ParisTech

TITLE: AI-DRIVEN QUALITY OF SMART ADDITIVE PRINTING: FROM CONCEPT TO MANUFACTURING

Topic number : ***2025_002***

Field : Energy, Processes - Material science, Mechanics and Fluids - Physics, Optics

Subfield: 3D printing

ParisTech School: Arts et Métiers
Research team : I2MP
Research team website:
Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés
Lab location: Châlons-en-Champagne
Lab website: https://www.msmp.eu/

Contact point for this topic: Nan KANG, nan.kang@ensam.eu

Advisor 1: Mohamed EL MANSORI - mohamed.elmansori@ensam.eu
Advisor 2: Nan KANG - nan.kang@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Laser Powder bed fusion (LPBF) additive manufacturing (AM) offers significant potential for producing complex, high-performance components across a range of industries. However, achieving defect-free parts remains challenging due to the layer-by-layer nature of the process and the enormous number of molten pools involved. This project presents an innovative AI-driven approach, incorporating multi-sensor data integration on a commercial Truprint 5000 system, to improve the quality of H13 steel components manufactured via LPBF for high-pressure die casting applications. By applying advanced AI algorithms—including machine learning and neural networks—the system enables in-situ detection and characterization of defects both on the powder bed and the as-built surfaces. Leveraging large datasets acquired during manufacturing, the developed AI models open new pathways for

accelerating the industrial adoption of AM, which facilitate the consistent production of high-quality components with more reliable and efficient.

Required background of the student:
1. Candidates should have a master's degree in the field of artificial intelligence;
2. A background in additive manufacturing will be a clear advantage;
3. Candidates should be able to work in a multidisciplinary environment and be fluent in English (both oral and written)

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

1. 1. Sahar Toorandaz , Katayoon Taherkhani , Farima Liravi , Ehsan Toyserkani, A novel machine learning-based approach for in-situ surface roughness prediction in laser powder-bed fusion, Additive Manufacturing 91 (2024) 104354.

2. 2. Pinku Yadav, Olivier Rigo, Corinne Arvieu, Emilie Le Guen, Eric Lacoste. Data Treatment of In Situ
Monitoring Systems in Selective Laser Melting Machines. Advanced Engineering Materials, 2021, 23
(5), pp.2001327.

3. 3. Huajing Zong, Nan Kang, Mohamed El Mansori, Laser powder bed fusion additive manufacturing of high-strength hot tool steel via in-situ heat treatment induced nano-scaled strengthening mechanism, Nano Materials Science Available online 8 July 2025, https://doi.org/10.1016/j.nanoms.2025.06.007.

ParisTech

TITLE: INVESTIGATION OF THE MECHANISMS OF ACTION OF METAL-BASED PHOTOSENTIZERS FOR PHOTODYNAMIC THERAPY

Topic number : ***2025_003***

Field : Life and Health Science and Technology - Chemistry, Physical chemistry and Chemical Engineering

Subfield: Biochemistry/Biology

ParisTech School: Chimie ParisTech - PSL
Research team :
Research team website: www.gassergroup.com
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: www.gassergroup.com

Contact point for this topic: Gilles Gasser - gilles.gasser@chimieparistech.psl.eu

Advisor 1: Gilles Gasser - gilles.gasser@chimieparistech.psl.eu
Advisor 2: Pierre Mesdom - pierre.mesdom@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Photodynamic Therapy (PDT) is an approved medical technique to treat certain types of cancer. It relies on the use of photosensitizer (PS) that is activated by light, producing reactive oxidative species (ROS) that kills cancer cells. In this project, in-depth biological evaluation of novel metal-based PSs just discovered in our group will be carried out in order to unveil the mechanisms of action of these compounds. Several biological/biochemical techniques will be used to elucidate the types of cell death induced by these metal complexes. It was recently shown that immunogenic cell death for example was involved. This will be one of the targets of this project.

Required background of the student:

The applicant should have a sound knowledge (theoretical and practical) in biochemistry/biology. They should have experience with in vivo studies. The applicant must be fluent in English since it is the language spoken in the Gasser group. Some theoretical and practical knowledge in chemistry would be an asset.

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

1. Metal-based Photosensitizers as Regulated Cell Death Inducers

Y. Zhang, B.-T. Doan* and G. Gasser,* Chem. Rev., 2023, 123, 10135-10155.

DOI: https://doi.org/10.1021/acs.chemrev.3c00161

2. A Triple Threat Against Ovarian Cancer: Os(II)-Pt(IV)-Ceritinib Conjugates for Photodynamic Therapy, Chemotherapy, and Immunogenic Cell Death Induction

M. Redrado, S. Acharya, P. Mesdom, T. Babu, J.W. Southwell, L.S. Oliveira, D. Gibson,* and Gasser,* Angew. Chem. Int. Ed., 2025, e202518623.

DOI: https://doi.org/10.1002/anie.202518623

OPEN ACCESS

3. Ruthenium(II) Polypyridyl Complexes containing COUBPY Ligands as Potent Photosensitizers for the Efficient Phototherapy of Hypoxic Tumors using Deep-Red and Near-Infrared Light

D. Abad-Montero, A. Gandioso, E. Izquierdo-García, S. Chumillas, A. Rovira, M. Bosch, M. Jordà-Redondo, D. Castaño, J. Bonelli, V.V. Novikov, A. Deyà, J.L. Hernández, J. Galino, M.E. Alberto, A. Francés-Monerris, S. Nonell, G. Gasser* and V. Marchán,* J. Am. Chem. Soc., 2025, 147, 7360-7376.

DOI: https://doi.org/10.1021/jacs.4c15036

4. Rationally Designed Ruthenium Complexes for 1- and 2-Photon Photodynamic Therapy

J. Karges, S. Kuang, F. Maschietto, O. Blacque, I. Ciofini, H. Chao,* and G. Gasser,* Nature Commun., 2020, 11, 3262.

DOI: https://www.nature.com/articles/s41467-020-16993-0

OPEN ACCESS

5. Inverse Correlation between Endoplasmic Reticulum Stress Intensity and Anti-Tumor Immune Response with Ruthenium(II)-based Photosensitizers for Photodynamic Therapy of Head and Neck Squamous Cell Carcinoma

C. Thibaudeau, C. Bour, M. Scarpi-Luttenauer, P. Mesdom, J. Karges, A. Gandioso, L. Zhou, S. Harlepp, M. Burgy, S. Martin, G. Mellitzer, C. Gaiddon,* G. Gasser,* and A.C. Jung,* J. Med. Chem., 2025, accepted.
DOI: https://doi.org/10.1021/acs.jmedchem.5c02147

ParisTech

TITLE: IDENTIFYING NOVEL FRAMEWORK META-MATERIALS WITH COMPUTATIONAL CHEMISTRY AND MACHINE LEARNING METHODS

Topic number : ***2025_004***

Field : Chemistry, Physical chemistry and Chemical Engineering - Material science, Mechanics and Fluids

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team :
Research team website: https://www.coudert.name
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr

Contact point for this topic: Coudert François-Xavier fx.coudert@chimieparistech.psl.eu

Advisor 1: François-Xavier Coudert - fx.coudert@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Framework materials, including metal–organic frameworks (MOFs), covalent organic frameworks (COFs) as well as inorganic framework materials, are increasingly present in materials science and demonstrate a variety of extraordinary physical and chemical behavior. The goal of this project is to identify novel materials with anomalous properties, such as negative Poisson's ratio, negative adsorption, very high anisotropic elasticity, etc. We will identify and design framework-based metamaterials based on three computational approaches at different scales: 1. High-throughput screening of materials databases, performed at the DFT level of theory, of tens of thousands of materials. This will identify trends in structure/property relationships, as well as provide training data for future models. 2. The development of machine learning models (based on equivariant graph neural nets) for the prediction of

tensorial properties of materials, based on their atomistic structure. 3. Scaling up this screening by relying on machine-learning potentials for the description of atomic interactions, allowing us to go beyond the screening of existing materials databases, but to integrate our calculations in a AI-based generative models to propose new material structures, and assess their feasibility. Our group already has significant experience in these areas of data-based computational chemistry, leveraging the latest advances in the field of machine learning to spur the development of novel materials.

