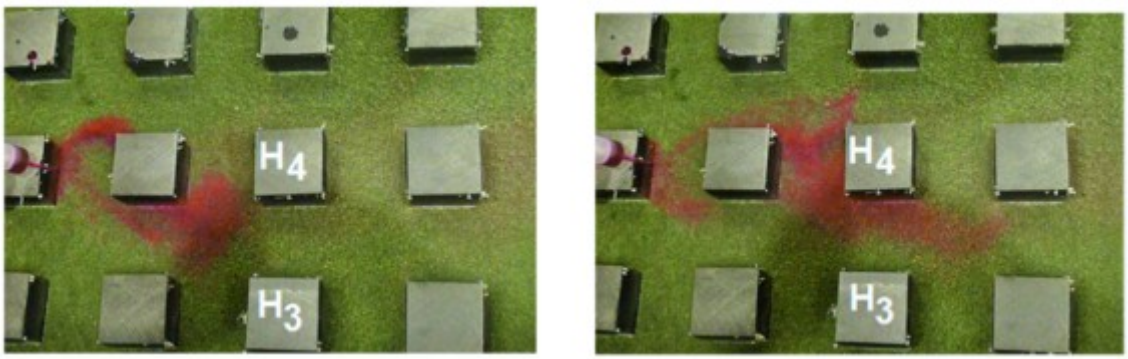


Illustration 1: PhD thesis of Marina Oukacine (p. 116). Étude expérimentale et numérique des écoulements à surface libre en présence d'obstacles émergés et faiblement submergés. Université Paris-Est, 2019. tel-02948861

ParisTech

École des Ponts
ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Mathematics and their applications

Subfield: Probability theory

Title: Central limit theorem for nonlinear functionals of the empririal mean of non i.i.d . samples

ParisTech School: Ecole des Ponts ParisTech

Advisor(s) Name: Benjamin JOURDAIN
Advisor(s) Email: benjamin.jourdain@enpc.fr
Research group/Lab: ENPC/CERMICS
Lab location: Champs-sur-Marne
(Lab/Advisor website): http://cermics.enpc.fr/~jourdain/home.html

Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)
The central limit theorem is with the strong law of large numbers one of the two fundamental limit theorems in probability theory. The confidence intervals that it permits to derive have major applications in Monte-Carlo methods as well as in statistics. In reference 1. below, B. Jourdain and his postdoctoral student A. Tse have extended to nonlinear functionals of the empirical measure of independent and identically distributed random vectors the central limit theorem which is well known for linear functionals given by the integral of a function against the measure. The main tool permitting this extension is the linear functional derivative, one of the notions of derivation on the Wasserstein space of probability measures that have recently been developed and are subject of an intensive research. Central Limit Theorems for linear functionals of non independent and identically distributed random variables such as the successive values of an ergodic Markov chain are long known. The PhD student will investigate extensions to nonlinear functionals in these settings.

Required background of the student: (What should be the main field of study of the applicant before applying?) Probability theory and/or mathematical statistics

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. B. Jourdain, A. Tse, *Central limit theorem over non-linear functionals of empirical measures with applications to the mean-field fluctuation of interacting particle systems*, Preprint arXiv:2002.01458
2. A. Alfonsi, J. Corbetta, B. Jourdain, *Sampling of probability measures in the convex order by Wasserstein projection*, Annales de l'Institut Henri Poincaré B, Probabilités et Statistiques, 56(3):1706-1729, 2020
3. A. Alfonsi, B. Jourdain, *Lifted and geometric differentiability of the squared quadratic Wasserstein distance* , accepted in ESAIM: Probability and Statistics, arXiv:1811.07787
4. G. Fort, B. Jourdain, T. Lelièvre, G. Stoltz, Co*nvergence and efficiency of adaptive importance sampling techniques with partial biasing*, Journal of Statistical Physics, 171(2):220-268, 2018
5. G. Fort, B. Jourdain, T. Lelièvre, G. Stoltz, *Self-Healing Umbrella Sampling: Convergence and efficiency*, Statistics and Computing 27(1):147-168, 2017

ParisTech

École des Ponts ParisTech

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Information and Communication Sciences and Technologies

Subfield: Smart Cities, Artificial intelligence, Environment

Title: Artificial intelligence and the Internet of Things to monitor and accommodate with urban pollution in smart cities

ParisTech School: Ecole des Ponts ParisTech (ENPC)

Advisor(s) Name: Françoise Lucas (Leesu, ENPC)
Advisor(s) Email: ***francoise.lucas@enpc.fr***, ***lucas@u-pec.fr***
Co-advisor: *Sami Souihi (LiSSi, University Paris-Est Créteil)*
co-advisor Email: *sami.souihi@u-pec.fr*
Research group/Lab: consortium of 3 laboratories: *Leesu (ENPC and University Paris-Est Créteil), LISA and LiSSi (University Paris-Est Créteil)*
Lab location: *Leesu, ENPC, Champs-sur-Marne, France*
(Lab/Advisor website): *https://www.leesu.fr/ and http://www.lissi.fr/*

Short description of possible research topics for a PhD:
This thesis is part of the Smart Cities paradigm. It aims to investigate the potential use of artificial intelligence to assess and reduce the pollution impact on human health in urban areas. Nowadays, the development of the Internet of Things allows the deployment of large sensor networks to monitor different aspects of Smart Cities. For instance, different applications and services inform the inhabitants of large cities about the degree of air or water pollution. This information, however, remains scattered through different databases, with very difficult interpretation and it does not take into account the cumulative impact of the various chemical, physical and biological perturbations, which remains difficult to quantify. The first objective of this research is to establish a unified knowledge plane (KP) that aggregates all the pollution data that can impact human health from aerial and aquatic monitoring programs in urban areas. The second objective is to use this KP, to produce and test an adaptive and predictive model of urban pollution assessment, which will be based on the techniques of belief functions and Deep Learning. The last objective of this thesis is to explore the possibility of an adaptive data visualization by considering a real application scenario.

Required background of the student:
- Good Python programming skills,
- Knowledge in Probabilistic theory,
- Knowledge in Machine Learning

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. ROGUET, Adélaïde, THERIAL, Claire, CATHERINE, Arnaud, et al. Importance of Local and Regional Scales in Shaping Mycobacterial Abundance in Freshwater Lakes. *Microbial ecology*, 2018, vol. 75, no 4, p. 834-846.
2. MARÉCAL, Virginie, PEUCH, V.-H., ANDERSSON, Camilla, et al. A regional air quality forecasting system over Europe: the MACC-II daily ensemble production. Geoscientific Model Development, 2015, vol. 8, no 9, p. 2777-2813.
3. MA, Jun, CHENG, Jack CP, LIN, Changqing, et al. Improving air quality prediction accuracy at larger temporal resolutions using deep learning and transfer learning techniques. *Atmospheric Environment*, 2019, vol. 214, p. 116885.
4. AMOUR, Lamine, SOUIHI, Sami, HOCEINI, Said, et al. A hierarchical classification model of qoe influence factors. In : *International Conference on Wired/Wireless Internet Communication*. Springer, Cham, 2015. p. 225-238.
5. RATHORE, M. Mazhar, AHMAD, Awais, PAUL, Anand, et al. Urban planning and building smart cities based on the internet of things using big data analytics. *Computer Networks*, 2016, vol. 101, p. 63-80.

ParisTech ESPCI PARIS | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Life and Health Science and Technology
Subfields: Neurosciences, Neuropathology

Title: **PROPAGATION OF NEURODEGENERATION IN PARKINSON'S DISEASE STUDIED IN *DROSOPHILA* MODELS**

ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Serge Birman
Advisor(s) Email: serge.birman@espci.psl.eu
Research group/Lab: Genes Circuits Rhythms and Neuropathology (GCRN group) /Brain Plasticity Laboratory
Lab location: 10 rue Vauquelin, 75005 Paris
(Lab/Advisor website): (https://www.bio.espci.fr/-Serge-Birman-Genes-Circuits-29-)

Short description of possible research topics for a PhD:

In our group, we are studying the role of specific neurotransmitter systems on brain functioning and behaviour, as well as their susceptibility to ageing and neurodegenerative conditions. This involves integrated studies that combine molecular biology, genetics and behavioural analysis to identify genes, neural circuits and mechanisms controlling locomotor activity and pathogenesis. Our model is the fruit fly *Drosophila*, which is used in laboratories around the world as it offers many tools and advantages for genetic and *in vivo* studies. The topic of the PhD will be to carry out research on Parkinson's disease models, with the aim to understand the mechanisms leading to the propagation of neurodegeneration from one neuron to another by a prion-like mechanism, as this may explain the clinical progression of the disease. This study will be based on solid preliminary results recently obtained in the laboratory by a previous doctoral student of the ParisTech/CSC PhD Program.

Required background of the student: Master's degree in Life Sciences (or Agriculture), ideally with previous training in Molecular Biology.

A list of 5 (max.) representative publications of the group:

1. YON, M., DECOVILLE, M., SAROU-KANIAN, V., FAYON, F., BIRMAN, S. (2020) Localized metabolic profiling of living *Drosophila* in neurodegenerative conditions using ^{1}H magic angle spinning NMR. **Sci. Rep.** 10(1), 9516–9. http://doi.org/10.1038/s41598-020-66218-z
2. HAJJI, K., MTEYREK, A., SUN, J., CASSAR, M., MEZGHANI, S., LEPRINCE, J., VAUDRY, D., MASMOUDI-KOUKI, O.*, BIRMAN, S.* (2019) Neuroprotective effects of PACAP against paraquat-induced oxidative stress in the *Drosophila* central nervous system. **Hum. Mol. Genet.** 28(11):1905-1918 doi:10.1093/hmg/ddz031
3. ISSA A.-R., SUN J., PETITGAS C., MESQUITA A., DULAC A., ROBIN M., MOLLEREAU B., JENNY A., CHÉRIF-ZAHAR B., BIRMAN S. (2018) The lysosomal membrane protein LAMP2A promotes autophagic flux and prevents SNCA-induced Parkinson disease-like symptoms in the *Drosophila* brain. **Autophagy** 14(11):1898–1910, doi:10.1080/15548627.2018.1491489
4. VACCARO A., ISSA A.-R., SEUGNET L., BIRMAN S., & KLARSFELD A. (2017) *Drosophila* Clock is required in brain pacemaker neurons to prevent premature locomotor aging independently of its circadian function. **PLOS Genet.** 13(1):e1006507, doi:10.1371/journal.pgen.1006507
5. RIEMENSPERGER T., ISSA A.-R., PECH U., COULOM H., NGUYỄN M. V., CASSAR M., JACQUET M., FIALA A. & BIRMAN S. (2013) A single dopamine pathway underlies progressive locomotor deficits in a *Drosophila* model of Parkinson disease. **Cell Rep.** 5:952–960 doi:10.1016/j.celrep.2013.10.032

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Energy, Processes
Subfield: Materials for photovoltaics
Title: Material Strategies for More Stable Perovskite Solar Cells
ParisTech School: ESPCI Paris
Advisor Name: Dr. Zhuoying Chen
Advisor Email: *zhuoying.chen@espci.fr*
Research group/Lab: *Micro & Nano Characterization Group/LPEM*
Website: *http://optoelec.lpem.espci.fr*

Short description of possible research topics for a PhD:

Research in the field of solution-processed organic-inorganic lead perovskite halide solar cells have witnessed remarkable progress over the past decade. The majority of research efforts have been focused on the improvement of the power-conversion efficiency, leading to a significant increase of this figure-of-merit reaching 25%. This progress and additional advantageous properties, such as ease of fabrication, low-cost, light-weight, flexibility and semi-transparency make these devices a bright contender for potential new industrial applications. However, when compared to silicon-based solar panels, which typically have a lifespan of 25 years, hybrid perovskite solar cells suffer from various degrees of material degradation related to the environment they are exposed to. Device stability, thus currently represents one of the utmost pressing issues preventing their large-scale application and exploitation.

