

## PROGRAMME INTITUTS ET INITIATIVES Appel à projet – campagne 2021 Proposition de projet de recherche doctoral (PRD) ISim - Initiative Sces et ingénierie moléculaires

# Intitulé du projet de recherche doctoral (PRD): Molecular tweezers for multifunctional switchable organogels

Directeur.rice de thèse porteur.euse du projet (titulaire d'une HDR) :

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École Doct doctorale	École Doctorale de rattachement de l'équipe (future école ED406-Chimie Moléculaire Paris Centre doctorale du.de la doctorant.e) :						
Doctorant.e.s actuellement encadré.e.s par la.e directeur.rice de thèse (préciser le nombre de doctorant.e.s leur année de 1 <sup>e</sup> inscription et la quotité d'encadrement) : (1) E. Liu (2019, 33%)							
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Doctorant.e.s actuellement encadré.e.s par la.e co-directeur.rice de thèse (préciser le nombre de doctorant.e.s, leur année de 1<sup>e</sup> inscription et la quotité d'encadrement) : (1) J. Lee (2020, 50 %)



NOM : Titre : Choisissez un élément : ou e-mail :

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HDR		

Unité de Recherche : Intitulé : Code (*ex. UMR xxxx*) :

École Doctorale de rattachement :

**Choisissez un élément :** Ou si ED non Alliance SU :

Doctorant.e.s actuellement encadré.e.s par la.e co-directeur.rice de thèse (préciser le nombre de doctorant.e.s, leur année de 1<sup>e</sup> inscription et la quotité d'encadrement) :

Cotutelle internationale : 🛛 Non 🗌 Oui, précisez Pays et Université :

Selon vous, ce projet est-il susceptible d'intéresser une autre Initiative ou un autre Institut ? Non Oui, précisez Choisissez l'institut ou l'initiative :

## Grandes lignes de la demande

## Title of the project:

Molecular tweezers for multifunctional switchable organogels

## Acronym

SwitchGel

## Summary of the project

(5 lignes)

We propose to develop multifunctional stimuli-responsive organogels by exploiting the mechanical motion of molecular tweezers. The tweezers will be composed of luminescent M-salen complexes bearing gelling groups connected to a coordination switchable terpyridine unit. The drastic geometric change between the open and closed conformations should trigger a transition from solution to gel associated to modified optical and recognitions properties.

## Scientific description (5 pages max.)

#### **Objectives and description of the project**

In recent years, molecular machines<sup>[1]</sup> have attracted increasing interest for their ability to control motion at the molecular level. Artificial machines can be defined as an assembly of molecular components designed to perform a mechanical movement in response to an external stimulus. Although a wide variety of systems have been developed, the exploitation of this mechanical motion to perform work or control properties remains a major concern in the field. In particular, the propagation of structural changes from the molecular level to higher meso- or macroscopic scales represents still a major challenge. Only limited proofs of concept using switches<sup>[2]</sup> rotaxanes<sup>[3]</sup> or motors<sup>[4]</sup> architectures have demonstrated such effect induced by molecular motion. In this project, we aim to develop an original concept to control a macroscopic transition from solution to gel by exploiting the mechanical motion of molecular machines and obtain switchable multifunctional gels.

Partner 1 has developed a family of switchable molecular tweezers for the control of properties at the molecular level by a mechanical motion. This versatile system is based on a terpyridine (terpy) unit connected to two arms carrying M-salen functional units. By coordination of a cation to the terpy, the tweezers can be switched from an open to a closed form bringing the two functional M-salen complexes into close proximity. The reversibility of the motion is achieved by the addition of a competitive ligand yielding to the decoordination of the cation and reopening of the tweezers. This controlled and large modification of the distance between the two functional units has been successfully applied to modulate various properties such as luminescence, magnetism, redox or catalysis with Pt(II),<sup>[5]</sup> Cu(II),<sup>[6]</sup> Ni(II)<sup>[7]</sup> and Zn(II)<sup>[8]</sup> salen complexes respectively.