Required background of the student:
computational chemistry, physical chemistry

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

1. “Best practices in machine learning for chemistry”, N. Artrith, K. T. Butler, F.-X. Coudert, S. Han, O. Isayev, A. Jain and A. Walsh, Nature Chem., 2021, 13 (6), 505–508. https://doi.org/10.1038/s41557-021-00716z

2. “Nanoscale metamaterials: Meta-MOFs and framework materials with anomalous behavior”, F.-X. Coudert and J. D. Evans, Coord. Chem. Rev., 2019, 388, 48–62. https://doi.org/10.1016/j.ccr.2019.02.023

3. “Artificial Intelligence Paradigms for Next-Generation Metal–Organic Framework Research”, A. Ozcan, F.-X. Coudert, S. M. J. Rogge, G. Heydenrych, D. Fan, A. P. Sarikas, S. Keskin, G. Maurin, G. E. Froudakis, S. Wuttke and I. Erucar, J. Am. Chem. Soc., 2025, 147 (27), 23367–23380. https://doi.org/10.1021/jacs.5c08214

4. “Machine learning interatomic potentials for amorphous zeolitic imidazolate frameworks”, N. Castel, D. André, C. Edwards, J. D. Evans and F.-X. Coudert, Digital Discovery, 2024, 3 (2), 355–368. https://doi.org/10.1039/d3dd00236e

5. “High-throughput computational screening of nanoporous materials in targeted applications”, E. Ren, P. Guilbaud and F.-X. Coudert, Digital Discovery, 2022, 1 (4), 355–374. https://doi.org/10.1039/d2dd00018k

ParisTech

TITLE: MULTI-PLATFORM INTERACTIVE DIGITAL TWINS FOR BETTER DATA INTELLIGIBILITY AND COLLABORATIVE DECISION SUPPORT

Topic number : ***2025_005***

Field : Information and Communication Science and Technology

Subfield: Human-computer interactions

ParisTech School: Arts et Métiers
Research team : Presence & Innovation
Research team website: https://lampa.ensam.eu/equipe-p-i-132195.kjsp?RH=1415871394252&RF=1478611858411
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website: https://lampa.ensam.eu/accueil-lampa-100748.kjsp

Contact point for this topic: sylvain.fleury@ensam.eu

Advisor 1: Sylvain Fleury - sylvain.fleury@ensam.eu
Advisor 2: Beatriz Moya Garcia - beatriz.moya_garcia@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
This thesis aims to design and evaluate ergonomic and interactive interfaces for Digital Twins (DT) to enhance the intelligibility of the complex data they provide and facilitate decision-making, particularly in a collaborative context. Building on the advancements of the CNRS@CREATE DesCartes project on urban digital twins and integrating into the ITTAI alliance for resilient territories, this research project will examine the contribution of interactivity compared to static visualizations and will compare the impact of different media (virtual reality, augmented reality, traditional screens, etc.) on the understanding of the information provided by a digital twin. A particular focus will be placed on user collaboration around the digital twin, assessing how a shared virtual environment can support collective decision-making. Finally, a specific innovative feature aimed at increasing the effectiveness of the

digital twin will be defined and integrated during the thesis (e.g., an intelligent analysis assistant or an additional interactive simulation tool). The candidate will be based at LAMPA in Laval or at PIMM in Paris, and co-supervised by experts in numerical modeling (CNRS, PIMM) and virtual reality (LAMPA), ensuring an interdisciplinary approach.

Required background of the student:
Background in cognitive psychology, ergonomics, design, or computer sciences.

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

1. Christmann, O., Fleury, S., Migaud, J., Raimbault, V., Poussard, B., Guitter, T., ... & Richir, S. (2022). Visualizing the invisible: User-centered design of a system for the visualization of flows and concentrations of particles in the air. Information Visualization, 21(3), 311-320.

2. Agnès, A., Sylvain, F., Vanukuru, R., & Richir, S. (2023). Studying the effect of symmetry in team structures on collaborative tasks in virtual reality. Behaviour & Information Technology, 42(14), 2467-2475.

3. Moya, B., Badías, A., González, D., Chinesta, F., & Cueto, E. (2023). A thermodynamics-informed active learning approach to perception and reasoning about fluids. Computational Mechanics, 72(3), 577-591.

4. Moya, B., Badias, A., Gonzalez, D., Chinesta, F., & Cueto, E. (2022). Physics perception in sloshing scenes with guaranteed thermodynamic consistency. IEEE Transactions on Pattern Analysis and Machine Intelligence, 45(2), 2136-2150.

5. Moya, B., Badías, A., Alfaro, I., Chinesta, F., & Cueto, E. (2022). Digital twins that learn and correct themselves. International Journal for Numerical Methods in Engineering, 123(13), 3034-3044.

ParisTech

TITLE: DYNAMIC CRACK PROPAGATION IN SOLIDS: A PHASE-FIELD APPROACH WITH THEORETICAL AND NUMERICAL DEVELOPMENTS

Topic number : ***2025_007***

Field : Material science, Mechanics and Fluids - Mathematics and their applications

Subfield: Fracture mechanics

ParisTech School: Arts et Métiers
Research team : DURABILITE, INGENIERIE DES PROCEDES ET PHYSIQUE DES ECOULEMENTS
Research team website: https://lampa.ensam.eu/equipe-dippe-134463.kjsp?RH=1415871394252
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website: https://lampa.ensam.eu/accueil-lampa-100748.kjsp

Contact point for this topic: Saber EL AREM saber.elarem@ensam.eu

Advisor 1: Amine Ammar - amine.ammar@ensam.eu
Advisor 2: Saber EL AREM - saber.elarem@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Here is a clean version in English that fits what you describe (dynamic crack propagation, phase-field theory, theory + numerics). --- ### Proposed PhD title **Dynamic crack propagation in solids: a phase-field approach with theoretical and numerical developments** (Shorter variant if needed: **Dynamic crack propagation in solids using phase-field fracture models**) --- ### Project description (for CSC file) Dynamic fracture in solids is a central topic in modern solid mechanics, with applications ranging from structural integrity and impact resistance to seismic rupture and fragmentation. Classical fracture mechanics, based on sharp crack representations, faces severe limitations when dealing with complex crack patterns, branching and coalescence, or three-

dimensional geometries. In this context, phase-field models of fracture have emerged as a powerful framework, in which cracks are described by a continuous damage-like field, allowing nucleation and propagation to be captured without explicit tracking of crack surfaces. The objective of this PhD project is to develop and analyse advanced phase-field models for **dynamic crack propagation** in brittle and quasi-brittle materials, with a balanced emphasis on **theoretical formulation** and **numerical implementation**. On the theoretical side, the work will build on thermodynamically consistent frameworks for gradient-enhanced damage and configurational forces, and will address the coupling between inertia, fracture energy dissipation, and possible rate-dependent effects. Special attention will be paid to the well-posedness of the model, the role of the internal length scale, and the prediction of crack speed and branching under dynamic loading. On the numerical side, the candidate will implement the proposed models in a finite element framework, using mixed or staggered solution strategies and robust time-integration schemes suitable for transient dynamics. Benchmark problems in dynamic fracture (dynamic tension, impact-induced cracking, etc.) will be simulated in order to assess the predictive capabilities and limitations of the approach. The final goal is to provide a consistent and efficient phase-field toolbox for simulating complex dynamic crack propagation in realistic structures, and to contribute to a better understanding of the underlying physics of dynamic fracture.

Required background of the student:
solid mechanics, fracture mechanics, numerical methods,

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

1. Nour Habib and Saber {El Arem} and Amine Ammar, Coupled crystal plasticity-cohesive zone modeling of rock salt viscoplasticity,Finite Elements in Analysis and Design,252,2025

2. N Habib, S El Arem, A Ammar, Numerical Simulation of the Viscoplastic Behavior of Rock Salt : Bridging Grain Boundary Cracking and Bulk Deformation, 26e Congrès Français de Mécanique, 2025

3. N Habib, S El Arem, A Ammar, On the strain energy decomposition in phase field brittle fracture: established models and novel cleavage plane-based techniques, Advanced Modeling and Simulation in Engineering Sciences, Volume 12, article number 7, 2025

4. Hela Gmati, Charles Mareau, Amine Ammar, Saber El Arem, A phase-field model for brittle fracture of anisotropic materials,Int J Numer Methods Eng. 2020; 121: 3362–3381

ParisTech

TITLE: OPTIMIZATION OF FILLING STAGE DURING CASTING PROCESS USING ARTIFICIAL INTELLIGENCE

Topic number : ***2025_008***

Field : Material science, Mechanics and Fluids

Subfield: Casting process, AI, Numerical methods, FE simulation

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website: https://lampa.ensam.eu/accueil-lampa-100748.kjsp

Contact point for this topic: BEN SAADA-MARIEM-mariem.bensaada@ensam.eu

Advisor 1: Amine AMMAR - amine.ammar@ensam.eu
Advisor 2: Mariem BEN SAADA - mariem.bensaada@ensam.eu
Advisor 3: Marie Bedel - marie.bedel@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Filling is a critical stage of casting as it directly impacts the final mechanical quality of the cast part. Indeed, if a mold cavity is filled too slowly, the metal solidifies before filling completion, inducing misrun defects. On the other hand, when filling too fast, the turbulent flow leads to oxide entrapment and mold erosion (1). In order to avoid those critical defects, an appropriate filling system has to be designed. Such design rules currently exist only for gravity casting, and are based on a very simplified approach, where a filling system is made of a sprue, runners and ingates whose dimensions are given by empirical expressions (2). If those standard design rules permit to avoid misrun defect, fluid flow is always turbulent in the filling system (3), thus systematically inducing oxides in the cast parts. Some recent studies proposed filling system optimization by using Machine Learning (ML) methods (4). However, only

the dimensions of a fixed filling system were optimized (5,6). Reconsideration of filling system design in itself is still hardly considered (7). To our best knowledge, such a design reconsideration has never been performed by using ML based algorithms without geometrical constrains. However, the revolution of sand printing technology makes the geometrical constrains associated with mold making totally outdated. When considering this new technology, innovative and much more optimized filling system design rules can be developed, by considering only thermal and fluid flow constrains. Today, foundry engineers can predict the cast products characteristics without having to perform numerous time-consuming trial-and-error experiments. It is hence possible nowadays in metal casting processes to apply powerful tools and models developed with reasonable number of simulations that allows predicting parts defects and controlling complex processes (8). On the other hand, approaches combining physics based reduced order models were recently developed, enabling parametric studies, and data-driven model enrichment in the so-called hybrid modelling framework. A high accuracy is obtained with respect to the experimental measurements, while proceeding under the stringent real-time constraint (9). Therefore, in this PhD study, these approaches could be extended and enriched with Generative Design approach to optimize the filling stage of casting. To do so, an adapted casting software will be used, which combines fluid flow dynamic and heat transfer, to study the impact of different parameters on head loss during filling; mold design, mold surface condition, metal viscosity or casting speed will be considered. Then the generated numerical data will be used to develop a predictive model of head loss by using hybrid physical-data driven techniques via Machine-Learning (ML) technologies and their integration into the detailed analytical and numerical modellings. Such a model will then be used to 2 optimize filling system design, therefore optimizing filling speed and flow rate while mastering casting yield and associated heat loss. The newly proposed design rules for filling systems will be eventually validated by experimental comparison, performed on the foundry facility of LAMPA laboratory, on both standard and optimized designs.