While there are existing methods (e.g. additives, different transport-layers and interface modifications) towards better perovskite solar cell stability, the fundamental processes happening in the material and the device by these methods are still to be fully understood. In addition, while perovskite solar cell stability can be slightly enhanced by current methods, it is still by far inferior compared to silicon solar cells. There is still much room for further improvement. This thesis program will therefore focus on understanding the fundamental roles of current methods in order to propose further innovative and more effective stability enhancement strategies. Specifically, the PhD candidate will first study the microstructure, chemical, and optical origins of the stability enhancement of hybrid perovskite halides when applying different materials and device modifications methods by a combination of optical, structural, microscopic, and spectroscopic investigations. Upon obtaining fundamental understandings, he/she will propose new strategies with more effective impact on the solar cell stability.

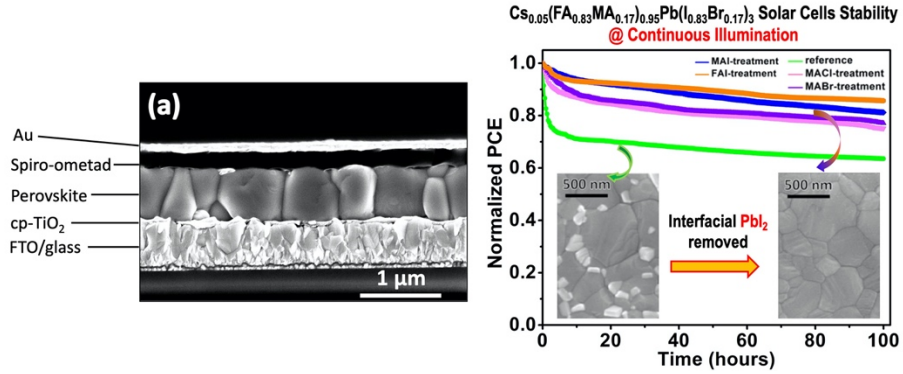


Figure: (a) Cross-sectional SEM image of a perovskite solar cell fabricated in our lab; (b) Efficiency evolution over 100 hrs of the unencapsulated $Cs_{0.05}(FA_{0.83}MA_{0.17})_{0.95}Pb(I_{0.83}Br_{0.17})_3$ perovskite solar cells with different surface treatments under continuous AM 1.5G 1-sun illumination measured inside an Ar glovebox in our lab.

Required background of the student: Solid academic background and a Master Degree on chemistry, material science, or applied physics. Good speaking & writing skills in English. Passionate in scientific experiments.

A list of representative publications of the group on this subject:

- "TiO_2 Nanocolumn Arrays for More Efficient and Stable Perovskite Solar Cells", ACS Applied Materials & Interfaces, 12, 5979-5989 (2020)
- "Microscopic Evidence of Upconversion-Induced Near-Infrared Light Harvest in Hybrid Perovskite Solar Cells", M. Schoenauer Sebag et al., ACS Applied Energy Materials, 1, 3537-3543 (2018)
- "Compact layer free mixed-cation lead mixed-halide perovskite solar cells", Z. Hu et al., Chemical Communications, 54, 2623-2626 (2018)
- "Effect of Ion Migration-Induced Electrode Degradation on the Operational Stability of Perovskite Solar Cells", ACS Omega, 3, 10042-10047 (2018)

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: ***Materials***
Subfield: (Applied Physics, Chemistry, Mathematics, Mech. Eng....)
Applied Physics-Chemistry.
Title: Electrostrictive and Triboelectric fibers for Vibrational Energy Harvesting.
ParisTech School: ESPCI Paris PSL
Advisor(s) Name: COLIN Annie
Advisor(s) Email: annie.colin@espci.fr
Research group/Lab: MIE CBI
Lab location: ESPCI Paris PSL 10 rue Vauquelin 75005 Paris
(Lab/Advisor website):https://www.cbi.espci.fr/accueil-22/
Short description of possible research topics for a PhD: The decreasing energy consumption of today's portable electronics has invoked the possibility of energy harvesting from the ambient environment for self-power supply. One common and simple method for vibration energy harvesting is to utilize triboelectricity or electrostriction. In this thesis, we propose to synthesize fibers to make smart fabrics. This fabric will be efficient and washable. Two types of fibers will be manufactured by dip-coating : electrostrictive fibers and triboelectric fibers. For this we will take advantage of the previous studies in the laboratory [1,2,3].
We will compare the performance of the two systems of fibers as a function of humidity. The second step will be to evaluate the performances of the fibers by preparing a self heating fabric. The garment will be heated by joule effect. Some conductive fibers will be used in the fabric and connected to the
In a third step we will store the produced energy and used it to cool the fabric.
Required background of the student: (What should be the main field of study of the applicant before applying?)
The student should have a solid training in chemistry , chemical formulation and be an experimentalist. Knowledge of electronics is recommended.
A list of 5 (max.) representative publications of the group:

1. M Pruvost, WJ Smit, C Monteux, P Poulin, A Colin - npj Flexible Electronics, 2019. Polymeric foams for flexible and highly sensitive low pressure capactive sensors.
2. W.Smit, C Kusina , JF Joanny, A Colin PRL 123(14) 148002. Stress field inside the bath determines dip coating with yield stress fluids in cylindrical geometry.
3. M.Pruvost, WJ Smit, C Monteux, P Poulin, A Colin Multifunctionnal Materials 1 (1) 015004 2018 Microporous electrostrictive materials for vibrational energy harvesting
4. Yuan, Jinkai, Alan Luna, Wilfrid Neri, Cécile Zakri, Annie Colin, and Philippe Poulin. "Giant electrostriction of soft nanocomposites based on liquid crystalline graphene." *ACS nano* 12, no. 2 (2018): 1688-1695.
5. Nesser, Hussein, Hélène Debéda, Jinkai Yuan, Annie Colin, Philippe Poulin, Isabelle Dufour, and Cedric Ayela. "All-organic microelectromechanical systems integrating electrostrictive nanocomposite for mechanical energy harvesting." *Nano Energy* 44 (2018): 1-6.

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Physics *Physics*
Subfield: (Applied Physics, Chemistry, Mathematics, Mech. Eng.…)
Soft Matter
Title: Characterization of the flow of concentrated suspensions under vibrations.
ParisTech School: ESPCI Paris PSL
Advisor(s) Name: COLIN Annie
Advisor(s) Email: annie.colin@espci.fr
Research group/Lab: MIE CBI
Lab location: ESPCI Paris PSL 10 rue Vauquelin 75005 Paris
(Lab/Advisor website):https://www.cbi.espci.fr/accueil-22/
Short description of possible research topics for a PhD:
Cements, sewage sludge, chocolate are dispersions, carbon suspensions are dispersions of non-Brownian particles. In industry, it is important to be able to prepare such highly concentrated dispersions in order to reduce the water impact of the processes while keeping systems with low viscosity.
In this thesis we will study the flows of highly concentrated suspensions of non Newtonian particles under vibration. Vibrating a suspension makes it possible to reduce the viscosity and to prepare dispersions with ultra high solid fraction. In this pHD, we will take advantages of the technics developed in our laboratory to characterize the features of the flow as a function of the amplitude of the external mechanical vibrations and of its frequency. We will use home made sensors to measure and characterize the shear stress map in a Couette cell[4]. These measurements will be complemented by solid fraction measurements under shear using Xray tomography [1], the friction coefficient and the forces profile between particles will be analyzed using a tuning fork[2,3,5] .
Required background of the student: (What should be the main field of study of the applicant before applying?)
The student should have a solid training in physics, fluid mechanics and be an experimentalist.***A list of 5 (max.) representative publications of the group:***

1:Ovarlez, G., Le, A.V.N., Smit, W.J., Fall, A., Mari, R., Chatté, G. and Colin, A., 2020. Density waves in shear-thickening suspensions. *Science Advances*, *6*(16), p.eaay5589.

2;Comtet, J., Chatté, G., Niguès, A., Bocquet, L., Siria, A. and Colin, A., 2017. Pairwise frictional profile between particles determines discontinuous shear thickening transition in non-colloidal suspensions. *Nature communications*, *8*(1), pp.1-7.

3.Chatté, Guillaume, Jean Comtet, Antoine Niguès, Lydéric Bocquet, Alessandro Siria, Guylaine Ducouret, François Lequeux, Nicolas Lenoir, Guillaume Ovarlez, and Annie Colin. "Shear thinning in non-Brownian suspensions." *Soft matter* 14, no. 6 (2018): 879-893.

4. Anais Gauthier, Mickael Pruvost, Olivier Gamache, Annie Colin, A new pressure sensor array for local normal stress measurement in complex fluids arXiv:2010.04474

5. Madraki, Y., A. Oakley, A. Nguyen Le, A. Colin, G. Ovarlez, and S. Hormozi. "Shear thickening in dense non-Brownian suspensions: Viscous to inertial transition." *Journal of Rheology* 64, no. 2 (2020): 227-238.

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RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Physics, Optics

Subfield: (Chemistry, Colloidal Sciences)

Title: Active Colloidal Gels

ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Olivier Dauchot
Advisor(s) Email: olivier.dauchot@espci.fr
Research group/Lab: Gulliver Lab
Lab location: Paris
(Lab/Advisor website): https://www.gulliver.espci.fr

Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)

Colloidal Gels are obtained from the aggregation of attractive colloids. Tuning the density of particles, and the attraction strength and range allow us to control the gel morphology. Embedding colloids, that can be activated by light, inside the gel, we can form an active material, the response of which is controlled by light.

The main goal of this project is to study experimentally the coupling between the activity level and the mechanical properties of the gel. In particular, one expects the strain field induced by the active forces to induce a feedback on the active units, eventually leading to some form of collective actuation. Unveiling such a process would be a major breakthrough both in our understanding of living bodies and I towards the design of new functional materials.

Required background of the student: (What should be the main field of study of the applicant before applying?)

A good knowledge of colloidal and interface science is mandatory. Being at ease with micro-manipulation, confocal microscopy is useful too. Finally mentoring data-processing using Matlab or python is important too.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. *Chemical Physics of Active Matter* O. Dauchot, H. Löwen J. Chem. Phys. **151**, 114901 (2019)
2. *Interrupted Motility Induced Phase Separation in Aligning Active Colloids*. Marjolein N. van der Linden, Lachlan C. Alexander, Dirk G. A. L. Aarts, Olivier Dauchot Phys. Rev. Lett. 123, 098001 (2019)
3. *The flow field around a confined active droplet*. C. de Blois, M. Reyssat, S. Michelin and O. Dauchot Physical Review Fluids **4,** 054001 (2019).
4. *Active versus Passive Hard Disks against a Membrane: Mechanical Pressure and Instability*, G. Junot, G. Briand, R. Ledesma-Alonso, and O. Dauchot, Phys. Rev. Lett. 119, 028002, (2017).
5. *Elastic interactions between topological defects in chiral nematic shells*, Alexandre Darmon, Olivier Dauchot, Teresa Lopez-Leon, Michael Benzaquem, *Phys. Rev. E* 94, (2016)

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RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Physics, Optics

Subfield: (Mech. Eng / Computer Science)

Title:Morphological Swarm Robotics

ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Olivier Dauchot
Advisor(s) Email: olivier.dauchot@espci.fr
Research group/Lab: Gulliver Lab
Lab location: Paris
(Lab/Advisor website): www.gulliver.espci.fr

Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)

In this project, we are interested in swarm robotics, where a large number of robots with limited computation and communication power are considered. Our goal is to propose new design methods, with a particular focus on collective decision making using both morphological and logical computation.