Figure 1. Principle of switchable molecular tweezers for multifunctional switchable organogels

The main objective of this doctoral project is to exploit the mechanical motion of switchable molecular tweezers carrying gelling groups to obtain multifunctional switchable organogels. Gels are soft materials composed of a liquid trapped in the three-dimensional network of a solid. Recently, organogels have attracted great interest due to their applications as new soft materials. This particular class of gels results from the self-assembly of low molecular weight gelators (LMWG) into fibrous gel networks.<sup>[9]</sup> The large structural reorganization driven by the opening and closing motion of the tweezers should modulate their gelation properties by promoting inter- or intramolecular interactions between tweezers depending on their conformation. By using emissive functional units, luminescent gels that can be activated by external stimuli should be obtained.

In order to obtain supramolecular gels, the control of non-covalent intermolecular interactions between gelators is essential. Using moieties such as amide or urea functions to establish hydrogen bonding networks, long alkyl chains to enhance Van der Waals interactions or aromatic systems to induce π stacking interactions have been commonly reported in the literature.<sup>[9-10]</sup> First, we will introduce long aliphatic or oligoethylene glycol chains as gelation-inducing groups at the level of the M-salen and/or terpyridine units. Indeed, salen complexes with this type of chain have been described as LMW organogelators.<sup>[11]</sup> Urea or amide units are also envisioned to increase intermolecular interactions via hydrogen bonds and induce the formation of large and well-organized assemblies.<sup>[12]</sup>

The use of Pt(II)-salen luminescent complexes will be favored for their capacity to induce Pt-Pt interactions that can favor the formation of supramolecular assemblies via this additional interaction.<sup>[13]</sup> Moreover, these Pt-Pt interactions modulate the remarkable phosphorescence properties of these complexes, which will thus allow us to probe optically their state of aggregation. Alternatively, Zn-salphen units will be considered as, in non-coordinating solvents, their dimerization has been observed and could lead to the formation of supramolecular fibers favorable to gelation.<sup>[11a]</sup> These complexes also present attractive fluorescence properties that are modulated by aggregation.



*Figure 2. Schematic representation of switchable tweezers with gelling substituents* 

Once obtained, solvent sampling will be performed to evaluate the self-assembly and gelation properties of the tweezers under these various conditions. Complementarily, a sergeant-soldier strategy by doping salen gelators with tweezers will also be investigated. The formation and structure of the organogels obtained will be studied by a combination of complementary physico-chemical techniques such as rheology, electron microscopy, light scattering, small angle scattering (X-rays, SAXS, or neutrons, SANS) that are accessible in the laboratory, on campus or on large instruments (Soleil Synchrotron - SWING beamline...).

The switching properties by metal coordination will also be studied by preparing the two forms separately or by applying the stimulus *in situ*. Depending on the substitution pattern of the terpyridine (in 6,6" or 4,4" positions)<sup>[5c]</sup> the default conformation is open or closed, offering a large modularity on the switching control. The dynamics of the mechanical motion and gel formation after the addition of the cation will also be monitored *in situ* by light scattering. The structure of the obtained fibrils and the parameters of the gelling network will be studied in real time by SAXS. These different analyses will allow a better understanding of the still little-known architecture of LMWGs and will shed light on the new role of the mechanical motion on gelling processes through real-time *in situ* monitoring of these transitions.

In addition to the modification of the gelation properties, the mechanical motion should lead to a variation of the optical properties with the appearance of an absorption and an emission at lower energy corresponding to a metal-metal ligand charge transfer (MMLCT) linked to Pt-Pt interactions. As platinum-based luminescent tweezers have shown recognition properties of ions<sup>[5a, 5b]</sup> or planar aromatic molecules,<sup>[5c]</sup> the recognition properties of these organogels will finally be studied. It is expected that different affinities between solution and gel will be achieved and controlled by the coordination stimulus, which should result in multifunctional and multi-activatable gels.

In conclusion, this multidisciplinary PhD project will allow the synthesis of innovative multifunctional molecular systems by exploiting the mechanical motion of a molecular machine. They will constitute smart-materials with potential applications in the field of sensors and recognition.