Required background of the student:
Continum Mechanics, Numerical methods, FE simulation

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

1. 1. Bedel M, Sanitas A, El Mansori M. Geometrical effects on filling dynamics in low pressure casting of light alloys. Journal of Manufacturing Processes. 1 sept 2019;45:194-207.

2. 2. Campbell J. Complete Casting Handbook: Metal Casting Processes, Metallurgy, Techniques and Design. Butterworth-Heinemann; 2015. 1055 p.

3. Cross M, McBride D, Croft TN, Williams AJ, Pericleous K, Lawrence JA. Computational modeling of mold filling and related free-surface flows in shape casting: An overview of the challenges involved. Metall Mater Trans B. 1 déc 2006;37(6):879-85.
3. 4. Ambekar SA, S.B.Jaju. A review on optimization of gating system for reducing defect. International Journal of Engineering Research and General Science. 2014;2(1):93-8.
5. He B, Lei Y, Jiang M, Wang F. Optimal Design of the Gating and Riser System for Complex Casting Using an Evolutionary Algorithm. Materials. janv 2022;15(21):7490.
6. Ktari A, El Mansori M. On the improvement of castings quality in hybrid low-pressure sand-casting (LPSC) process in a fully integrated CAE environment. Int J Adv Manuf Technol. juill 2023;127(5-6):2309-26.
4. 7. Sama SR, Badamo T, Lynch P, Manogharan G. Novel sprue designs in metal casting via 3D sand-printing. Additive Manufacturing. 2019;25:563-78.
8. Nouri M, Artozoul J, Caillaud A, Ammar A, Chinesta F, Köser O (2022) Shrinkage porosity prediction empowered by physics-based and data-driven hybrid models. Int J Mater Form 15(3).
5. 9. Ammar, A., Ben Saada, M., Cueto, E. et al. Casting hybrid twin: physics-based reduced order models enriched with data-driven models enabling the highest accuracy in real-time. Int J Mater Form 17, 16 (2024).

ParisTech

TITLE: MIXED REALITY FOR INTUITIVE 3D MODELING AND DESIGN SIMULATION

Topic number : ***2025_009***

Field : Information and Communication Science and Technology - Design, Industrialization

Subfield: Computer-aided design, Geometry modelling, Virtual reality, Computer graphics

ParisTech School: Arts et Métiers
Research team : Chalon Institute - XR
Research team website: https://institutchalon.ensam.eu/
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Chalon-sur-Saône
Lab website: https://lispen.artsetmetiers.fr/

Contact point for this topic: LOU - Ruding ruding.lou@ensam.eu

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Advisor 2: Ruding LOU - ruding.lou@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Recent advances in Mixed Reality (MR) technologies are transforming the way users interact with 3D digital models. Traditional Computer-Aided Design (CAD) systems such as CATIA or SolidWorks remain powerful but are often complex, requiring extensive training and experience to use effectively. Their desktop-based interfaces constrain direct spatial interaction and limit accessibility for novice users. In contrast, Mixed Reality environments provide intuitive, spatially aware, and gesture-based interactions that can significantly lower the barrier to entry for 3D modeling and prototyping [1-2]. Moreover, MR also enables designers and users to simulate real-world usage contexts and assembly interactions (for example, collecting data [3], real sensor to locate in the

virtual world [4]). Such design and usage simulations support the “Design for X” philosophy, allowing users to virtually test and iterate on their ideas rapidly while maintaining a strong connection with the intended use environment. This PhD project aims to investigate and compare the usability, efficiency, and accuracy of MR-based modeling and simulation workflows against traditional CAD software. The research will focus on two main aspects: 1. Intuitive modeling and geometric operations in MR, where users—without formal CAD training—can easily create and manipulate 3D shapes using natural interactions such as hand gestures or voice commands; 2. Simulative Design for X (DfX), where MR enables direct evaluation of design performance, such as assembly fit or functional testing, without the need for physical prototypes. This approach has been shown to reduce prototyping time and material waste in recent MR-enhanced rapid prototyping studies [5-6]. The proposed research will involve designing experimental modeling tasks that can be replicated in both CATIA and MR environments. Through controlled experiments, task completion time, model precision, and user workload will be measured. Quantitative data will be complemented by qualitative evaluations through usability questionnaires and interviews. The expected outcome is a comprehensive assessment framework for comparing immersive modeling tools with traditional CAD systems, offering new insights into human–computer interaction design, accessibility in 3D modeling, and the integration of MR for Design for X simulations in engineering and manufacturing contexts. References: [1] Horvat, N., Škec, S., Martinec, T., Lukačević, F., & Perišić, M. M. (2019). Comparing Virtual Reality and Desktop Interface for Reviewing 3D CAD Models. Proceedings of the Design Society: International Conference on Engineering Design, 1(1), 1923–1932. doi:10.1017/dsi.2019.198 [2] Lee, J. G., Seo, J., Abbas, A., & Choi, M. (2020). End-Users’ Augmented Reality Utilization for Architectural Design Review. Applied Sciences, 10(15), 5363. https://doi.org/10.3390/app10155363 [3] M. Murnane, M. Breitmeyer, C. Matuszek and D. Engel, "Virtual Reality and Photogrammetry for Improved Reproducibility of Human-Robot Interaction Studies," 2019 IEEE Conference on Virtual Reality and 3D User Interfaces (VR), Osaka, Japan, 2019, pp. 1092-1093. https://doi.org/10.1109/VR.2019.8798186 [4] Y. Liu, G. Novotny, N. Smirnov, W. Morales-Alvarez and C. Olaverri-Monreal, "Mobile Delivery Robots: Mixed Reality-Based Simulation Relying on ROS and Unity 3D," 2020 IEEE Intelligent Vehicles Symposium (IV), Las Vegas, NV, USA, 2020, pp. 15-20, doi: 10.1109/IV47402.2020.9304701. [5] Yin, Y., Zheng, P., Li, C., & Pang, Y. M. (2023). A mixed reality-enhanced rapid prototyping approach for industrial articulated products. Procedia CIRP, 119, 1035-1040. https://doi.org/10.1016/j.procir.2023.02.178 [6] Snider, C., Kukreja, A., Cox, C. M. J., Gopsill, J., & Kent, L. (2024). Mixed reality prototyping: a framework to characterise simultaneous physical/virtual prototyping. Proceedings of the Design Society, 4, 775–784. doi:10.1017/pds.2024.80

Required background of the student:

Computer Aided Design, Geometry processing, Virtual reality, Computer graphics

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

1. Horvat, N., Škec, S., Martinec, T., Lukačević, F., & Perišić, M. M. (2019). Comparing Virtual Reality and Desktop Interface for Reviewing 3D CAD Models. Proceedings of the Design Society: International Conference on Engineering Design, 1(1), 1923–1932. doi:10.1017/dsi.2019.198

2. Lee, J. G., Seo, J., Abbas, A., & Choi, M. (2020). End-Users' Augmented Reality Utilization for Architectural Design Review. Applied Sciences, 10(15), 5363. https://doi.org/10.3390/app10155363

3. B. Li, F. Segonds, C. Mateev, R. Lou, F. Merienne, "Design in context of use: An experiment with a multi-view and multi-representation system for collaborative design", Computers in Industry, 103: 28 - 37, 2018

4. B. Faliu, A. Siarheyeva, R. Lou, F. Merienne, "Design and Prototyping of an Interactive Virtual Environment to Foster Citizen Participation and Creativity in Urban Design", Lecture Notes in Information Systems and Organisation, 34: 55 - 78, Springer, Cham, 2019.