To do so, we aim at new kind of swarm bots, where the shape factor guarantees the group dynamics, while each robot embeds a lightweight system-on-chip, sensors and actuators that can be used to modulate the robot behaviors on-the-fly.

We will then look for specific educated collective behaviors: starting from the spontaneous phase obtained from the purely physical interactions of our robots we aim at applying minimal control from embodied capabilities on each bot, to induce specific collective behavior, which we will refer to as operational phases. Optimizing such behavior, we will aim at the realization of complex collective tasks.

Required background of the student: (What should be the main field of study of the applicant before applying?)

Our approach towards this topic is definitely the one of physicists; it is therefore important to have a good background in physics. At the same time, the object of studies, the robot swarm, requires a good knowledge of Fablab tools, such as 3D printers, laser cutter, electronics, which is closer to mechanical engineering. Finally being familiar with computer sciences, sensor-controllers is important too.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

This is a new topic of the group. Before the group was focusing on physical active matter (not involving robots). This is why in the five publication below, only one is directly related to robotics.

1. *Distributed On-line Learning in Swarm Robotics with Limited Communication Bandwidth*. Nicolas Fontbonne, Olivier Dauchot and Nicolas Bredeche. Proceedings of the IEEE Congress on Evolutionary Computation (CEC), 2020
2. *Dynamics of a Self-Propelled Particle in a Harmonic Trap*. O. Dauchot, and V. Démery. Phys. Rev. Lett. **122,** 068002 (2019).
3. *Spontaneously Flowing Crystal of Self-Propelled Particles*. G. Briand, M. Schindler and O. Dauchot. Phys. Rev. Lett 120**,** 208001 (2018).
4. *Active versus Passive Hard Disks against a Membrane: Mechanical Pressure and Instability*, G. Junot, G. Briand, R. Ledesma-Alonso, and O. Dauchot, Phys. Rev. Lett. 119, 028002, (2017).
5. *Self-propelled hard disks: implicit alignment and transition to collective motion* Khanh-Dang Nguyen Thu Lam, Michael Schindler, Olivier Dauchot New Journal of Physics (2015)

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Materials Science, Mechanics, Fluids

Subfield: (Applied Physics and electrical engineering)

Title: Contact effects at metal/insulator interfaces

ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Stéphane Holé
Advisor(s) Email: stephane.hole@espci.fr
Research group/Lab: Physics and Material Study (LPEM)
Lab location: ESPCI – 10, rue Vauquelin – 75005 Paris – France
(Lab/Advisor website):

Short description of possible research topics for a PhD:
When two materials are brought into contact, electric charge transfer from one material to another occurs at the interface. This gives rise to a contact potential. Though it is well described when metals and semiconductors are concerned, this is still not well established when an insulator is concerned, because no measurement can be carried out.
We have proposed a new measurement method for directly accessing the contact voltage in the case of metal/insulator contacts based on an electro-elastic coupling. The advantage of the method is that no material model is required to obtain the information.
The aim of the PhD is to improve the calibration procedure, test various metal/insulator interfaces and propose an interface model from the observed results.

Required background of the student: (What should be the main field of study of the applicant before applying?)
The applicant should have skills in solid state physics, instrumentation (in electronics bases at least) and matlab or python language.

A list of 5 (max.) representative publications of the group:

1. Holé S., *Contact potential measurement at metal/insulator interface*, ISE, p. 51, 2019. available at https://ise2019.mosaicteam.eu/wp-content/uploads/2019/09/ISE17_2019_AbstractBook.pdf.
2. Salamé B. and Holé S., *Elasto-electric coupling for direct electric field distribution measurement in semiconductor structures*, J. Appl. Phys., vol. 120, p. 175702 (2016)
3. Salamé B.and Holé, S, *The pressure wave propagation method for the study of interface electric field*, EIC, pp. 53-56 (2015)
4. Salamé B. and Holé, S., *Electrode induced signal with Pressure-Wave-Propagation Method*, ISE, p. IX.7 (2014)
5. Ravat C., Absil, É., Holé, S. and Lewiner, J., *Acoustoelectric coupling for direct electrical characterization of semiconductor devices*, J. Appl. Phys., vol. 99, pp. 063712-1-5 (2006)

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Materials Science, Mechanics, Fluids

Subfield: Applied Physics and electrical engineering

Title: High spatial resolution space charge distribution measurement by electro-acoustic reflectometry (EAR)

ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Stéphane Holé
Advisor(s) Email: stephane.hole@espci.fr
Research group/Lab: Physics and Material Study (LPEM)
Lab location: ESPCI – 10, rue Vauquelin – 75005 Paris – France
(Lab/Advisor website):

Short description of possible research topics for a PhD:
Insulating materials should prevent electric charges from flowing. However, charges enter and become trapped resulting in damage to the system in which the material is included. This is particularly problematic to high voltage integrated devices, but existing measurement methods have not a sufficient spatial resolution for studying this problem.
LPEM has developed a new measurement method based on the material impedance variation due to electromechanical couplings. It allows to greatly increase the spatial resolution, but still needs to be improved to obtain even better resolution. This implies working with micro-wave techniques up to 10 GHz.

Required background of the student: (What should be the main field of study of the applicant before applying?)
The applicant should have skills in electronics, microwave and interested in advanced instrumentation.

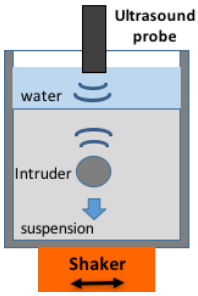
A list of 5 (max.) representative publications of the group:

1. Hamidouche L., Holé S. and Géron E., An overview on the sensitivity of Electro-Acoustic-Reflectometry (EAR) method, IEEJ Trans. FM, vol. 139, pp. 99-104 (2019)
2. Hamidouche L., Géron E. and Holé, S., Physical investigation of the Electro-Acoustic-Reflectometry method for space charge measurements, Phys. Scr., vol. 94, pp. 115006-1-9 (2019)
3. Hamidouche L., Géron E. and Holé S., Very high spatial resolution space charge measurement using electro-acoustic reflectometry (EAR), IEEE Electrical Insulation Magazine, vol. 33, pp. 9-16 (2017)
4. Hamidouche L., Géron E. and Holé S., Electro-Acoustic Reflectometry, a new method toward very high spatial resolution space charge measurements, ICD, vol. 1, pp. 46-48 (2016)
5. Hamidouche L., Géron E., Ditchi T. and Holé S., High Frequency Spectroscopy for High Spatial Resolution Space Charge Measurements, ISE, p. IX.8, (2014)

Research Topic for the ParisTech/CSC PhD Program

***Field: Physics, Optics;* Materials Science, Mechanics**
Subfield: Applied Physics, Acoustics
ParisTech School: ESPCI Paris – PSL University
Title: Acoustic imaging and pumping in granular sediments
Advisor: Professor Xiaoping JIA
Advisor Email: xiaoping.jia@espci.fr
Research group/Lab: Institut Langevin
***Lab location*:** 1 rue Jussieu, 75005 Paris
Website: https://www.institut-langevin.espci.fr

Short description of possible research topics for a PhD:
Imaging and understanding the motion of an intruder or buried object inside opaque dense suspensions such as quicksand or ocean sediments are of practical and fundamental importance. In this PhD project, we use the ultrasonic echography with one or multiple elements to monitor the sinking dynamics of a steel ball in vibrated dense glass bead packings (3D) saturated by water [1,2]. Unlike a falling ball reaching a terminal velocity in Newtonian liquids (viscometer), the ball in gravitational granular suspensions may stop sinking at a given depth due to the yield stress, which depends on the packing density and confining pressure. We will investigate the ball motion fluidized by horizontal vibration (Fig. a) or by acoustic pumping within the framework of granular rheological models [3]. In particular, we will focus on the transition of granular sediments from solid state to liquid state resulted from a mechanism of acoustic lubrication that reduces the inter-particle friction and shear contact stiffness due to the micro-slip [4], without visible macroscopic rearrangement of grains as in usual liquefaction phenomena. This work also help a better understanding of landslides and avalanches caused by vibrations, related to human activities or to natural events such as volcanoes [5].



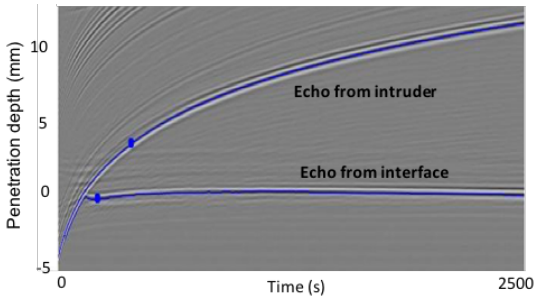


Figure : (a) Diagram of experimental setup *(b)Intruer sinking tracked by ultrasound*

Required background of the student: a good background in physics in general and particularly acoustics and mechanics

***A list of 5 (max.) representative publications of the group:* author(s)** of the group in **bold**
[1] S. van den Wildenberg, **X. Jia**, J. Léopoldès, and A. Tourin, *Sci. Rep.* 9, 5460 (2019)
[2] J. Brum, J.L. Gennisson, M. Fink, A. Tourin & **X. Jia**, Phys. Rev. E 84, 020301 (2019)
[3] B. Andreotti, Y. Forterre & O. Pouliquen, Granular Media (Cambridge University Press, 2013)
[4] **X. Jia,** T. Brunet, J. Laurent, *Phys. Rev. E* 84, 020301(R) (2011); P. Johnson and **X. Jia**, *Nature* 437, 871 (2005)
[5] J. Léopoldès, **X. Jia**, A. Tourin, A. Mangeney, Phys. Rev. E 102, 042901 (2020)

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Physics, Optics
Subfield: Condensed Matter

Title: Local electronic properties of a remarkable ionic conductor

ParisTech School: ESPCI Paris | PSL
Advisors Name: Guillaume LANG, Brigitte LERIDON
Advisors Email: guillaume.lang@espci.fr brigitte.leridon@espci.fr
Research lab: LPEM (CNRS, ESPCI Paris, PSL, Sorbonne Université)
Lab location: ESPCI Paris, 10 rue Vauquelin, 75005 Paris
Advisor website: https://em.lpem.espci.fr/home/

The 2D oxide $Rb_2Ti_2O_5$ has a **colossal low-frequency dielectric constant** ($\simeq 10^9$) and an **exceptional electric polarization** (0.1 C/cm^2). This is related to the very large ionic conductivity of this electronic insulator and to the accumulation of charges at its boundaries. While $Rb_2Ti_2O_5$ is promising for super-capacitors and memory applications, the transport properties of the diffusing ionic species and the spatial variations of the electronic properties are not well understood.