#### Feasibility. Risk assessment and management

The proposal is ambitious but the key risk, that switchable molecular tweezers could not be obtained and available for study, is minimized based on partner 1 previous publications<sup>[6-7]</sup> and our preliminary results. Indeed, during the course of a master internship, we have obtained Pt-salphen complexes with long alkyl chains either by direct ligand synthesis and coordination or by post-functionalization of the Pt-salen complex already formed via alkylation reactions of free phenol functions or Sonogashira couplings on iodine derivatives. Such inert Pt(II) complexes can be used as building block in a "chemistry on complex" strategy that we have developed using cross-coupling reactions for the connection to the switchable terpyridine unit.<sup>[4-6]</sup> Alternative strategies for more labile Zn(II) complexes by synthesizing the free ligand followed by a metallation in the last step are also available<sup>[14]</sup> demonstrating the feasibility to obtain the targeted tweezers.

The formation of an organogel can be challenging as the gelation conditions (solvent,

concentrations...) are difficult to predict. However, Zn(II)-salen complexes have been described to form organogels in some organic solvents<sup>[11]</sup> and some planar Pt(II) complexes can form supramolecular assemblies via Pt-Pt interactions. A preliminary study allowed us to observe the formation of organogels with Pt(II) and Zn(II) salphen complexes with C12 chains at low concentration (~5 mg/mL) in toluene or xylene. Both organogels are luminescent with emissions in the visible and preliminary SAXS experiments performed by partner 2 have shown that the temperature dependent sol-gel transitions could be followed in real time by SAXS. Moreover, depending on the metallic cation, they display interesting discrepancies in their order parameters and in their behavior with the temperature change.



Organogels of Zn and Ptsalen with C<sub>12</sub> chains in toluene and xylene

Finally, the risk of not obtaining stimuli-responsive gel is unlikely because of by the drastic geometric change induced by the mechanical motion. Moreover, the versatility of the building block strategy will enable an easy optimization of the response through the modification of the substituents and the fine tuning of the inter- and intramolecular interactions depending on the tweezer's conformation. Since gels can be sensitive to ionic strength, the effect of the addition of a cation to the system might need to be differentiated from the effect of the mechanical motion. The availability of tweezers with a default open or closed conformation (depending on the substitution on the terpy in 6,6" and 4,4") should enable a fine evaluation of both effects on gelation properties and offers additional modularity.

Thus, combining the expertise of Partner 2 in soft materials and their characterization with the switchable systems developed by Partner 1 holds great potential for the development of multifunctional smart molecules and materials.

## Position of the project within national and international context

The exploitation of artificial molecular machines as responsive building blocks to develop new types of stimuli-responsive materials is a fundamentally disruptive approach compared to others that have been developed so far.<sup>[15]</sup> It aims to exploit precisely controlled mechanical motions at molecular level and to amplify them in collective mechanical motions taking place at larger dimensions up to the material length scale. Some examples of incorporation of molecular motor or switches into liquid crystalline materials resulting in macro or mesoscopic changes have been described by Feringa,<sup>[4]</sup> Stoddart<sup>[16]</sup> Aprahamian<sup>[2b]</sup> or Katsonis.<sup>[2a]</sup> Giuseppone, in Strasbourg, has exploited a pH-responsive [ $c_2$ ]daisy chain rotaxane as the constituent of a supramolecular polymer to achieve a reversible gel–sol transition using either pH or temperature as external triggers.<sup>[17]</sup> However, very limited examples of low molecular weight gelator based on molecular machine are reported and none are switchable molecular tweezers despites their potential due to drastic change in shape between their two forms. Stoddart has described the formation of an organogel by a cholesterol-stoppered bistable

[2]Rotaxane<sup>[18]</sup> but no sol-gel transition was observed upon switching. In 2010, Chen and Chiu reported the first switchable organogelator based on a [2]rotaxane.<sup>[19]</sup> The gelation of this molecular machine originated from a free urea station involved in intermolecular hydrogen bonding that can be disrupted by the shuttling of the macrocycle over the urea moiety. More recently, the group of Chung has reported a similar strategy to achieve a sol-gel transition in organic solvents using an amphiphilic calix[4]arene-based [2]rotaxanes.<sup>[20]</sup> Theses studies demonstrate the potential of molecular machines to influence the stability and the morphology of the self-assembled structures in which they operate and the growing interest of the scientific community for this kind of systems.