5. A. Scalas, Y. Zhu, F Giannini, R. Lou, K. Lupinetti, M. Monti, M. Mortara, M. Spagnuolo, "A first step towards cage-based deformation in Virtual Reality", Eurographics - STAG, 2020

ParisTech

TITLE: MIXED REALITY FOR PHYSICAL VAPOR DEPOSITION

Topic number : ***2025_010***

Field : Information and Communication Science and Technology - Material science, Mechanics and Fluids

Subfield: Virtual reality, Physical simulation

ParisTech School: Arts et Métiers
Research team : Chalon Institute - XR
Research team website: https://institutchalon.ensam.eu/
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Chalon-sur-Saône
Lab website: https://lispen.artsetmetiers.fr/

Contact point for this topic: LOU - Ruding ruding.lou@ensam.eu

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Advisor 3: Ruding LOU - ruding.lou@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Sputtering is one of the technic grouped under the denomination of Physical Vapor Deposition (PVD). The objective of these processes is to deposit matter on the surface of a piece by the mean of a vapor generated physically (i.e. thermally or mechanically). The deposition results in a film, or coating, few micrometres thick and from centimetre to meter in lateral dimension. The deposited film changes the surface properties of the piece. The applications are found in microelectronics, optics, data storage devices, energy (photovoltaic solar panel, batteries, fuel cells), medical devices (implants, prosthesis, tools), cutting tools and many others. In the context of Industry 4.0, Mixed reality (MR) plays a crucial role by merging the physical and digital worlds, providing immersive and interactive experiences. MR in Industry 4.0 enhances productivity, efficiency, and innovation by bridging the gap between the physical and digital realms, enabling new ways of working, training, and problem-

solving in the industrial context. MR allows engineers and designers to visualize complex 3D models and data in a realistic environment. This aids in designing, prototyping, and optimizing products and processes. MR enables the integration of digital twins, allowing real-time monitoring, simulation, and analysis of physical assets and processes. MR supports predictive maintenance by providing real-time data visualization and analytics. The aim of this project is to develop a new interactive MR application for PVD based on scientific data obtain by experimental measurements and numerical computations. • Process Visualization: MR can overlay relevant data, such as temperature, pressure, and deposition rates, onto the physical PVD equipment in real-time. This enables operators to monitor the process parameters more effectively and make informed decisions for process optimization. • Maintenance and Troubleshooting: MR can assist maintenance personnel in identifying and addressing issues with PVD equipment. By overlaying digital information on the physical equipment, maintenance procedures can be guided step by step, reducing downtime and improving the overall reliability of the system. • Customization and Design: MR can aid in the design and customization of coatings. By visualizing virtual prototypes and simulations in the physical environment, engineers and designers can make informed decisions about the composition and thickness of coatings, leading to improved product performance. The following research questions will be addressed during the proposed PhD : • What is the best interaction metaphor to let user visualize the virtual coating film ? o Under different representations: point cloud (for atoms) or surface mesh (for volume) o Through different scales: macroscope (coating pièce) or microscope (column-like structure) • How to design the augmented reality visualization for virtual PVD process in real machine ? o When the real PVD is stopped, how to visualize the simulated PVD results o During the real PVD process, how to synchronize the virtual PVD with which data ? • How to real-time and imprecisely simulate the PVD process in mixed reality application ? o Using scientific simulation software to simulate multiple cases o Using AI to train a black box model that can predict simulation result in MR References: [1] B. Li, F. Segonds, C. Mateev, R. Lou, F. Merienne, "Design in context of use: An experiment with a multi-view and multi-representation system for collaborative design", Computers in Industry, 103: 28 - 37, 2018. [2] Watiez, N. et al. (2023). Finite Element Mesh Generation for Nano-scale Modeling of Tilted Columnar Thin Films for Numerical Simulation. In: Noël, F., Nyffenegger, F., Rivest, L., Bouras, A. (eds) Product Lifecycle Management. PLM in Transition Times: The Place of Humans and Transformative Technologies. PLM 2022. IFIP Advances in Information and Communication Technology, vol 667. Springer, Cham [3] Watiez, N., Cotton, D., Besnard, A., Lou, R., Birembaux, H., & Outeiro, J, Augmented reality representation for the investigation of simulated inclined chromium thin films, In PLATHINIUM, Antibes, France, September 2023 [4] A. Besnard, R. Lou "“Virtual PVD”: A Virtual Reality approach to explore PVD Magnetron sputtering", Lecture Notes in Computer Science, 15740: 81-94, Springer, Cham, 2025

Required background of the student:

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

1. B. Li, F. Segonds, C. Mateev, R. Lou, F. Merienne, "Design in context of use: An experiment with a multi-view and multi-representation system for collaborative design", Computers in Industry, 103: 28 - 37, 2018.

2. Watiez, N. et al. (2023). Finite Element Mesh Generation for Nano-scale Modeling of Tilted Columnar Thin Films for Numerical Simulation. In: Noël, F., Nyffenegger, F., Rivest, L., Bouras, A. (eds) Product Lifecycle Management. PLM in Transition Times: The Place of Humans and Transformative Technologies. PLM 2022. IFIP Advances in Information and Communication Technology, vol 667. Springer, Cham

3. Watiez, N., Cotton, D., Besnard, A., Lou, R., Birembaux, H., & Outeiro, J, Augmented reality representation for the investigation of simulated inclined chromium thin films, In PLATHINIUM, Antibes, France, September 2023

4. A. Besnard, R. Lou "“Virtual PVD”: A Virtual Reality approach to explore PVD Magnetron sputtering", Lecture Notes in Computer Science, 15740: 81-94, Springer, Cham, 2025

ParisTech

TITLE: TOWARD MORE PREDICTABLE PHOTOPOLYMERIZATIONS IN DISPERSED MEDIA: A MIXED THEORY/PRACTICAL APPROACH

Topic number : ***2025_011***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: polymer synthesis, radical chemistry

ParisTech School: Chimie ParisTech - PSL
Research team : COCP
Research team website:
https://www.ircp.cnrs.fr/en/research-groups/cocp-group/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/

Contact point for this topic: Lacote - Emmanuel - emmanuel.lacote@chimieparistech.psl.eu

Advisor 1: Emmanuel Lacote - emmanuel.lacote@chimieparistech.psl.eu
Advisor 2: François-Xavier Coudert - fx.coudert@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Tha aim of the project is to build a predictive in-silico method to assess and describe photopolymerization processes in dispersed media. This is a joint synthetic/theory approach, whose final goal is to streamline the process optimization by determining the key parameters responsible for the reactivity.

Required background of the student:
experience in organic and polymer synthesis, basic coding skills

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

1. Schoumacker, M.; Subervie, D.; Dugas, P.-Y.; Lalevée, J.; Montarnal, D.; Lansalot, M.; Lacôte, E.; Bourgeat-Lami, E. Adv. Funct. Mater. 2024, 35, 2407914

2. Kalout, H.; Lansalot, M.; Bourgeat-Lami, E.; Morlet-Savary, F.; Lacôte, E.; Lalevée, J. Adv. Funct. Mater. 2024, 2406299

3. Canterel, R.; Lalevée, J.; Bourgeat-Lami, E.; Lacôte, E.; Lansalot, M. Angew. Chem. Int. Ed., 2023, e202309674

4. Artrith, N.; Butler, K. T.; Coudert, F.-X.; Han, S.; Isayev, O.; Jain, A.; Walsh, A. Nat. Chem. 2021, 13, 505

5. Gaillac, R.; Pullumbi, P.; Beyer, K. A.; Chapman, K. W.; Keen, D. A.; Bennett, T. D.; Coudert, F.-X. Nature Mater. 2017, 16, 1149

ParisTech

TITLE: PRODUCTION OF SUSTAINABLE POLYMERS BY ONE-POT CATALYSIS

Topic number : ***2025_012***

Field : Chemistry, Physical chemistry and Chemical Engineering - Environment Science and Technology, Sustainable Development, Geosciences

Subfield: Chemistry

ParisTech School: Chimie ParisTech - PSL
Research team : Organometallic Chemistry and Polymerization Catalysis
Research team website:
https://www.ircp.cnrs.fr/en/research-groups/cocp-group/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/en/chemistry-research-institute-of-paris/

Contact point for this topic: THOMAS Christophe
christophe.thomas@chimieparistech.psl.eu

Advisor 1: Christophe THOMAS - christophe.thomas@chimieparistech.psl.eu
Advisor 2: Régis GAUVIN - regis.gauvin@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
The development of new methods to transform biomass into resources suitable for polymer production remains a crucial obstacle on the way to a more sustainable chemical economy.1 In this regard, the creation of renewable polymers through one-pot catalysis represents an important tool to support more sustainable plastics production.2,3 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.4 These will then be polymerized through stereoselective ring opening polymerization, providing novel polyesters or polyamides.5 An intense emphasis will be placed on the design of new

organometallic catalysts based on Earth-abundant metals, as well as on establishing the physicochemical properties of the polymers.

Required background of the student:
organic and:or polymer chemistry

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

1. Fouilloux, H.; Rager, M.-N.; Ríos, P.; Conejero, S.; Thomas, C. M. Angew. Chem., Int. Ed. 2022, 61, e202113443.

2. Upitak, K.; Thomas, C. M. Acc. Chem. Res. 2022, 55, 2168.

3. a) Robert, C.; De Montigny, F.; Thomas, C. M. Nat. Commun. 2011, 2, 586. b) Fouilloux, H.; Qiang, W.; Robert, C.; Placet V.; Thomas, C. M. Angew. Chem., Int. Ed. 2021, 60, 19374.

4. Nguyen, D. H.; Trivelli, X.; Capet, F.; Paul, J.-F.; Dumeignil, F.; Gauvin R. M. ACS Catal., 2017, 7, 2022.

5. Marin, P.; Tschan, M. J.-L.; Isnard, F.; Robert, C.; Haquette, P.; Trivelli, X.; Chamoreau, L.-M.; Guérineau, V.; del Rosal, I.; Maron, L.; Venditto, V.; Thomas C. M. Angew. Chem. Int. Ed. 2019, 58, 12585.