In the context of a joint study (LPEM Paris, ICCMO Orsay), we rely on Nuclear Magnetic Resonance (NMR), **an excellent probe of the spin and charge properties at the atomic scale**. It allows here to show that, contrary to expectations in an electronic insulator, the nanoscale charge and magnetic fluctuations are quantitatively similar as well as correlated with one another. A tentative scenario is that of the ionic diffusion inducing electronic changes in the Ti/O layers.

Using NMR and cryogenics, the Ph.D. student will focus on studying:

- Ionic diffusion and its connection to the local electronic properties.
- The *macro-scale* variation of the *nano-scale* electronic properties in samples having undergone macroscopic electrical polarization.
- How the observations hold in related compounds, to help develop an optimization strategy with an eye towards applications.

Required background: Education in condensed matter (or solid-state) physics. Interest in experimental physics. Knowledge of NMR is NOT needed.

Representative publications of the group:

1 R. Rani *et al.*, Materials Letters 258, 126784 (2020)
2 G. Lang *et al.*, Phys. Rev. B 94, 014514 (2016)
3 S. de Sousa Coutinho *et al.*, Solid State Ionics 333, 72 (2019)
4 R. Federicci *et al.*, Journal of Applied Physics 124, 152104 (2018)
5 R. Federicci *et al.*, Phys. Rev. Materials 1, 032001 (2017)

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Mathematics and their applications

Subfield: (Statistical mechanics, statistics, applied mathematics)

Title: Irreversible algorithms for molecular modeling

ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Anthony Maggs
Advisor(s) Email: anthony.maggs@espci.fr
Research group/Lab: *Gulliver*
Lab location: ESPCI, 10 rue Vauquelin Paris 75005
(Lab/Advisor website): https://www.gulliver.espci.fr/

Short description of possible research topics for a PhD:

Molecular modeling (research rooted in particle-based computation) is central to our understanding of the material world. Its methods allow one to investigate complex phenomena in biophysics and materials research, and to describe the fundamental phase behavior of the universe that surrounds us. Molecular modeling has provided methods for many other fields, from astrophysics to hydrodynamics, statistical mechanics and field theory. Molecular modeling is an interdisciplinary research field, in which the development of algorithms plays an important role. Improved sampling methods, constrained ensembles, and novel approaches beyond molecular dynamics stand out in their promise for the future.

Although the principal methods have been developed for over half a century, disruptive development continues to take place. An example is the irreversible Markov-chain Monte Carlo methods which violate the fundamental detailed-balance condition yet converge towards equilibrium. They illustrate that past algorithms were overly restrictive. Radically new Markov-chain Monte Carlo algorithms have already led to the resolution of long-standing controversies (as for example in two-dimensional melting studied through the use of irreversible Markov chains). We wish to extend these methods to standard interaction potentials in soft-matter physics, in the belief that this can lead to highly efficient codes that explore equilibrium configurations using irreversibility flows.

Required background of the student:

We are looking for students with background in statistical mechanics, applied mathematics or statistics who are interested in joining an open collaboration between several groups in the historic center of Paris.

A list of 5 (max.) representative publications of the group:

All-atom computations with irreversible Markov chains, M.F. Faulkner, Liang Qin, A.C. Maggs and Werner Krauth, J.Chem Phys (2018).
https://aip.scitation.org/doi/10.1063/1.5036638

Event-chain Monte Carlo with factor fields, Ze Lei, Werner Krauth, and A. C. Maggs, PRE (2019). https://doi.org/10.1103/PhysRevE.99.043301

Research Topic for the ParisTech/CSC PhD Program

Field : Physical chemistry, Chemical engineering

Subfield: material sciences, mechanics, fluids

Title: **Bio inspired hydrogels for water filtration**

ParisTech School: ESPCI Paris

Advisor(s) Name: Cecile Monteux
Advisor(s) Email:cecile.monteux@espci.fr
Research group/Lab: SIMM, Soft Matter Science and Engineering
(Lab/Advisor website):

Short description of possible research topics for a PhD: Hydrogels are polymer based materials composed of a network of polymer chains in water, which are covalently or physically bound. In nature, some bio-hydrogels have outstanding filtration properties. As an example, mucus prevents the entrance of toxic nanoparticles into the lungs. In the kidney, the glomerular barrier, which is composed of collagen fibers, filters proteins and nanoparticles. Such hydrogels are highly permeable to water but very efficiently filter nanoparticles. Our goal is to conduct a biomimetic approach to design bioinspired hydrogels that present similar properties to natural hydrogels. Our challenge will be to tune the toughness of the hydrogels so that they can sustain high filtration pressures. Indeed we expect that the deformation of hydrogels under pressure and their eventual compression may lead to a permeability decrease. Moreover we will design hydrogels with controlled spatial heterogeneity to control the water permeability.

Required background of the student: background in chemical engineering or materials science

A list of 5(max.) representative publications of the group:

Foaming of Transient Polymer Hydrogels, Deleurence, R., Saison, T., Lequeux, F. & Monteux*, C. *ACS Omega* **3**, 1864–1870 (2018). 10.1021/acsomega.7b01301

Cross-flow filtration for the recovery of lipids from microalgae extracts: membrane screening and filtration of model and real products, E. Claveijo, C. Monteux, E. Couallier*, *Process Biochemistry*, in press (10.1016/j.procbio.2019.10.016)

ParisTech ESPCI PARIS | PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Biology, Biophysics and Bio Chemistry

Subfield: Biophysics, Soft-Matter, Synthetic Biology, Chemistry, Applied Physics

Title: A microfluidic reactor for the emergence, assembly and evolution of life's biopolymers and cellular structures

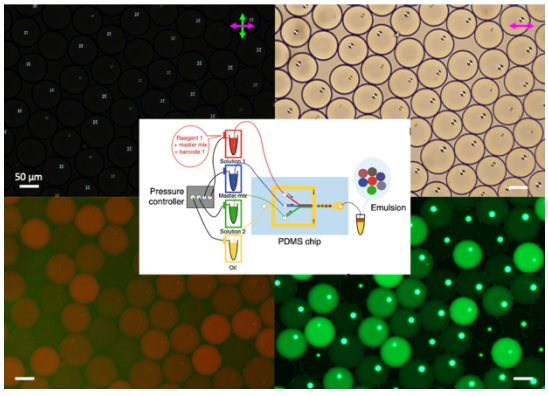
ParisTech School: ESPCI Paris | PSL

Advisors Name: Philippe Nghe, Tommaso Fraccia
Advisors Email: philippe.nghe@espci.psl.eu, tommaso.fraccia@espci.fr
Research group/Lab: Laboratoire de Biochimie / CBI
Lab location: IPGG, 3rd and 6th floors, 6 rue Jean Calvin, 75005, Paris
Lab/Advisor websites: blog.espci.fr/nghe, blog.espci.fr/tfraccia, www.lbc.espci.fr

Short description of possible research topics for a PhD:

It remains unknown how biological building blocks can polymerize and self-organize into compartmentalized reaction networks capable of evolution, thus making the bridge between physico-chemistry and biology. Solving this problem requires considering the self-assembly of such molecules into phases typical of soft-matter, such as liquid crystals and coacervates[1,2]. Indeed, these phases have been shown to template polymerization[3] and allow evolution through compartmentalization[4,5].

We will set-up an experiment to test for the emergence, assembly and evolution of life's biopolymers and cellular structures in complex mixtures of biomolecular building blocks (RNA, peptides, lipids) submitted to cyclical variations of different physico-chemical conditions (concentration, temperature, pH, ionic strength and valence). To achieve this goal, this project exploits cutting-edge optical microscopy techniques coupled to innovative microfluidic platforms allowing the high throughput screening of reaction conditions in parallel.



Liquid crystal coacervates produced with a high-throughput multi-parameter automated titration method based on microfluidics

Required background of the student:
Supramolecular chemistry or Biochemistry or Soft-Matter Physics or Biophysics

A list of 5 (max.) representative publications of the group:

1. Fraccia, T. P.; Jia, T. Z. Liquid Crystal Coacervates Composed of Short Double-Stranded DNA and Cationic Peptides. *ACS Nano* **2020**, *xxx*, xxx–xxx, doi:10.1021/acsnano.0c05083

2. Smith, G. P.; Fraccia, T. P. & al. Backbone-free duplex-stacked monomer nucleic acids exhibiting Watson–Crick selectivity. *Proc. Natl. Acad. Sci. U. S. A.* **2018**, *115*, E7658–E7664, doi:10.1073/pnas.1721369115.
3. Todisco, M.; Fraccia, T. P. & al. Nonenzymatic Polymerization into Long Linear RNA Templated by Liquid Crystal Self-Assembly. *ACS Nano* **2018**, *12*, 9750-9762, doi:10.1021/acsnano.8b05821.
4. Matsumura, S. & al.Transient compartmentalization of RNA replicators prevents extinction due to parasites. *Science* **2016**, *354*, 1293-1296, doi:10.1126/science.aag1582.
5. Blokhuis, A. & al. Selection Dynamics in Transient Compartmentalization. *Phys. Rev. Lett.* **2018**, *120*, 158101, doi:10.1103/PhysRevLett.120.158101.

Research Topic for the ParisTech/CSC PhD Program

Field : Life and Health Science and Technology; Physics, Optics

Subfield: ***High resolution eye imaging***

Title: ***Imaging and dynamic of the retina cells***

ParisTech School: ESPCI

Advisor(s) Name: ***Olivier Thouvenin, Pedro Mece, Claude Boccara***
Advisor(s) Email:olivier.thouvenin@espci.fr pedro.mece@espci.fr claude.boccara@espci.fr
Research group/Lab: Institut Langevin
(Lab/Advisor website): https://www.institut-langevin.espci.fr/home?lang=en

Short description of possible research topics for a PhD:

The goal of this research will be to design a dynamic in-vivo cell imaging device to observe microscopic changes in single neurons, called ganglion cells, in the retina of patients. By combining an optical interference imaging technique, such as full-field optical tomography, with wavefront shaping approaches, and the extraction of new contrasts linked to the metabolic activity of cells, this project promises to open up promising perspectives in the following fields: physics, engineering, biology, neuroscience, pharmacology and medicine.
This work will be carried out the Langevin Institute, ESPCI Paris laboratory in connection with Quinze-Vingt Eye Hospital in Paris.

Required background of the student:
The recruitment of a doctoral student with a good background in physics in general and particularly optics as well as a marked interest in the interface with ophthalmology, or medicine, through imaging methods is desired.
The candidate will have initial experience in optics with a taste for microscopy and image processing. Knowledge of biology would be appreciated.
The management and interpretation of images generally use the MATLAB and / or Python language with which the candidate should be familiar.

A list of 5(max.) representative publications of the group:

Dynamic full-field optical coherence tomography: 3D live-imaging of retinal organoids
Scholler, J., K. Groux, O. Goureau, J. A. Sahel, M. Fink, S. Reichman, C. Boccara, and K. Grieve
Light: Science and Applications **9**, 140 (2020)

Real-time non-contact cellular imaging and angiography of human cornea and limbus with common-path full-field/SD OCT
Mazlin, V., P. Xiao, J. Scholler, K. Irsch, K. Grieve, M. Fink, and A. C. Boccara
Nature Communications **11**, 1868 (2020)

Coherence gate shaping for wide field high-resolution in vivo retinal imaging with full-field OCT
Pedro Mecê, Kassandra Groux, Jules Scholler, Olivier Thouvenin, Mathias Fink, Kate Grieve, and Claude Boccara. Biomedical Optics Express 11, n°9, 4928 (2020)

High-resolution in-vivo human retinal imaging using full-field OCT with optical stabilization of axial motion. Pedro Mecê, Jules Scholler, Kassandra Groux, and Claude Boccara. Biomedical optics express, 11(1), 492-504 (2020).