While Pt-Pt interactions have been exploited to form self-assembled luminescent supramolecular architecture in particular by the group of Vivian Yam<sup>[21]</sup> with Pt(II)-terpyridine complexes, there is no example of organogels based on Pt(II)-salen complexes. Thus, the combination of the mechanical motion of switchable molecular tweezers with luminescent Pt-salen moieties to achieve stimuli responsive organogels is original and offers great potential for the development of smart multifunctional materials.

## Position of the project in regard to the iSiM objectives

This project is clearly within the scope of the iSiM initiative since it proposes to tackle a major scientific challenge around the implementation of the mechanical movement of molecular machines. Our original approach uses the tools of molecular chemistry for the synthesis of well-defined molecular species that will be used to generate effects on a mesoscopic scale by controlling self-assembly processes. These effects will then be characterized by physico-chemical techniques adapted to the study of the formed materials. This multidisciplinary project will benefit from the complementarity between the two partners belonging to Sorbonne University. The location of the two laboratories on the Pierre and Marie Curie campus will facilitate collaboration through discussions and access to the necessary equipment.

Although preliminary experiments have started on this topic, this proposal is the first shared research project between the two main investigators. The joint supervision of a PhD student would then strengthen the ties between the two research teams, in accordance with the iSiM objective to foster collaborations between research groups within Sorbonne University. Lastly, this project would provide initial results and new elements to apply for national and European funding.

## Highlight partners complementarity

Partner 1 (**G. Vives**, IPCM, SU) will provide the necessary expertise in organic synthesis, supramolecular and coordination chemistry and photophysics. Since his appointment in Paris in 2010, G. Vives has been working in supramolecular chemistry on the development of rotaxanes and cyclodextrin polyrotaxanes and switchable molecular tweezers (PI ANR JCJC SMARTEES 2015-20). He is author of 37 scientific publications (~1250 citations, h-index 22) and has experience in national project management (ANR JCJC) and participation in consortia (ANR, Labex...) as well as student supervision (7 PhD, 12 M2). He will supervise the PhD student who will work in the GOBS team of the IPCM and will benefit from his scientific environment in supramolecular chemistry.

Partner 2 (**C. Guibert**, LRS, SU) will co-supervise the PhD student and will bring his skills in the implementation and characterization of self-assembled systems. Lecturer at Sorbonne University since 2017, he is interested in understanding the interactions governing the properties of materials at interfaces and their structure, in particular using radiation scattering techniques. He has worked on several studies of supramolecular assemblies (ref. <sup>[22]</sup>, <sup>[23]</sup>) and in particular on one of them involving the formation of gels (ref. <sup>[24]</sup>). He regularly works on light or neutron lines of large instruments (about 15 measurement campaigns over the last 9 years) and will be able to use this particular expertise in the framework of this project. He will welcome

and supervise the PhD student in the LRS laboratory and will train him or her to classical physico-chemical characterization techniques.

In summary, combining the expertise of Partner 2 in the characterization of self-assembled systems with the switchable molecular system developed by Partner 1 holds great potential for the development of multifunctional smart molecules and materials. Funding of a PhD would help to start a new collaboration beneficial for both teams within the framework of iSiM initiative.

## Références

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## Programme de travail

## Research program (1 page max.)

The work program will be composed of 3 main tasks:

• WP1. Synthesis and characterization of the tweezers

This work will be devoted to the synthesis and characterization of tweezers with Pt(II) or Zn(II) salen units and gelling substituents that should form organogels. For Pt(II) tweezers, our building block strategy <sup>[4-6]</sup> using Sonogashira coupling reactions between alkyne terminated Pt-salen units and dibromo-terpyridine will be adapted with salen bearing gelling substituents. The incorporation of gelling substituents on the terpyridine unit will also be investigated using Hantzsch conditions between a substituted benzaldehyde and bromo-acetylpyridine. For more labile Zn(II) tweezers a final Zn(II)-templated condensation between an hemi-salen moiety and a salicylaldehyde substituted terpyridine is envisioned as previously reported.<sup>[8]</sup> This will result in an alternate connection mode that might change the gelling properties. All the tweezers will be fully characterized at the molecular level by MS, NMR, UV-Vis and emission spectroscopies. This task will be conducted in Partner 1 lab which is fully equipped for synthesis.