ParisTech

TITLE: ECO-EFFICIENT PROCESSES FOR THE SYNTHESIS OF SUSTAINABLE POLYMERS

Topic number : ***2025_013***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: catalysis, organometallic chemistry, polymer chemistry

ParisTech School: Chimie ParisTech - PSL
Research team : Organometallic Chemistry and Polymerization Catalysis
Research team website: http://www.ircp.cnrs.fr/la-recherche/equipe-cocp/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: http://www.ircp.cnrs.fr/

Contact point for this topic: regis.gauvin@chimieparistech.psl.eu

Advisor 1: REGIS M. GAUVIN - regis.gauvin@chimieparistech.psl.eu
Advisor 2: Christophe Thomas - christophe.thomas@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
The development of new methods to transform biomass into resources suitable for polymer production remains a crucial obstacle on the way to a more sustainable chemical economy.[1] In this regard, the creation of renewable polymers through one-pot catalysis represents an important tool to support more sustainable plastics production.[2,3] 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.[4] These will then be polymerized through stereoselective ring opening polymerization, providing novel polyesters or polyamides.[5] An intense emphasis will be placed on the design of new organometallic catalysts based on Earth-abundant metals, as well as on establishing the physicochemical properties of the polymers.
[1] Fouilloux, H.; Rager, M.-N.; Ríos, P.; Conejero, S.; Thomas, C. M.

Angew. Chem., Int. Ed. 2022, 61, e202113443. [2] Upitak, K.; Thomas, C. M. Acc. Chem. Res. 2022, 55, 2168. [3] a) Robert, C.; De Montigny, F.; Thomas, C. M. Nat. Commun. 2011, 2, 586. b) Fouilloux, H.; Qiang, W.; Robert, C.; Placet V.; Thomas, C. M. Angew. Chem., Int. Ed. 2021, 60, 19374. [4] Nguyen, D. H.; Trivelli, X.; Capet, F.; Paul, J.-F.; Dumeignil, F.; Gauvin R. M. ACS Catal., 2017, 7, 2022. [5] Marin, P.; Tschan, M. J.-L.; Isnard, F.; Robert, C.; Haquette, P.; Trivelli, X.; Chamoreau, L.-M.; Guérineau, V.; del Rosal, I.; Maron, L.; Venditto, V.; Thomas C. M. Angew. Chem. Int. Ed. 2019, 58, 12585.

Required background of the student:
Required background of the student : organic and polymer chemistry.

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

1. Fouilloux, H.; Rager, M.-N.; Ríos, P.; Conejero, S.; Thomas, C. M. Angew. Chem., Int. Ed. 2022, 61, e202113443.

2. Upitak, K.; Thomas, C. M. Acc. Chem. Res. 2022, 55, 2168.

3. a) Robert, C.; De Montigny, F.; Thomas, C. M. Nat. Commun. 2011, 2, 586. b) Fouilloux, H.; Qiang, W.; Robert, C.; Placet V.; Thomas, C. M. Angew. Chem., Int. Ed. 2021, 60, 19374.

4. Nguyen, D. H.; Trivelli, X.; Capet, F.; Paul, J.-F.; Dumeignil, F.; Gauvin R. M. ACS Catal., 2017, 7, 2022.

5. Marin, P.; Tschan, M. J.-L.; Isnard, F.; Robert, C.; Haquette, P.; Trivelli, X.; Chamoreau, L.-M.; Guérineau, V.; del Rosal, I.; Maron, L.; Venditto, V.; Thomas C. M. Angew. Chem. Int. Ed. 2019, 58, 12585.

ParisTech

TITLE: NEW METHOD TO PREDICT THE VIBRATION CHARACTERISTICS OF NANOPARTICLES IN BIOLOGICAL TISSUE USING A HIGHER-ORDER NONLOCAL ELASTICITY AND STRAIN GRADIENT THEORIES: AN EMERGING AVENUE IN BIOMECHANICS.

Topic number : ***2025_014***

Field : Material science, Mechanics and Fluids - Mathematics and their applications - Life and Health Science and Technology

Subfield: Nonlocal elasticity and strain gradient, viscoelastic media, vibration of nanoparticles, characterization by Raman effect, scale effect.

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LAMPA - Laboratoire angevin de mécanique, procédés et innovation
Lab location: Angers
Lab website: https://lampa.ensam.eu/accueil-lampa-100748.kjsp

Contact point for this topic: el baroudi - adil - adil.elbaroudi@ensam.eu

Advisor 1: Adil EL BAROUDI - adil.elbaroudi@ensam.eu
Advisor 2: Ammar Amine - amine.ammar@ensam.eu
Advisor 3: Stéphane CHAMPMARTIN - stephane.champmartin@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Interest in nanomaterials has continued to grow over the past twenty years. The work carried out to date has made it possible to understand and use these new materials which have physical and chemical properties completely different from those known until now thanks to their small size. This work gave birth to nanotechnology, a vast disciplinary field which deals with the synthesis, characterization and exploitation of nanostructured materials. Nanomedicine, still at the development stage, is part of nanotechnology. In particular, gold nanoparticles are used in many applications such as catalysis, biology and medicine. In oncology,

these nanoparticles are the subject of growing interest. Three applications are currently being developed: aid in diagnosis and radiotherapy, transport of therapeutic molecules (vectorization) and photothermal therapy. The interest in nanoparticles in oncology is linked to the fact that nanoparticles injected through the bloodstream concentrate on tumors. In addition, these particles are chemically inert and therefore biocompatible. The network of blood vessels around the tumors promotes this concentration. Moreover, these nanoparticles are also used as nanovectors for the delivery of therapeutic molecules. Otherwise, the fixation of gold particles on tumors has given rise to another very promising application, the photothermal therapy. Finally, another solution is to vibrate the nanoparticles using a magnetic field. This vibration activates the cell death mechanisms of cancer cells without affecting healthy tissues. This perspective makes it necessary to study resonance frequencies and quality factor.

Required background of the student:
Master in Mechanics or in Applied Mathematics or in Physics.

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

1. X. Huang, A. El Baroudi and A. Ammar. An analytical approach to characterize the breathing mode vibration for thermoelastic nanosphere, Acta Mechanica (2025).

2. A. El Baroudi and J. Y. Le Pommellec. Gradient elasticity theories and instability criterion for the vibration of nanoparticles, Applied Physics A (2025).

3. X. Huang, A. El Baroudi, J. Y. Le Pommellec and A. Ammar. On the importance of modified continuum mechanics to predict the vibration of an embedded nanosphere in fluid, Zeitschrift für angewandte Mathematik und Physik (2024).

4. X. Huang, A. El Baroudi and B. Wu. Vibration properties of an elastic gold nanosphere submerged in viscoelastic fluid, Modern Physics Letters B (2023).

5. Y-S Borghei, S. Hosseinkhani and M. R. Ganjali. Plasmonic Nanomaterials: An emerging avenue in biomedical and biomedical engineering opportunities, Journal of Advanced Research (2022).

ParisTech

TITLE: SYNTHESIS AND FORMULATION OF BIODEGRADABLE POLYMERS FROM RENEWABLE RESOURCES

Topic number : ***2025_015***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Chemistry and material science

ParisTech School: Chimie ParisTech - PSL
Research team : Organometallic Chemistry and Polymerization Catalysis
Research team website:
https://www.ircp.cnrs.fr/en/research-groups/cocp-group/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/en/chemistry-research-institute-of-paris/

Contact point for this topic: BOUCHEMAL Kawthar
kawthar.bouchemal@chimieparistech.psl.euu

Advisor 1: Christophe THOMAS -
christophe.thomas@chimieparistech.psl.eu
Advisor 2: Kawthar BOUCHEMAL -
kawthar.bouchemal@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Ring-opening polymerization (ROP) of N-carboxyanhydrides (NCA) can produce homopolymers and block-copolymers with well-controlled structures where repeat units are natural amino acids. Similar to proteins, these synthetic polypeptides possess well-defined secondary structures, whereas synthetic polymers generally present a disordered coil structure. Therefore, these biomimetic polymers produce sophisticated superstructures with new material properties. We will aim to develop an efficient route from readily available reactants to synthesize new polypeptide analogs with a conserved ability to form well-defined secondary structures. In this regard, bimetallic catalysts are ideal

candidates for this purpose since the polar organometallic moiety will act as a strong nucleophile with 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 one-pot catalytic transformation, where cyclic urethanes or ureas are synthesized from, respectively, epoxides or aziridines and subsequently polymerized by ROP. In the second set of experiments, the physicochemical properties of the polypeptide analogs will be characterized, and their ability to self-assemble as supramolecular nanostructures will be investigated. The morphology, surface charge, and nanomechanical properties will be assessed using conventional physicochemical and physical characterization methods. Once prepared and characterized, the behaviors of the polypeptide analogs' nanostructures regarding biological systems will be investigated.