Probing dynamic processes in the eye at multiple spatial and temporal scales with multimodal full field OCT
Scholler, J., V. Mazlin, O. Thouvenin, K. Groux, P. Xiao, J. A. Sahel, M. Fink, C. Boccara, and K. Grieve
Biomedical Optics Express 10, no. 2, 731-746 (2019)

**Please choose one or more from the following fields:*

1. Biology, Biophysics and Bio Chemistry
2. Chemistry, Physical Chemistry and Chemical Engineering
3. Economics, Management and Social Sciences
4. Energy, Processes
5. Environment Science and Technology, Sustainable Development, Geosciences
6. Information and Communication Sciences and Technologies
7. Life and Health Science and Technology
8. Materials Science, Mechanics, Fluids
9. Mathematics and their applications
10. Physics, Optics
11. Design, Industrialization
12. Life Science and Engineering for Agriculture, Food and the Environment
13. Urban planning, Transport

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Physics, Optics

Subfield: Applied Physics

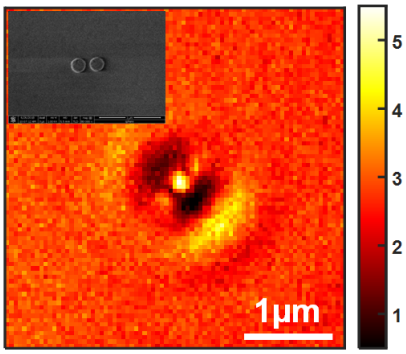
Title: Nanostructures fabrication and characterization for implementation in optoelectronic devices

ParisTech School: ESPCI Paris | PSL

Advisor(s) Name: Lionel Aigouy / Zhuoying Chen
Advisor(s) Email: *lionel.aigouy@espci.fr / zhuoying.chen@espci.fr*
Research group/Lab: MNC Group / LPEM
Lab location: ESPCI
(Lab/Advisor website): https://www.lpem.espci.fr

Short description of possible research topics for a PhD:

Optoelectronic devices such as solar cells, photodetectors constantly need to be improved and optimized in terms of sensitivity and detection range. For that, conventional, 'flat', devices are often associated to nanostructures whose presence change the local optical, electronic, or thermal properties of the devices and lead to better performances. Nano-antenna, meta-surfaces, plasmonic or dielectric nanostructures can be used but the visualization of their effect at the sub-micron scale is necessary for a fundamental comprehension and final device optimization. As seen in the figure, the near-field around two adjacent plasmonic nanodisks exhibit a strong increase in their gap which can lead to better absorption and a local temperature increase. The goal of this thesis is to design and study plasmonic and dielectric nanostructures with particular local properties able to modify and improve the characteristics of a real device like a solar cell, a photodetector, or a photothermo-electric detector. The local optical and thermal properties will be correlated to the device tested in operation, so that a direct optimization will be made.



Required background of the student: master degree in Chemistry, Physics, Materials Science.

A list of 5 (max.) representative publications of the group:

- 'Mapping plasmon-enhanced upconversion fluorescence of Er/Yb-doped nanocrystals near gold nanodisks.', L. Aigouy, M.-U. González, H.-J. Lin, M. Schoenauer-Sebag, L. Billot, P. Gredin, M. Mortier, Z. Chen and A. García-Martín. Nanoscale 11, 10365-10371 (2019)
- 'TiO2 nanocolumn arrays for more efficient and stable perovskite solar cells.', Z. Hu, J.-M. García-Martín, Y. Li, L. Billot, B. Sun, F. Fresno, A. García-Martín, M.-U. González, L. Aigouy, Z. Chen. ACS Applied Materials & Interfaces 12(5), 5979-5989 (2020).
- 'Exploring the Magnetic and Electric Side of Light through Plasmonic Nanocavities.', C. Ernandes, H.-J. Lin, M. Mortier, P. Gredin, M. Mivelle, and L. Aigouy. Nano Letters 18 (8), 5098-5103 (2018)

ParisTech ESPCI PARIS PSL

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Physics
Subfield: Hydrodynamics
Title: Micro-helices in flows
ParisTech School: ESPCI Paris | PSL
Advisor(s) Name: Anke Lindner and Olivia du Roure
Advisor(s) Email: anke.lindner@espci.fr, Olivia.duroure@espci.fr
Research group/Lab: Complex Suspensions/PMMH
Lab location: Campus Jussieu, 75005 PARIS
(Lab/Advisor website): https://blog.espci.fr/alindner/ or oliviaduroure/

Short description of possible research topics for a PhD:

The study of fluid structure interactions between helix-shaped particles and viscous flows is of importance for both fundamental science and technological applications. The chirality of such particles induces breaking of the time reversal symmetry associated with viscous flows; an effect exploited by microorganisms, such as E. coli bacteria, which propel themselves through viscous media by rotating helically shaped flagella. Particle chirality has also been shown to induce a lateral drift in shear flows, responsible for example for bacterial rheotaxis. Possible applications include swimming micro-robots for targeted drug delivery or flow micro-sensors. We have recently developed several experimental model systems to investigate the interaction between helical micro-particles and viscous flows (see figure). These micro-objects are put under flow in specifically designed microchannels and followed during their transport.

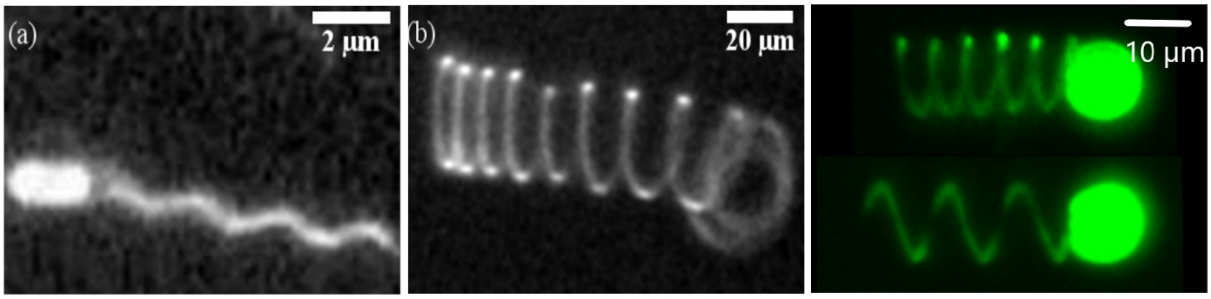


Figure 1a) Fluorescent imaging of E-coli bacteria, (copyright H. C. Berg). (b) Flexible helix observed under fluorescent microscopy, clamped on its right. (c) Microprinted helix with a head.

In this PhD we suggest tackling some of the many questions still open in this field, using one of our model systems. These questions include determining the magnitude of the chirality induced drift as a function of helix shape, using microprinted helices or flagella of different micro-organisms. Another possibility is to study the role of flexibility using the nano-ribbon helices on their transport in chosen microflows.

Required background of the student: Physics, if possible, Hydrodynamics, Complex fluids or Soft Matter. Taste for performing experiments is necessary and skills in microfabrication or microfluidics would be a plus.

A list of 5 (max.) representative publications of the group:

Chakrabarti, et al. Nature Physics 16 (6), 689-694
du Roure, et al Annual Review of Fluid Mechanics. 51:539
Pham, J. et al. Physical Review E, 92, 011004(R)
Liu et al. PNAS 115 (38) 9438-9443.
Cappello et al. Physical Review Fluids 4, 034202

Research Topic for the ParisTech/CSC PhD Program

Subfield: Polymer materials and chemistry, Mechanics, Material science
ParisTech School: ESPCI Paris-PSL
Title: Cutting soft materials
Advisors: Matteo Ciccotti (matteo.ciccotti@espci.fr), Frederic Lechenault (frederic.lechanault@phys.ens.fr)
Website: http://www.simm.espci.fr/

Short description of possible research topics for a PhD:

Cutting is a ubiquitous process with wide ranging implications, culturally and technologically. Experimenting on the kitchen table, we quickly learn that the easiest way to cut soft solids with a knife is by a slicing action, i.e., dragging the sharp blade over the soft surface without pushing too strongly into it; indeed, pushing the edge of a knife too strongly into a soft solid only squashes it. Moreover, applying a compression in a plane orthogonal to the direction of cutting can be of great help for guiding the cut. However, more generally the forces applied for both cutting and holding the object are responsible for uncomfortable large strains, which induce strong perturbations in the final shape of the parts. Beyond these everyday examples, the cutting of soft materials is of great interest in industrial food processing, in tissue analysis in the context of histology, etc..

The initial developments of cutting science and technology were mostly devoted to metal machining and focused on plastic deformations induced by the motion of the blades though the material. The importance of fracture toughness in cutting was only acknowledged in the 60's after the development of linear elastic fracture mechanics, leading to important advances in the understanding of cutting mechanics of more brittle materials. However, a unifying physical view of cutting that may be suitable for a larger class of materials is still lacking, especially for soft materials. The standard tools of linear elastic fracture mechanics are not suited to treat a problem where the driving arises directly at the crack lips instead of remotely. The local crack fields are strongly coupled with the shape and motion of the blade, involving subtle adhesion and friction problems. In this context the fracture energy and direction of propagation are not independent of shape of the blade and new tools have to be developed to describe them. Although the case of soft materials is of particular importance for many industrial applications, very few tools are available to deal with the very strong nonlinear deformations at different scales, which make it difficult to cut parts of the desired shape and with good surface finish.

This project aims at performing cutting experiments on model soft materials in controlled situations, in order to bridge this gap, while profiting of the significant advances that have recently been made on fracture and adhesion of soft dissipative materials. On the one hand, we aim at clarifying the relevant notions of cutting energy and directionality of the cut as a function the shape and motion of the blade. On the other hand, we intend to develop tools for predicting the final shape of the cut parts in order to allow forward design.