• WP2. Gel formation and characterization

This task will be focused on the studies and optimization of the gelation properties of the tweezers and will provide a permanent feedback to the synthetic task. The M-salen precursors with gelling units will first be studied as model enabling some parallel work even before the final tweezers are obtained. Solvent sampling will be performed to evaluate the self-assembly and gelation properties under various conditions of the tweezers and M-salen precursors. The formation and structure of the organogels will be studied by a combination of complementary physico-chemical techniques, in particular with the help of light scattering experiments. These studies will be conducted in Partner 2 lab or on large instruments to which he has regular access.

• WP3. Switching studies and guest recognition

This final task will be devoted to the studies of the mechanical switching of the tweezers and their guest binding activity. The dynamics of the mechanical motion and gel formation after the addition of the cation will be monitored in situ UV-Vis and luminescence spectroscopy and by light and small-angle scattering. The binding of planar aromatic molecules and intercalation of bidentate ligands in the closed form will be investigated by UV-vis titrations for Pt(II) and Zn(II) tweezers respectively. These studies will be conducted conjointly between Partner 1 & 2 labs.



## **Guillaume Vives**

Maître de Conférences Institut Parisien de Chimie Moléculaire UMR 8232 Sorbonne Université 4 place Jussieu, 75005 Paris, France Born 12/01/1981 guillaume.vives@sorbonne-universite.fr http://www.ipcm.fr/VIVES-Guillaume ResearcherID: <u>G-4248-2010</u>

#### **Education and Employment**

Since 2010 Maître de conférences, Sorbonne Université. Institut Parisien de Chimie Moléculaire.

2016 Habilitation à Diriger des Recherches, Université Pierre et Marie Curie, Paris

- 2009-2010 *Post-doctoral fellow*, Institut des Sciences Moléculaires, Université de Bordeaux. "Communication between functional molecules using photocontrolled ions" Supervisor: *Dr. Nathan D. McClenaghan*
- 2007-2009 *Post-doctoral fellow*, Chemistry department, Rice University, Houston, TX, (USA). "Synthesis of functionalized nanovehicles" Supervisor: *Prof. James M. Tour*
- 2004-2007 *PhD Université Paul Sabatier*, CEMES, Toulouse. "Synthesis of a familly of rotary molecular motors" Supervisors: *Dr. Gwénaël Rapenne, Prof. Jean-Pierre Launay*

2003-2004 *DEA*, Université Paul Sabatier, Toulouse.

2003 Agrégation de Sciences Physiques option Chimie.

2000-2004 Elève de l'ENS Lyon.

#### **Research interests**

Supramolecular Chemistry. Polyrotaxanes of cyclodextrin for multimodal imaging. Switchable Molecular Tweezers. Molecular machines.

Supervisions: 7 PhD students, 1 post-doc, 12 M2, 3 M1, 10 L3, 1 L2 students.

## Funding

Coordinator ANR JCJC SMARTEES (2015-2020) 'Switchable molecular tweezers'; participation to Labex Michem (2013-16, coordinator B. Hasenknopf) 'Polyrotaxanes for multimodal imaging', ANR Rotaximage (2016-20, coordinator B. Hasenknopf), ANR SMAC (2019-23, coordinator V. Marvaud).

#### Awards and Prizes

Research and doctoral supervision award, Sorbonne University (2015-...). French Chemical Society 'Young Observer' at IUPAC general assembly, Istanbul (2013). Poster prize ESF Research conference: Supramolecular Chemistry, Obernai, France (2005).