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

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

1. J. Control. Release, 2022, 342, 93.

2. Nature Comm., 2011, 2, 586.

3. Chem. Soc. Rev., 2013, 42, 9392.

4. Colloids Surf. B, 2021, 205, 111916.

ParisTech

TITLE: MODELLING MECHANOCHEMICAL ACTIVATED REACTIONS USING NOVEL DFT-BASED COMPUTATIONAL PROTOCOLS

Topic number : ***2025_016***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Theoretical Chemistry, Modelling of reaction mechanisms

ParisTech School: Chimie ParisTech - PSL
Research team : Chemical Theory and Modelling Group
Research team website: https://www.quanthic.org/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr/

Contact point for this topic: ilaria.ciofini@chimieparistech.psl.eu

Advisor 1: Ciofini Ilaria - ilaria.ciofini@chimieparistech.psl.eu
Advisor 2: Labat Frédéric - frederic.labat@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Mechanochemistry has emerged as an elegant and efficient approach providing alternative energy inputs for chemical transformations under mild conditions. [1] It can be used to facilitate reactions with insoluble reactants, it enables high-yielding solvent-free synthetic procedures, and can provides access to reactivity pathways inaccessible under solution-based conditions.[2] Not surprisingly, different computational models and methods have been recently developed to describe mechanochemical activated reactions [3]. In this general context, the aims of this thesis are : i) develop novel computational protocols allowing to overcome the limitations of existing models ; and ii) apply these approaches to both model reactions (such as Diels-Alder), to test their accuracy, and experimentally challenging reaction mechanisms, involving for instance transition metal complexes. [1] Do, J.-L. and Friščić, T., ACS Cent. Sci., 2017, 3, 13–19. [2] Hernández, J. G. and Bolm, C., J. Org. Chem., 2017,

82, 4007–4019. [3] F. Zeller, C.-M. Hsieh, W. Dononelli, T. Neudecker WIREs Comput Mol Sci. 2024;14:e1708.

Required background of the student:
Strong background in quantum chemistry. Knowledge of DFT approaches.

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

1. N. Al Assaad, A. Chamayou, R. Calvet,. M. Pedrón, I. Ciofini, F. Labat Mechanistic insights on hydrazones synthesis: a combined theoretical and experimental study PCCP 27 (2025) 7084-7092

2. L. Wilbraham, M. Louis, D. Alberga, A. Brosseau, R. Guillot, F. Ito, F. Labat, R. Métivier, C. Allain, I. Ciofini “Revealing the origins of mechanically-induced fluorescence changes in organic molecular crystals” Adv. Mat 30(2018) 1800817

3. T. Yan, A. Bonardi, C. Adamo, I. Ciofini Adaptable Range Separated Hybrids for the description of excited states : tuning the range separation parameter on effective charge transfer distance J. Chem. Theory Comput. 21 (2025) 1892–1904

4. N. Al Assaad, M. Pedrón, M.Ferrer, A. Chamayou, R. Calvet I. Ciofini, F. Labat, Addressing the importance of non-covalent interactions in the selectivity of Diels-Alder reactions under pressure : a theoretical study submitted

ParisTech

TITLE: DEVELOPMENT OF ORGANOMETALLIC COMPOUNDS FOR ANTIMICROBIAL APPLICATIONS

Topic number : ***2025_017***

Field : Chemistry, Physical chemistry and Chemical Engineering - Life and Health Science and Technology

Subfield: Medicinal Chemistry, Bioorganometallic Chemistry

ParisTech School: Chimie ParisTech - PSL
Research team : Institute of Chemistry for Life and Health Sciences - Inorganic Chemical Biology
Research team website: www.gassergroup.com
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: www.gassergroup.com

Contact point for this topic: kevin.cariou@chimieparistech.psl.eu

Advisor 1: Kevin Cariou - kevin.cariou@chimieparistech.psl.eu
Advisor 2: Gilles Gasser - gilles.gasser@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Antimicrobial resistance, whether for bacteria or for fungi, is a highly worrying topic that has been declared critical by the World Health Organization. Part of the solution is to explore new chemical space[1] to develop new drugs that can overcome the resistance. Our group is at the forefront of the development of organometallic anti-infectious compounds with a particular focus on antiparasitic and antifungal drugs. [2-5] In this project, we envision the development of organometallic antibiotic drugs, following the same successful approach. At this end of this project, we hope to have unveiled a compound that works on high priority resistant bacteria and mitigate the risk of new resistances emerging.

Required background of the student:

The applicant should have a sound knowledge (theoretical and practical) in both organic and organometallic synthetic 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 Inorganic Chemical Biology group led by Prof. Gilles GASSER. Practical knowledge in biology would be an asset.

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

1. C. Ludwig, A. Massiot, E. Dolcher, O. Blacque K. Cariou,* G. Gasser,* Organometallics, 2025, 44, 2182

2. S. Zhong, A. Kalamatianou, G. Scalese, C. O'Beirne, M. Redrado, O. Blacque, C. Tomasoni, C. Logé, M. Albassier, I. Ourlac-Garnier, F. Pagniez, P. Le Pape, L. Pérez-Díaz, D. Gambino, M.A. Comini, K. Cariou,* and G. Gasser,* Inorg. Chem., 2025, 64, 16192.

3. T. Karpstein, A. Kalamatianou, S. Keller, P. Späne, C. Häberli, A. Odermatt, O. Blacque, K. Cariou,* G. Gasser,* and J. Keiser,* ACS Infect. Dis., 2025, 11, 2037

4. Y. Lin, G. Scalese, C.A. Bulman, R. Vinck, O. Blacque, M. Paulino, A. Ballesteros-Casallas, L. Pérez Díaz, G. Salinas, M. Mitreva,* T. Weil,* K. Cariou,* J.A. Sakanari,* D. Gambino,* and G. Gasser,* ACS Infect. Dis., 2024, 10, 938-950.

5. Y. Lin, H. Jung, C.A. Bulman, J. Ng, R. Vinck, C. O'Beirne, S. Zhong, M.S. Moser, N. Tricoche, R. Peguero, R. Li, J.F. Urban Jr, P. Le Pape, F. Pagniez, M. Moretto, T. Weil,* S. Lustigman,* K. Cariou,* M. Mitreva,* J.A. Sakanari* and G. Gasser,* J. Med. Chem., 2023, 6, 15867-15882.

ParisTech

TITLE: P(III)-DIRECTED ROLLOVER CYCLOMETALATION AS A PLATFORM FOR LIGAND DESIGN

Topic number : ***2025_018***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Organic chemistry, catalysis, transition metal

ParisTech School: Chimie ParisTech - PSL
Research team : Catalysis, Synthesis of Biomolecules and Sustainable Development Team (CSB2D Team)
Research team website: https://iclehs.fr/research/csb2d/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr

Contact point for this topic: SOULE - Jean-François - jean-francois.soule@chimieparistech.psl.eu

Advisor 1: Jean-François Soulé - jean-francois.soule@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Phosphine ligands are foundational in transition-metal catalysis, shaping activity, stability, and selectivity across cross-coupling, hydrofunctionalization, and C–H activation. Yet expanding the structural diversity of diphosphines—especially beyond a few established scaffolds—remains challenging because conventional routes rely on multistep syntheses and hazardous building blocks. This project develops a C–H bond functionalization approach to build diphosphine libraries directly on the disphosphine backbone. A key obstacle is the strong σ-donor/π-acceptor character of two P(III) centers, which favors bis-coordination and blocks metalation. We address this by leveraging P(III)-directed rollover cyclometalation: an auxiliary ligand is used to tune the trans effect, promote transient decoordination of one phosphorus, and enable

selective C–H bond activation. This platform is designed to map how backbone substitution, bite angle, and electronic profiles can be diversified efficiently. The resulting diphosphines will be evaluated across representative catalytic reactions (e.g., cross-coupling, and selected C–H functionalizations) to establish structure–performance relationships. When a chiral auxiliary ligand is employed, the same strategy can be extended to atroposelective C–H bond functionalization to access chiral diphosphines for asymmetric catalysis.

Required background of the student:
The applicant must have good English language. She/he should have a Master's degree in molecular chemistry with solid skills in organic synthesis and organometallic complex preparations (theoretical and practical), including working under an inert atmosphere and mastering the usual characterization techniques. Experience in asymmetric catalysis will be appreciated but not mandatory.

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

1. Zhang, Z.; Roisnel, T.; Dixneuf, P. H.; Soulé, J.-F. Angew. Chem. Int. Ed. 2019, 58, 14110.

2. Rzayev, J.; Zhang, Z.; Durand, N.; Soulé, J.-F. Org. Lett. 2022, 24, 6755. [

3. M. Peng, C.-S. Wang, P.-P. Chen, T. Roisnel, H. Doucet, K. N. Houk, J.-F. Soulé, J. Am. Chem. Soc. 2023, 145, 4508-4516.

4. Peng, D. Ari, T. Roisnel, H. Doucet, J.-F. Soulé, Chem. Sci. 2023, 14, 9055-9062.

5. J. Zhang, J.-F. Soulé, ACS Catal. 2025, 2839-2846.

ParisTech

TITLE: DESIGN OF SMART PHOTOCAGES FOR ON-DEMAND RELEASE OF BIOMEDICAL PAYLOADS

Topic number : ***2025_019***

Field : Chemistry, Physical chemistry and Chemical Engineering - Life and Health Science and Technology

Subfield: Photochemistry

ParisTech School: Chimie ParisTech - PSL
Research team : Inorganic Chemical Biology (ICB)
Research team website: https://www.gassergroup.com/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr/

Contact point for this topic: Klausen Maxime - maxime.klausen@chimieparistech.psl.eu

Advisor 1: Maxime Klausen - maxime.klausen@chimieparistech.psl.eu
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Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
The controlled release of bioactive molecules triggered by light has emerged as a transformative approach in chemical biology and medicine, enabling the study of complex biochemical processes and the activation of therapeutic drugs “on-demand”. Photo-cleavable protecting groups (PPGs) offer such control by covalently “caging” drugs in an inactive form and releasing them upon light exposure.1 Recent breakthroughs from the group have allowed the development of remarkable systems with combined dual photo-therapeutic functionality.2-4 The proposed project aims to develop novel NIR-activatable photocage architectures by applying rational molecular engineering strategies to tune their light-responsiveness. The project will combine multi-step organic synthesis, coordination chemistry, and rigorous mechanistic investigation of the photochemical and photophysical processes at play using advanced

spectroscopic techniques. The most promising photocages will be adapted to targeted cancer therapy applications by releasing chemotherapy drug payloads and investigating bio-orthogonal targeting strategies.