Required background of the student: polymer materials, mechanics, soft matter physics

A list of 5 representative publications of the group:

1. Creton C., Ciccotti M. *Rep Prog Phys* **2016,** 79, (4), 046601.
2. Chopin J., Villey R., Yarusso D., Barthel E., Creton C., Ciccotti M. Macromolecules 51 (21), 8605-8610
3. Ciccotti M. Journal of physics D: Applied physics 42 (21), 214006.
4. Lechenault F., Dauchot O., Biroli G., Bouchaud JP. EPL 83 (4), 46003.
5. Lechenault F., Thiria B., Adda-Bedia M. Physical Review Letters 112 (24), 244301

Research Topic for the ParisTech/CSC PhD Program

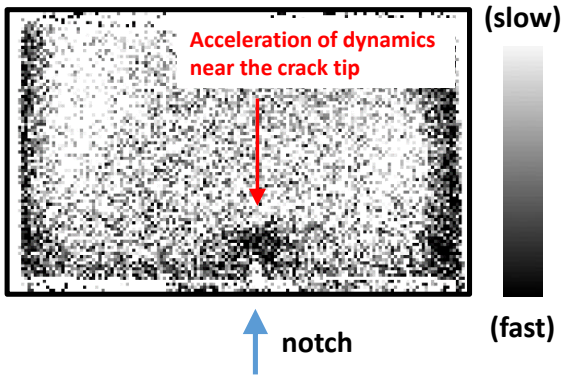
Subfield: Polymer materials and chemistry, Mechanics, Material science
ParisTech School: ESPCI Paris-PSL
Title: Bridging Chemistry, Physics and Mechanics: Understanding how needles and blades damage chemical bonds in soft materials
Advisors: Tetsuharu Narita (tetsuharu.narita@espci.fr, Costantino Creton (costantino.creton@espci.fr), Matteo Ciccotti (matteo.ciccotti@espci.fr)
Website: http://www.simm.espci.fr/

Short description of possible research topics for a PhD:
Hydrogels, networks of crosslinked polymers swollen in water, are soft squishy solids abundant in nature and everyday life and in food and biomedical industries. Although hydrogels are generally brittle, some tough hydrogels that are resistant to fracture have been developed. Especially for medical applications, biological tissues or artificial implants need to be incised, sutured and punctured by sharp blades or needles. While very common, this kind of mechanical damage combining very large deformations and chemical bond scission of the polymer is poorly understood and very multiscale. (1) molecules break at the nanometric scale, (2) local damage occurs at the microscopic scale, and (3) stress strain relation are at the macroscopic scale.

Recently our laboratory developed a low-force indentation by sharp needles, and a non-invasive optical technique MSDWS (multi-speckle diffusing-wave spectroscopy), to map the local dynamics change felt by probe nanoparticles in the network, related to the damage at the microscopic scale.

The objective of this thesis is to combine mechanical (see left figure) and dynamic light scattering optics (right figure), to map the local damage (to know when and where chain breaking occurs) of the gel as it is indented or cut with a sharp object like a needle, blade or sharp edged cylinder and ultimately design better puncture and cutting resistant gels.

The overall thesis project involves preparing well defined model soft hydrogels, developing an original setup combining the two techniques, and characterizing the fracture properties of the model systems.



Required background of the student: polymer materials, mechanics, soft matter physics

A list of 5 representative publications of the group:

1. Mayumi, K.; Guo, J.; Narita, T.; Hui, C. Y.; Creton, C. *Extreme Mechanics Letters* **2016,** 6, 52-59.
2. Mayumi, K.; Marcellan, A.; Ducouret, G.; Creton, C.; Narita, T. *ACS Macro Letters* **2013,** 2, (12), 1065-1068.
3. Rose, S.; Dizeux, A.; Narita, T.; Hourdet, D.; Marcellan, A. *Macromolecules* **2013,** 46, (10), 4095-4104.
4. Creton, C.; Ciccotti, M. *Rep Prog Phys* **2016,** 79, (4), 046601.
5. Ducrot, E., Chen, Y., Bulters, M., Sijbesma, R.P., Creton, C. Science 2014, 344(6180), 186.

ParisTech

INSTITUT d'OPTIQUE GRADUATE SCHOOL ParisTech | université PARIS-SACLAY

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Physics, Optics

Subfield: Applied Physics

Title: Highly sensitive sensors for detection of pollutants based on optical nanofibers

ParisTech School: Institut d'Optique Graduate School

Advisor(s) Name: Lebrun
Advisor(s) Email:sylvie.lebrun@institutoptique.fr
Research group/Lab: Laboratoire Charles Fabry
Lab location: Palaiseau
(Lab/Advisor website): https://www.lcf.institutoptique.fr/

Short description of possible research topics for a PhD: Our research group is working since more than 10 years on non linear effects in optical nanofibers. We have developed a pulling machine with performances at the state of the art that enabled us to realize several first ever experimental demonstrations. As shown on the fig., the nanofiber is linked to the two unstretched parts of a standard fiber through two tapers. At these small diameters the optical mode shows a high evanescent field around the nanofiber which is very sensitive to the external environment. In this thesis we propose to study a new type of sensor using Raman scattering in the evanescent field of nanofibers immersed in liquids or gas to detect pollutants. This sensor will be highly compact, low cost and sensitive compared to other techniques.

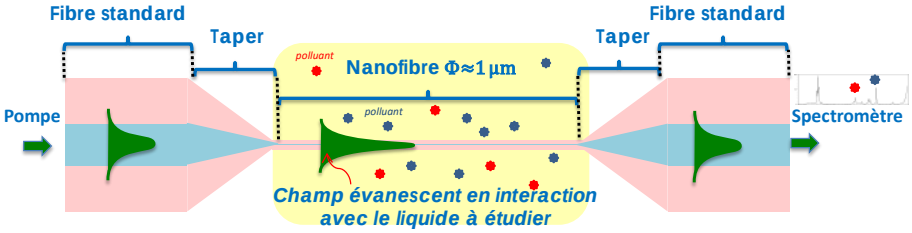


Figure 1. Scheme of the pollutant sensor based on a silica nanofiber.

Required background of the student: Master in physics with a pronounced interest in optics and experimental work. Knowledge in non linear optics and/or guided optics and/or sensors are welcome.

A list of 5 (max.) representative publications of the group:

1. L. Shan, G. Pauliat, G. Vienne, L. Tong, and S. Lebrun, Appl. Phys. Letters, 102, (2013).
2. M. Bouhadida, J. C. Beugnot, P. Delaye, K. Phan Huy and S. Lebrun, Appl. Phys. B 125,228 (2019).
3. J.-C. Beugnot, S. Lebrun, G. Pauliat, H. Maillotte, V. Laude, and T. Sylvestre. Nature Communications, 5:5242, October 2014.

ParisTech

INSTITUT d'OPTIQUE GRADUATE SCHOOL ParisTech | université PARIS-SACLAY

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

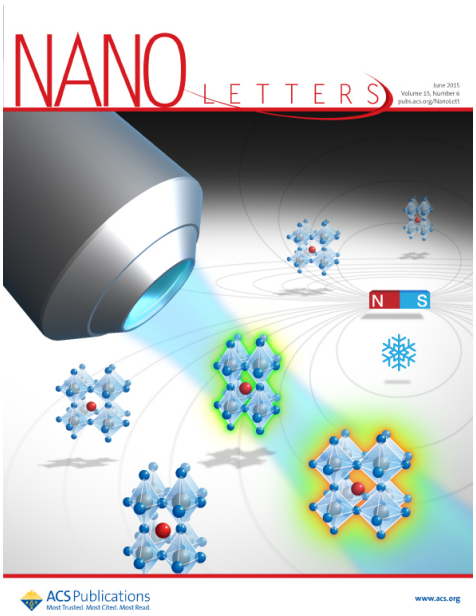
Field: Physics, Optics ***Subfield***: Nanophotonics

Title: **Exploring the optical properties of perovskite single nanocrystals and superlattices**

ParisTech School: Institut d'Optique Graduate School
Advisor(s) Name: Brahim LOUNIS, Philippe TAMARAT
Advisor(s) Email: brahim.lounis@u-bordeaux.fr; philippe.tamarat@u-bordeaux.fr
Research group/Lab: LP2N, UMR5298/Nanophotonics group
Lab location: Bordeaux
(Lab/Advisor website): https://sites.google.com/site/bordeauxnanophotonicsgroup/home

Short description of possible research topics for a PhD:

Lead halide perovskites exhibit outstanding optical and electronic properties for a wide range of applications in optoelectronics and for light-emitting devices. Yet, the physics of the band-edge exciton, whose recombination is at the origin of the photoluminescence, is the subject of ongoing debate. In particular, the long-lived ground exciton of lead halide perovskite nanocrystals plays a major role in the quantum properties of the emitted light, since it promotes the formation of biexcitons and thus the emission of correlated photon pairs. Future investigations will aim at reducing the dephasing rate and spectral diffusion in these materials and improve the indistinguishability character of the emitted photons. With a view to the realization of ideal sources of entangled photons, we will aim at achieving degenerate bright triplet emission. We will also study the quantum optical properties of the photoluminescence stemming from lead halide NCs that are self-organized into highly ordered three-dimensional superlattices. We will investigate the spectroscopic and temporal signatures of collective coupling of the nanocrystals, which should give rise to the many-body quantum phenomenon of superfluorescence. Such entangled multi-photon quantum light sources should fuel the development of next-generation devices for quantum technologies.



These activities will be led in close collaboration with the group of chemists of M. Kovalenko (ETH Zürich).

Required background of the student: quantum physics, optics, solid-state physics, lab training.

A list of representative publications of the group:

1. « The ground exciton state of formamidinium lead bromide perovskite nanocrystals is a singlet dark state », P. Tamarat et al. Nature Materials, 18 (2019) 717.
2. « Neutral and charged exciton fine structure in single lead halide perovskite nanocrystals revealed by magneto-optical spectroscopy », M. Fu et al., Nanoletters, 17 (2017) 2895.
3. "Unravelling exciton-phonon coupling in individual $FAPbI_3$ nanocrystals emitting near-infrared single photons", M. Fu et al., Nature Communications, 9, 3318 (2018).
4. « Spectroscopy of Single Nanocrystals», M.J. Fernée, P. Tamarat, B. Lounis, Chem. Soc. Rev. 43 (2014) 1311.

ParisTech

INSTITUT d'OPTIQUE GRADUATE SCHOOL ParisTech | université PARIS-SACLAY

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

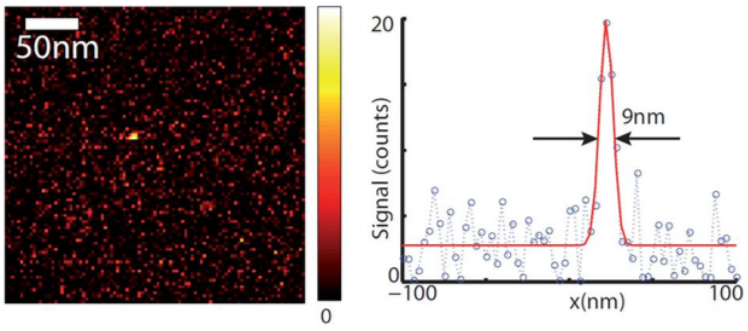
Field: Physics, Optics ***Subfield***: Quantum Optics

Title: **Coherent dipole-dipole coupling of organic molecules at cryogenic temperatures**

ParisTech School: Institut d'Optique Graduate School
Advisor(s) Name: Brahim LOUNIS, Jean-Baptiste Trebbia
Advisor(s) Email: brahim.lounis@u-bordeaux.fr
Research group/Lab: LP2N, UMR5298/Nanophotonics group
Lab location: Bordeaux
(Lab/Advisor website): https://sites.google.com/site/bordeauxnanophotonicsgroup/home

Short description of possible research topics for a PhD:

The controlled, coherent manipulation of quantum systems is an important challenge in modern science, with significant applications in quantum technologies. Solid-state quantum emitters such as single molecules, quantum dots and defect centers in diamond are promising candidates for the realization of quantum bits and quantum networks. Collective quantum dynamics resulting from coherent dipole–dipole coupling is challenging, since they require nanometric distances between emitters, the degeneracy of their optical resonances and low temperatures. We will aim at developing experimental schemes to find coupled quantum emitters and manipulate their degree of entanglement with external fields. The optical super-resolution nanoscopy technique built in the group (with sub 10-nm far-field optical resolution at cryogenic temperatures) will be used to reveal the rich space-frequency signatures of coherent coupled quantum emitters. The formation of collective quantum states from coupled optical emitters being a general phenomenon, these experimental schemes can also be useful for the study of many other systems including light harvesting complexes polymer conjugates, quantum dots molecules and hybrid systems.