#### **Outreach activities**

Participation in chemistry workshops at Fête de la Science and for the International Year of Chemistry. Popularization conferences on molecular motors for High school Teachers and Middle-school children. Contributing author for the International Chemistry Olympiad (Paris, 2019)

#### Scientific production

37 articles (h-index 22, ~1250 citations), 1 book chapter

5 invited international conferences, 10 invited seminars (2 int. - 8 nat.)

22 oral communications (14 int. - 8 nat.) and 21 poster communications. (13 int. - 8 nat.)

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## Fields of interest

Physical chemistry of interfaces:

- surface nanostructuring in solution and functionalisation of interfaces,
- stability of colloidal dispersions (nanoparticles, microemulsions),
- control and characterisation of colloidal interactions (X-ray or neutrons scattering),
- responsive systems (pH, temperature, magnetic field),
- comprehension of self-assembling systems.

#### Professional Experience

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sept. 2017	Maître de conférences (assistant professor) at Sorbonne Université.		
2016-2017	PrAg (lecturer) at the ENS Paris-Saclay.		
2015-2016	Post-doc position in SPC at TUE (Eindhoven, NL) under the supervision of Ilja Voets.		
2012 -2015	Master degree internship then PhD thesis in PHENIX (UPMC, Paris) under the supervision of Véronique Peyre, Vincent Dupuis and Jérôme Fresnais.		
ducation and diplomas			

#### Education and diplomas

2012-2015	PhD in physical chemistry at the UPMC (ED 388).
2011-2012	Second year of the Master's degree of Chemistry, specialities: materials/theoretical chemistry at the UPMC.
2009-2010	Preparation for and admission to the agrégation de chimie (a contest giving the position of teacher in Chemistry at university level).
2007-2012	ENS Paris diploma in Chemistry.

#### Outreach activities

<ul> <li>2008- Increasing involvement in the selection and the preparation of French team for International Chemistry Olympiad (IChO) and member of the scientific committe the international competition in 2018 (Bratislava &amp; Prague) and in 2019 (Paris).</li> <li>2020 Member of the beam of the setebut division of the Second Content (CCE)</li> </ul>
<ul> <li>ongoing International Chemistry Olympiad (IChO) and member of the scientific committe the international competition in 2018 (Bratislava &amp; Prague) and in 2019 (Paris).</li> <li>Adverse of the beard of the established of the Science of the Science (SCE)</li> </ul>
the international competition in 2018 (Bratislava & Prague) and in 2019 (Paris).
2020 Manuban of the bound of the east-burt division of the French Chamistry (CCF)
<b>2020</b> Wember of the board of the catalyst division of the French Chemistry Society (SCF)
ongoing representative of the young chemists.

## Scientific production

summary	17 articles (h-index 11, ~480 citations), 5 articles in educational or popular scien journals, 1 book chapter	
recent significant publications	<ol> <li>Calcium phosphate mineralization through homogenous enzymatic catalysis: Investigation of the early stages, E. Colaço, D. Brouri, C. Méthivier, L. Valentin, F. Oudet, K. El Kirat, C. Guibert, J. Landoulsi, Journal of colloid and interface science, 565, 43-54 (2020)</li> <li>Strain stiffening hydrogels through self-assembly and covalent fixation of semi-flexible fibers, R.P. Sijbesma, M. Fernandez-Castano Romera, C. Guibert, I.K. Voets, C. Storm, Angewandte Chemie International Edition (2017)</li> <li>Morphological evolution of complex coacervate core micelles revealed by iPAINT microscopy, A. Aloi, C. Guibert, L.L.C. Olijve, I.K. Voets, Polymer 107, 450-455 (2016)</li> <li>Hyperthermia of magnetic nanoparticles: experimental study of the role of aggregation, C. Guibert, V. Dupuis, V. Peyre, J. Fresnais, The Journal of Physical Chemistry C 119 (50), 28148-28154 (2015)</li> <li>Controlling nanoparticles dispersion in ionic liquids by tuning the pH, C. Guibert, V. Dupuis, J. Fresnais, V. Peyre, Journal of colloid and interface science 454, 105-111 (2015)</li> </ol>	