Required background of the student:
The successful candidate should possess strong theoretical and practical expertise in multi-step organic synthesis, purification and chemical characterization techniques (HPLC, NMR, mass spectrometry), as well as fundamental knowledge of spectroscopy and photophysics. Prior experience working with bioconjugation protocols and/or with biological assays and cell-based models would be a strong asset. The candidate should be fluent in English, demonstrate intellectual curiosity, problem-solving ability, and the capacity to work effectively within an interdisciplinary research environment bridging chemistry, photophysics, and biology.

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

1. M. Klausen and M. Blanchard-Desce, J. Photochem. Photobiol. C: Photochem. Rev., 2021, 48, 100423.

2. P. A. Shaw, M. Klausen and M. Bradley, Polym. Chem., 2024, 15, 54-58.

3. B. Mills, A. Kiang, S. M. P. C. Mohanan, M. Bradley and M. Klausen, JACS Au, 2023, 3, 3014-3023.

4. K. M. Kuznetsov, P. Mesdom, K. Purkait, O. Blacque, A. H. Winter, K. Cariou and G. Gasser, Chem. Sci., 2025, 16, 14553-14563.

ParisTech

TITLE: ENHANCED PASSIVITY AND CORROSION RESISTANCE OF MULTI PRINCIPAL ELEMENT ALLOYS

Topic number : ***2025_020***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team : PCS
Research team website:
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/

Contact point for this topic: Dimitr Mercier

Advisor 1: Dimitri MERCIER - dimitri.mercier@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Multi principal element alloys (MPEA), also called high entropy alloys (HEA), is a new class of metallic alloys (first elaborated in 2004) having a great interest as engineering alloys. Their mechanical properties have been widely studied and currently a detailed approach of the design of these alloys (microstructure, composition) allows elaborating specific alloys with excellent mechanical properties, that may outperform those of conventional alloys. In contrast to the mechanical properties, the surface reactivity of these materials, and particularly their corrosion resistance, has only been slightly studied. Different studies have shown that the original “Cantor” alloy does not provide good corrosion resistance, due to its high (equimolar) Mn content. Combining what we know of the origin of the corrosion resistance of Ni and Fe-based stainless alloys, and applying a thermodynamic approach for the composition optimization, our research group was able to design and synthesize two new single-phase HEA/MPEA alloys containing molybdenum, which show excellent

corrosion resistance. The purpose of this research program is to understand the detailed relationship between alloy composition, surface reactivity and corrosion behavior (passivity, passivity breakdown, localized corrosion resistance) of MPEA/HEA alloys with high Cr and Mo contents, and explore a range of compositions that can be maintained as single fcc phase after rapid cooling or contain Mo-rich secondary phases. The surface oxides (native and passive films), which are key factors for the corrosion resistance, will be characterized for the different alloy compositions by advanced surface analysis techniques, including X-ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Spectrometry (ToF-SIMS), combined with electrochemical measurements. A focus will be placed on the stability and the growth mechanisms of these layers using an original approach developed by our research group, using in situ isotopic labelling (18O2).

Required background of the student:
Corrosion Science, Surface Science, Materials Science, Electrochemistry

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

1. Study of the surface oxides and corrosion behaviour of an equiatomic CoCrFeMnNi high entropy alloy by XPS and ToF-SIMS
Corrosion Science,167, 2020, 108507
10.1016/j.corsci.2020.108507

2. Enhanced passivity of Cr-Fe-Co-Ni-Mo multi-component single-phase face-centred cubic alloys: design, production and corrosion behaviour
Corrosion Science, 200, 2022, 110233
10.1016/j.corsci.2022.110233

3. Origin of enhanced passivity of Cr-Fe-Co-Ni-Mo multi-principal element alloy surfaces
npj Materials Degradation, 7, 2023, 13

4. XPS study of the thermal stability of passivated NiCrFeCoMo multi-principal element alloy surfaces
Surface and Interface Analysis, 55, 2023, 457
10.1002/sia.7193

5. Hydroxyl transport mechanisms upon passivation of Cr-Fe-Co-Ni-Mo multi-principal element alloy surfaces investigated by isotopic labelling
Applied Surface Science, 655, 2024, 159558
10.1016/j.apsusc.2024.159558

ParisTech

TITLE: CO-DESIGNING WITH EMERGING DIGITAL TECHNOLOGIES

Topic number : ***2025_021***

Field : Design, Industrialization - Information and Communication Science and Technology

Subfield: Co-design, User-Centered Design, Artificial Intelligence, Digital Twin, Immersive Technologies, Innovation

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LCPI - Laboratoire conception de produits et innovation
Lab location: Paris
Lab website: https://lcpi.ensam.eu/

Contact point for this topic: LOU - Ruding ruding.lou@ensam.eu

Advisor 1: Frédéric SEGONDS - Frederic.SEGONDS@ensam.eu
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Advisor 3: Ruding LOU - ruding.lou@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Contemporary product design processes increasingly incorporate advanced digital technologies to enhance their outcomes. Specifically, Artificial Intelligence (AI), Digital Twin (DT) and eXtended Reality (XR) technologies offer exclusive capabilities that designers can leverage to support user-centric design approaches (Cui et al., 2025). Indeed, altogether, they facilitate the creation of actionable and dynamic artifacts to support co-design with end-users. AI plays a pivotal role in such design activities. It can quickly generate design alternatives while dynamically integrating user cognitive feedback thereby improving the propositions (Guillaume et al., 2023). DT provides a virtual representation of the product, serving as the foundational artifact for co-design. The digital model can incorporate real-world data collected from physical prototypes while also executing functional and usage simulations for iterative refinement (Tao et al., 2019). XR offers the immersive interaction tools to

integrate virtual product and usage simulations into various environments. This capability allows designers to comprehensively design and test the products with their end-users (Li et al., 2018). Despite the synergies among these technologies, their systematic integration into user-centered design methodologies remains underexplored. Few studies have proposed structured frameworks or tools to fully leverage their combined potential in collaborative design contexts with end-users (Bertoni, 2023). This thesis aims to address this gap by developing a methodological approach that bridges the capabilities of AI, DT and XR to support effective co-design practices. Beyond theoretical contributions, the study will deliver practical tools validated in real-world co-design scenarios. The research will thus be divided into three main phases: The first year will be dedicated to conducting a comprehensive state of the art on existing methodologies for augmented user-centered design. Particular attention will be given to frameworks integrating AI, DT and/or XR in collaborative processes. This review will inform the formulation of possible research contributions. By the end of this phase, a roadmap will be established to guide their development and validations. The second and third years will focus on developing and iteratively refining the method and its tools. Experimental campaigns will be conducted to test the propositions in real-world co-design contexts. The fourth and final year will aim to synthesize all research contributions into a coherent and optimised methodological framework. This phase will thus consolidate and formalise a comprehensive set of practices and tools to bridge AI, DT and XR in effective co-design processes.

Required background of the student:
Product Design, User Interaction Design, User Experience Design, Industrial Design or related fields

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

1. Bertoni, M. (2023). Towards Digital Immersive Experiences for Collaborative Value Co-creation in Design. In L. M. Camarinha-Matos, X. Boucher, & A. Ortiz (Éds.), Collaborative Networks in Digitalization and Society 5.0 (Vol. 688, p. 193 206). Springer Nature Switzerland. https://doi.org/10.1007/978-3-031-42622-3_14

2. Cui, J., Mantelet, F., Jean, C., Lou, R., & Segonds, F. (2025). Exploring the usability and creativity enhancement of augmented reality in additive manufacturing-based product design. Computers in Human Behavior Reports, 20, 100816. https://doi.org/10.1016/j.chbr.2025.100816

3. Guillaume, R., Pailhès, J., Gruhier, E., Laville, X., Baudin, Y., & Lou, R. (2023). Intent Detection for Virtual Reality Architectural Design. In F.