Required background of the student: quantum physics, optics, light-matter interaction, lab training. The thesis will be mainly experimental. The candidate will also develop theoretical simulations and acquire a strong background in laser spectroscopy, single photon detection, quantum optics...

A list of representative publications of the group:

1- A solid state source of photon triplets based on quantum dot molecules, M. Khoshnegar *et al.*, Nature Communications 8 (2017) 15716.
2- Optical Manipulation of Single Flux Quanta, I. S. Veshchunov *et al.*, , Nature Communications 7 (2016) 12801.
3- Optical Nanoscopy with Excited State Saturation at Liquid Helium Temperatures B. Yang, *et al.*, Nature Photonics, 9 (2015) 658-662.
4- Indistinguishable near-infrared single photons from an individual organic molecule J.-B. Trebbia *et al.*, Phys. Rev. A. 82 (2010) 063803.
5- 3D optical nanoscopy with excited state saturation at liquid helium temperatures, J.-B. Trebbia, R. Baby, P. Tamarat, and B. Lounis, Optics Express, 27 (2019) 23486

ParisTech

INSTITUT d'OPTIQUE GRADUATE SCHOOL ParisTech | université PARIS-SACLAY

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

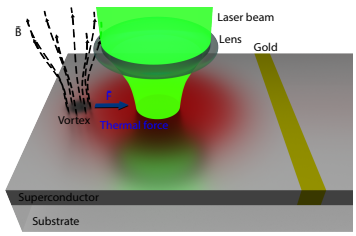
Field: Physics, Optics ***Subfield***: Superconductivity and magnetism, Josephson transport

Title: **Fast Josephson-junction control by optical manipulation of a flux quantum**

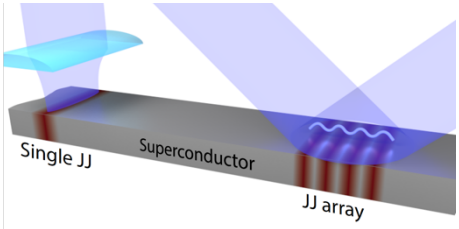
ParisTech School: Institut d'Optique Graduate School
Advisor(s) Name: Brahim LOUNIS, Philippe Tamarat
Advisor(s) Email: brahim.lounis@u-bordeaux.fr
Research group/Lab: LP2N, UMR5298/Nanophotonics group
Lab location: Bordeaux
(Lab/Advisor website): https://sites.google.com/site/bordeauxnanophotonicsgroup/home

Short description of possible research topics for a PhD:

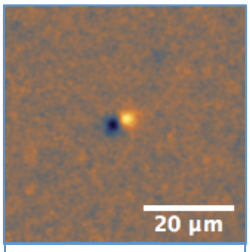
The miniaturization of semiconductor-based electronic components could reach its limits within a decade. Superconducting electronics, based on quantum flux superconducting logic circuits (Josephson junctions), is a promising alternative offering both high operating rates and low switching energies. Full optical control of Josephson junctions would enable low-power, wideband communication between logic circuits at cryogenic temperatures and room-temperature mass memories. In this context, the thesis objective is the fundamental exploration of the interplay between optics, magnetism and superconductivity, an emerging research field. Innovative optical methods of individual Abrikosov vortex manipulation recently developed in our group offer promising perspectives such as fast optical Josephson junction control by moving a quantum of flux near a junction by photo-thermal effect.



Control of a Josephson junction with a single vortex.



Sculpting a normal region in a superconductor with light.



Generation of a vortex-antivortex pair with a laser pulse.

We will also aim at creating the Josephson junction itself by photo-thermal effect, by illuminating the section of a superconducting ribbon. The Josephson electrical transport signatures will be studied according to the geometry and power of the laser beam used to locally weaken the superconductivity. Finally, in the perspective of an all-optical control of superconducting electronic devices, part of the thesis will be dedicated to the creation of flux quanta with a laser pulse, using the inverse Faraday effect.

Required background of the student: quantum physics, optics, light matter interaction, superconductivity and magnetism.

A list of representative publications of the group:

« Optical Manipulation of Single Flux Quanta», I. S. Veschunov et al. Nature Communications 7 (2016) 12801.
Patent "Control of the displacement of an individual Abrikosov vortex », A. Bouzdine, B. Lounis, P. Tamarat.
"Anomalous Josephson effect controlled by an Abrikosov vortex", S. Mironov et al., PRB 96, 214515 (2017).
"On-Demand Optical Generation of Single Flux Quanta" A. Rochet et al. Nano Letters 20 (2020) 6488.

ParisTech

INSTITUT d'OPTIQUE GRADUATE SCHOOL ParisTech | université PARIS-SACLAY

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

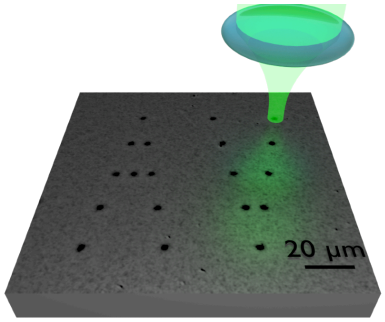
Field: Physics, Optics ***Subfield***: Quantum physics, molecular physics, condensed matter

Title: **Towards single spin control with an optically driven Abrikosov vortex**

ParisTech School: Institut d'Optique Graduate School
Advisor(s) Name: Brahim LOUNIS, Philippe Tamarat
Advisor(s) Email: brahim.lounis@u-bordeaux.fr
Research group/Lab: LP2N, UMR5298/Nanophotonics group
Lab location: Bordeaux
(Lab/Advisor website): https://sites.google.com/site/bordeauxnanophotonicsgroup/home

Short description of possible research topics for a PhD:

Abrikosov vortices are the most compact magnetic objects, with a size of a few tens to a few hundred nanometers. These flux tubes, which penetrate type II superconductors (such as Niobium), carry a quantum of flux h/2e and are surrounded by super-currents. Recently, our group demonstrated the ability to manipulate single flux quanta with a laser beam, as simply as with optical tweezers.



The main goal of the doctoral project is to explore the magnetic interaction between an optically manipulated individual Abrikosov vortex and a single spin present in a quantum nano-emitter such as the nitrogen-vacancy color center in diamond. The entanglement between the vortex mesoscopic system and the spin will be studied. The 3D optical nanoscopy methods developed in our group will be applied to precisely map the distribution of magnetic field (or electric field) around a vortex. Finally, we will investigate the ability to manipulate the spin state with the magnetic field carried by the vortex.

Required background of the student: quantum physics, optics, light matter interaction, superconductivity and magnetism. The thesis will be mainly experimental. The candidate will also develop the theoretical simulations and acquire a strong background in laser spectroscopy, single photon detection, quantum optics...

A list of representative publications of the group:

1- Ivan S. Veshchunov et al., Optical Manipulation of Single Flux Quanta, Nature communications 7 (2016) 12801.
2- Bin Yang, et al., Optical Nanoscopy with Excited State Saturation at Liquid Helium Temperatures, Nature Photonics, 9 (2015) 658-662.
3- « Anomalous Josephson effect controlled by an Abrikosov vortex », S. Mironov et al. PRB 96, 214515 (2017).
4- "Optical nanoscopy with excited state saturation at liquid helium temperatures", Yang et al. Nature Photonics 9 (2015) 658.
5- "On-Demand Optical Generation of Single Flux Quanta" A. Rochet et al. Nano Letters 20 (2020) 6488.

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RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: *Materials Science, Mechanics, Fluids*

Subfield: Bio-based polymers, Biomaterials, Aerogels, Fluid mechanics

Title: 3D printing of gels and aerogels for biomedical applications

ParisTech School: MINES ParisTech | PSL

Advisor(s) Name: Tatiana BUDTOVA, Co-advisors: Sijtze BUWALDA and Rudy VALETTE

Advisor(s) Email: *Tatiana.Budtova@mines-paristech.fr*

Research group/Lab: *Center for Materials Forming (CEMEF), Biobased Polymers and Composites group (BIO) and Computing and Fluids group (CFL)*

Lab location: *Sophia Antipolis*

(Lab/Advisor website): https://www.cemef.mines-paristech.fr/en/homepage/

Short description of possible research topics for a PhD:

Additive manufacturing is a very promising technology for biomedical applications such as regenerative medicine, tissue engineering and drug delivery. In this project 3D printing will be used to make bio-based gels in complex shapes, which will then be transformed into bio-aerogels. The goal is to use bio-aerogels as matrices for drug delivery in smart patches. Bio-aerogels are 100% bio-based ultra-lightweight nanostructured materials with a high internal surface area.
Two approaches for printing gels from polysaccharide solutions will be considered: either printing in a fluid in which the polymer is cross-linked, or printing in a non-solvent which induces phase separation. The rheology of solutions in the capillary of the printer nozzle and near its exit will be studied experimentally and modelled using finite element analysis approaches developed in CEMEF. Special attention will be paid to solution liquid-"solid" (gel) transitions. Bio-aerogels will be characterized, loaded with drugs and their release kinetics studied.

Required background of the student: polymer chemical physics; materials science

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. F. Chen, W. Xiang, D. Sawada, L. Bai, M. Hummel, H. Sixta, T. Budtova «Exploring Large Ductility in Cellulose Nanopaper Combining High Toughness and Strength », *ACS Nano*, 14, 11150 (2020)
2. S. Buwalda, T. Vermonden, W. Hennink, «Hydrogels for therapeutic delivery: current developments and future directions», *Biomacromolecules*, 18, 316 (2017)
3. L. Druel, P. Niemeyer, B. Milow, T. Budtova, "Rheology of cellulose-[DBNH][CO2Et] solutions and shaping into aerogel beads", *Green Chem*., 20, 3993 (2018)
4. S. Zhao, W. J. Malfait, A. Demilecamps, Y. Zhang, S.L Brunner, L. Huber, P. Tingaut, A. Rigacci, T. Budtova, M. M. Koebel "Strong, Thermally Superinsulating, Biopolymer-Silica Aerogel Hybrids by Cogelation of Silicic Acid with Pectin", *Angew. Chemie Intl. Edition*, 54, 14282 (2015)
5. A. Pereira, R. Valette, E. Hachem, « Inertia-dominated coiling instabilities of power-law fluids", *J. Non-Newt. Fluid Mech*., 282, 104321 (2020)

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Energy, Processes

Subfield: Electrical engineering, applied mathematics, smart grid

Title: Big data based forecasts for the electric power system

ParisTech School: MINES ParisTech | PSL

Advisor(s) Name: Andrea Michiorri,
Advisor(s) Email: andrea.michiorri@mines-paristech.fr
Research group/Lab: *PERSEE*
Lab location: *Sophia Antipolis*
(Lab/Advisor website): http://www.mines-paristech.eu/Research-valorization/Fields-of-Research/Energy-and-processes/PERSEE-Centre-for-processes-renewable-energies-and-energy-systems/

Short description of possible research topics for a PhD:
Context: This research is based on the following considerations: 1) Energy forecasts are used for decision making by system's actors. 2) They are partially correlated, and this can be used to improve their precision. 3) Data sources increase in terms of size, variety and quality.
Objectives: The objectives of this research are: A) to develop forecast models for the state of the electric power system (production, consumption, prices) with attention to extreme and rare events. B) To integrate alternative data sources such as climate models or natural language processing.
Methodology: The research will be organized according to the following plan: i) preparation (bibliographic research, learning tools and datasets, with attention to open data). ii) A second phase regarding the development of the forecast models (point A). iii) A third phase for the evaluation of the models.

Required background of the student: Applied mathematics, informatics, machine learning

A list of 5 (max.) representative publications of the group:
1. Andrea Michiorri, Huu-Minh Nguyen, et al., "Forecasting for dynamic line rating", Renewable and Sustainable Energy Reviews, 2015/12/31, Vol 52, pp 1713-1730
2. Andrea Michiorri, Philip C Taylor, "Forecasting real-time ratings for electricity distribution networks using weather forecast data", Electricity Distribution-Part 1, 2009. CIRED 2009. 20th International Conference and Exhibition on
3. Arthur Bossavy, Robin Girard, Andrea Michiorri, Georges Kariniotakis, "The impact of available data history on the performance of photovoltaic generation forecasting models", Electricity Distribution (CIRED 2013), 22nd International Conference and Exhibition on
4. Romain Dupin, Andrea Michiorri, Georges Kariniotakis, "Dynamic Line Rating Forecasting and Evaluation", EWEA Technology Workshop, Wind Power Forecasting 2015

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM

Field: Energy, Processes

Subfield: Electrical engineering, applied mathematics, smart grid

Title: Dynamic Line Rating: risk and impact on investment planning

ParisTech School: MINES ParisTech | PSL

Advisor(s) Name: Andrea Michiorri,
Advisor(s) Email: andrea.michiorri@mines-paristech.fr
Research group/Lab: *PERSEE*
Lab location: *Sophia Antipolis*
(Lab/Advisor website): http://www.mines-paristech.eu/Research-valorization/Fields-of-Research/Energy-and-processes/PERSEE-Centre-for-processes-renewable-energies-and-energy-systems/

Short description of possible research topics for a PhD:
Context: Dynamic line rating (DLR) is a technology able to modify in real time the current carrying capacity of power system components such as overhead lines, power transformers and electric cables. It has the potential to reduce network charges, but several challenges needs to be addressed before its implementation.
Objectives: This thesis is focused on two points: 1) to develop a methodology to safely determine DLR to be applied. 2) To study the impact of the application of DLR on investment planning, both for the network (network reinforcements) and for network users (reduced connection cost).
Methodology: The focus will be kept on overhead lines, but transformers and electric cables can be investigated as well. For point 1) several approaches will be considered and/or combined: a) the use of historical data, weather reanalysis and climate projections to create a DLR climatology, b) the use of daily probabilistic forecasts, c) a risk-based approach. For point 2) simulations will be carried out on well-defined use cases comparing the benefits and drawbacks of the application of DLR. Examples are: a) retarding network reinforcements following load or renewable production increase, b) reducing renewable's connection cost.;

Required background of the student: Electrical engineering (power systems)

A list of 5 (max.) representative publications of the group:
1. Andrea Michiorri, Huu-Minh Nguyen, et al., "Forecasting for dynamic line rating", Renewable and Sustainable Energy Reviews, 2015/12/31, Vol 52, pp 1713-1730
2. Andrea Michiorri, Philip C Taylor, "Forecasting real-time ratings for electricity distribution networks using weather forecast data", Electricity Distribution-Part 1, 2009. CIRED 2009. 20th International Conference and Exhibition on
3. Romain Dupin, Andrea Michiorri, Georges Kariniotakis, "Dynamic Line Rating Forecasting and Evaluation", EWEA Technology Workshop, Wind Power Forecasting 2015

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RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Information and Communication Sciences and Technologies

Subfield: Computer Science

Title: Scaling Up Polarized Deduction Modulo Theory

ParisTech School: MINES ParisTech | PSL

Advisor(s) Name: Olivier Hermant
Advisor(s) Email: olivier.hermant@mines-paristech.fr
Research group/Lab: Centre de recherche en informatique
Lab location: Fontainebleau, France
(Lab/Advisor website): http://www.cri.mines-paristech.fr

Short description of possible research topics for a PhD:
Formal methods aims at ensuring *provably bug-free* software. An industrial benchmark of ten of thousands of problems has given us the opportunity to jointly develop automated theorem provers and proof checkers.
The research subject aims at extending those tools and their logical foundations in the direction of polarized rewriting, where conditional computation steps are embedded into reasoning step, a feature that gave excellent preliminary results on the benchmark. Our tools are also critically dependent on the strategy adopted. As this strategy is dependent on the shape of the problem, another part of the research subject is to learn automatically how to trigger the best heuristics.

Required background of the student: an M.Sc.-level specialization in any field of computer science or in the foundations of mathematics. More specialized courses, among which machine learning, compilers, logics, theoretical computer science, or functional programming are a plus.

Representative publications of the group:
1. G. Burel, G. Bury, R. Cauderlier, D. Delahaye, P. Halmagrand, and O. Hermant. *Automated deduction: When deduction modulo theory meets the practice.* Journal of Automated Reasoning 64(6), pp. 1001–1060, 2020.
2. M. Boespflug, Q. Carbonneaux, and O. Hermant. *The λΠ-calculus modulo as a universal proof language*. In Second Workshop on Proof Exchange for Theorem Proving (PxTP), volume 878, pp. 28–43, CEUR-WS.org, 2012.
3. G. Dowek. *Polarized deduction modulo*. In IFIP Theoretical Computer Science, 2010.
4. The BWare Project, 2012. http://bware.lri.fr/

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Materials Science, Mechanics, Fluids

Subfield: (Mechanics of materials, physical metallurgy)

Title: A Self consistent crystal plasticity model coupled to a mean field model for microstructural evolution predictions

ParisTech School: MINES ParisTech | PSL

Advisor(s) Name: François Bay, Daniel Pino Muñoz, Charbel Moussa
Advisor(s) Email: *francois.bay@mines-paristech.fr, daniel.pino_munoz@mines-paristech.fr, charbel.moussa@mines-paristech.fr*
Research group/Lab: *Centre de mise En Forme des matériaux (CEMEF)*
Lab location: *06904 Sophia Antipolis, France*
(Lab/Advisor website): *www.cemef.mines-paristech.fr*

Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)

Controlling the microstructures of metallic alloys can lead to an improvement of in use properties. Therefore, prediction of the microstructure evolution during thermomechanical treatments is of utmost importance in many industrial applications. Physical mechanisms responsible for microstructural evolution take place at different scales. At the structural parts scale, it is not possible model explicitly all those mechanisms. For this reason, simplified models based on an implicit description of the microstructure, so-called mean-field models, can be used. Because of the complexity and the heterogeneity of the thermomechanical conditions, mean-field models predictions need to be built on strong physical basis. In this project we aim at implementing mechanical homogenization techniques, based on self-consistent approaches, in order to accurately describe the mechanical response of a polycrystal. This accurate mechanical response will then be used to propose reliable mean-fields models of the evolution of the microstructure. The developed technique will be applied to thermo-mechanical loading paths induced by electromagnetic forming processes.

Required background of the student: (What should be the main field of study of the applicant before applying?)
Mechanics of materials, Material Science, Numerical methods

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Maire L., Fausty J., Bernacki M., Bozzolo N., De Micheli P., Moussa C., "A new topological approach for the mean field modeling of dynamic recrystallization", Materials and Design, 146 (2018) p.194-207
2. Maire L., Scholtes B., Moussa C., Bozzolo N., Pino Muñoz D., Settefrati A., Bernacki M., "Modeling of dynamic and post-dynamic recrystallization by coupling a full field approach to phenomenological laws", Materials and Design, 133 (2017) p.498-519
3. Ruiz Sarraloza D.A., Maire L., Moussa C., Bozzolo N., Pino Muñoz D., Bernacki M., "Full field modeling of Dynamic Recrystallization in a CPFEM context - Application to 304L steel", Computational Materials Science, 184 (2020) p.109892
4. Ruiz Sarraloza D.A., Pino Muñoz D., Bernacki M., "A new numerical framework for the full field modeling of dynamic recrystallization in a CPFEM context", Computational Materials Science, 179 (2020) p.109645
5. Alves Zapata J., Bay F., “Modeling and Analysis of Electromagnetism in Magnetic Forming Processes”,IEEE Transactions on Magnetics, Volume: 52, Issue: 5 , (2016)

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Logo de votre école (ne garder que le bon logo)

RESEARCH TOPIC FOR THE PARISTECH/CSC PHD PROGRAM
(one page maximum)

Field: Economics, Management and Social Sciences

Subfield: Logistics and Supply Chain and Management

Title: Performance of interconnected logistics networks under uncertainty

ParisTech School: MINES ParisTech | PSL

Advisor(s) Name: Eric BALLOT, Shenle PAN
Advisor(s) Email: eric.ballot@mines-paristech.fr; shenle.pan@mines-paristech.fr
Research group/Lab: Centre de gestion Scientitique
Lab location: 60, boulevard Saint-Michel, 75006 Paris, France
(Lab/Advisor website): www.cgs.mines-paristech.fr

Short description of possible research topics for a PhD: (10-15 lines in English + optional figure)

Due to economic globalization, today's supply chain and logistics networks are more complex and stringent than ever before, and facing many uncertainties like market volatility, global transportation service and lead-time, or global or local disruptions like the COVID pandemic. How to effectively and efficiently manage supply chains and the operations under such uncertainties remains a major challenge in the field of supply chain management (SCM). Physical Internet, aiming at the interconnection of independent logistics or supply networks via physical and informational interoperability, is a recent breakthrough logistics paradigm, and that seems promising. Its potential on improving logistics efficiency and sustainability has been demonstrated by former research works. However, the question of how it could alleviate the uncertainties by enhancing the agility and resilience is not yet studied in the literature. The thesis will focus on the later question, and apply modelling approaches (especially, robust optimization, coupling optimization-simulation) for quantitative and qualitative research. The PhD candidate will join the team and the Physical Internet Chair, in order to work closely with researchers and industrial partners.

Required background of the student: (What should be the main field of study of the applicant before applying?)

The applicant should have master degree in logistics or supply chain management. Solid knowledge on mathematic modelling is also required, for example, Operational Research, multi-agent or discrete event simulation.

A list of 5 (max.) representative publications of the group: (Related to the research topic)

1. Pan S, Trentesaux D, Ballot E. and Huang G. (2019). "Horizontal collaborative transport: survey of solutions and practical implementation issues". International Journal of Production Research, 57 (15-16). 10.1080/00207543.2019.1574040.
2. Lafkihi M., Pan, S. & Ballot, E. (2019). "Freight Transportation Service Procurement: A literature review and future research opportunities in Omnichannel E-commerce". Transportation Research Part E, 125, 348-365 doi.org/10.1016/j.tre.2019.03.021
3. Yang Y, Pan S, and Ballot E (2016). "Mitigating supply chain disruptions through interconnected logistics services in the Physical Internet". International Journal of Production Research, 55(14): 3970-3983.
4. Sarraj R, Ballot E, Pan S, Montreuil B. and Hakimi D. (2014). "Interconnected logistic networks and protocols: simulation-based efficiency assessment." International Journal of Production Research. 52(11): 3185-3208
5. Pan S, Ballot E. and Fontane F. (2013). "The reduction of greenhouse gas emissions from freight transport by merging supply chains." International Journal of Production Economics. 143(1): p. 86-94