Noël, F. Nyffenegger, L. Rivest, & A. Bouras (Éds.), Product Lifecycle Management. PLM in Transition Times : The Place of Humans and Transformative Technologies (Vol. 667, p. 420 430). Springer Nature Switzerland. https://doi.org/10.1007/978-3-031-25182-5_41

4. Li, B., Segonds, F., Mateev, C., Lou, R., & Merienne, F. (2018). Design in context of use : An experiment with a multi-view and multi-representation system for collaborative design. Computers in Industry, 103, 28-37. https://doi.org/10.1016/j.compind.2018.09.006

5. Tao, F., Sui, F., Liu, A., Qi, Q., Zhang, M., Song, B., Guo, Z., Lu, S. C.-Y., & Nee, A. Y. C. (2019). Digital twin-driven product design framework. International Journal of Production Research, 57(12), 3935 3953. https://doi.org/10.1080/00207543.2018.1443229

ParisTech

TITLE: MODELLING CONFORMATION-CONFINED POLYMORPHISM AND PHOTOPHYSICAL TUNING IN MOLECULAR CRYSTALS

Topic number : ***2025_022***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Theoretical Chemistry, Modelling of materials

ParisTech School: Chimie ParisTech - PSL
Research team : Chemical Theory and Modelling Group
Research team website: https://www.quanthic.org
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr

Contact point for this topic: Labat - Frederic - frederic.labat@chimieparistech.psl.eu

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Advisor 4:

Short description of possible research topics for a PhD:
Conformation-confined molecular crystals offer a powerful platform for tuning solid-state photophysical properties, with applications across a wide range of fields [1]. These materials can exhibit distinct polymorphs that arise from restricting vibrational and rotational molecular motions, thereby creating rigid structures that resist significant deformation under packing forces within the crystal lattice, thus dictating specific photophysical properties [1,2]. In particular, butterfly-like molecular skeletons are very promising systems, as their pi-conjugation length can be tuned depending on the polymorph, leading to markedly different photophysical behaviors in the aggregated state. Building on these butterfly-like frameworks, the objectives of this thesis are: (i) to develop and apply DFT-based computational protocols combined with electrostatic embedding techniques [3] to investigate conformation-confined polymorphism in molecular crystals and to tune their

photophysical properties, and (ii) to clarify the structure-property relationships in these unique systems.

Required background of the student:
Strong background in quantum chemistry. Knowledge of DFT approaches with periodic boundary conditions.

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

1. Angew. Chem. Int. Ed. 64, e202414960 (2025)

2. Chem. Rev. 115, 11718−11940 (2015)

3. J. Chem. Theory Comput. 12, 3316-3324 (2016)

ParisTech

TITLE: CONTEXTUAL CHARACTERIZATION AND DECISION FRAMEWORK FOR OPTIMAL HUMAN-AI COLLABORATION IN INDUSTRIAL SUPERVISION

Topic number : ***2025_023***

Field : Information and Communication Science and Technology - Design, Industrialization

Subfield:

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Aix-en-Provence
Lab website: https://lispen.artsetmetiers.fr/

Contact point for this topic: Amzil - Kenza - kenza.amzil@ensam.eu

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Advisor 3: Nathalie Klement - nathalie.klement@ensam.eu
Advisor 4: Lionel Roucoules - lionel.roucoules@ensam.eu

Short description of possible research topics for a PhD:
This PhD project aims to determine under which conditions industrial system supervision should rely on humans, AI systems, or a specific form of Human-AI collaboration. While AI is increasingly used for anomaly detection, diagnostics, predictive maintenance, and decision support, its performance remains highly dependent on data quality, operational variability, and explainability constraints. Conversely, human operators provide contextual reasoning and ethical responsibility but face cognitive load, fatigue, and time pressure. The project will first develop a formal ontology describing roles, tasks, autonomy levels, collaboration modes, and contextual factors relevant to industrial supervision. It will then define measurable descriptors to characterize scenarios and build a multi-criteria evaluation framework that integrates technical, human, organizational, and normative KPIs. Experimental studies, via simulations

or through real case studies, will assess the effectiveness of different collaboration configurations. The outcome will be a recommendation framework that links scenario characteristics to the most suitable collaboration mode, enabling industries to make informed, context-aware decisions about Human-AI collaboration strategies. Ultimately, this work aims to ensure that investments in AI are rigorously justified and that AI is deployed only when it provides clear and demonstrable value beyond human-only supervision.

Required background of the student:
Industrial Engineering, Computer Science, Artificial Intelligence

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

1. Song, Binyang, Qihao Zhu, et Jianxi Luo. « Human-AI Collaboration by Design ». Proceedings of the Design Society 4 (mai 2024): 2247-56. https://doi.org/10.1017/pds.2024.227.

2. Heinzl, B., Silvina, A., Krause, F., Schwarz, N., Kurniawan, K., Kiesling, E., ... & Moser, B. (2024, April). Towards Integrating Knowledge Graphs into Process-Oriented Human-AI Collaboration in Industry. In International Conference on Software Quality (pp. 76-87). Cham: Springer Nature Switzerland.

3. Fragiadakis, George, Christos Diou, George Kousiouris, et Mara Nikolaidou. « Evaluating Human-AI Collaboration: A Review and Methodological Framework ». arXiv, 9 juillet 2024. http://arxiv.org/abs/2407.19098.

4. Amzil K., Yahia E., Klement N., Roucoules L. (2021) Causality Learning Approach for Supervision in the Context of Industry 4.0. In: Roucoules L., Paredes M., Eynard B., Morer Camo P., Rizzi C. (eds) Advances on Mechanics, Design Engineering and Manufacturing III. JCM 2020. Lecture Notes in Mechanical Engineering. Springer, Cham. https://doi.org/10.1007/978-3-030-70566-4_50

5. Hartikainen, M., Spurava, G., & Väänänen, K. (2024). Human-AI Collaboration in Smart Manufacturing: Key Concepts and Framework for Design. HHAI 2024: Hybrid Human AI Systems for the Social Good, 162-172.

ParisTech

TITLE: REINFORCEMENT LEARNING-BASED TOPOLOGY-PRESERVING NON-RIGID DEFORMATION OF CAD MODELS FROM POINT CLOUDS FOR FIRST-TIME-RIGHT PRODUCTION IN SMART MANUFACTURING

Topic number : ***2025_024***

Field : Design, Industrialization - Information and Communication Science and Technology - Mathematics and their applications

Subfield: Reverse engineering and geometric modeling

ParisTech School: Arts et Métiers
Research team : Digital Engineering and Geometric Representations
Research team website: https://lispen.ensam.eu
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Aix-en-Provence
Lab website: https://lispen.ensam.eu

Contact point for this topic: PERNOT - Jean-Philippe - jean-philippe.pernot@ensam.eu

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Advisor 2: Arnaud POLETTE - arnaud.polette@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
This PhD program addresses the way CAD models can be adapted and deformed to capture the manufacturing defaults and thus maintain the coherence between the digital model and its physical and manufactured counterpart. This is particularly useful to optimize tool paths and manufacturing parameters. New deformation operators will be developed to simulate and reproduce various state-of-the-art manufacturing behaviors and deviations, including free-form and non-rigid deformations. Those operators will be applied until the deviation between the CAD model and the acquired point cloud of the manufactured counterpart is minimized. During the deformation process, the topology of the CAD models will be preserved, to be able to maintain the whole coherency and

possibly available semantic information. Based on these newly defined capabilities, it will also be possible to deform CAD models a priori, i.e. without any point cloud to serve as a reference and prior to the start of the manufacturing process or before a new manufacturing step, in order to compensate for future deviations and allow for first-time-right production. This will be made possible thanks to the use of a reinforcement learning strategy, wherein an autonomous agent will learn how to define the deformation sequence to be applied to compensate the coming shape deviations between the theoretical model and its manufactured counterpart. Following this strategy, it will therefore be possible to mix both known rules coming from existing machine fault modeling theories, as well as unknown rules to be learned from experience. The proposed framework will be implemented and validated on academic as well as industrial examples.

Required background of the student:
Computer science, machine learning, computer-aided design.

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

1. Peuzin-Jubert M., Polette A., Nozais D., Mari J-L., Pernot J-P., Survey on the View Planning Problem for reverse engineering and automated control applications, Computer-Aided Design, vol. 141, 103094, 2021.

2. Shah G. A., Polette A., Pernot J-P., Giannini F., Monti M., Simulated annealing-based fitting of CAD models to point clouds of mechanical parts' assemblies, Engineering with Computers, vol. 37(4), pp. 2891-2909, 2021.

3. Hu S., Polette A., Pernot J-P., SMA-Net: Deep learning-based identification and fitting of CAD models from point clouds, Engineering with Computers, vol. 38, pp. 5467-5488, 2022.

4. Zhang C., Pinquié R., Polette A., Carasi G., De Charnace H., Pernot J-P., eCAD-Net: editable parametric CAD models reconstruction from dumb B-Rep models using deep neural networks », Computer-Aided Design, vol. 178, 2025.

5. Zhang C., Polette A., Pinquié R., Iida M., De Charnace H., Pernot J-P., Reinforcement Learning-Based Parametric CAD Models Reconstruction From 2D Orthographic Drawings, Computer-Aided Design, vol. 188, 2025.

ParisTech

TITLE: REINFORCEMENT LEARNING-BASED 3D RECONSTRUCTION OF CAD MODELS FROM POINT CLOUDS FOR SMART MANUFACTURING APPLICATIONS

Topic number : ***2025_025***

Field : Design, Industrialization - Information and Communication Science and Technology - Mathematics and their applications

Subfield: Geometric modeling and reverse engineering

ParisTech School: Arts et Métiers
Research team : Digital Engineering and Geometric Representations
Research team website: https://lispen.ensam.eu
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Aix-en-Provence
Lab website: https://lispen.ensam.eu

Contact point for this topic: PERNOT - Jean-Philippe - jean-philippe.pernot@ensam.eu

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Advisor 2: Arnaud POLETTE - arnaud.polette@ensam.eu
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Advisor 4:

Short description of possible research topics for a PhD:
This PhD program addresses the way CAD models can be reverse engineered from point clouds to discover the possible building trees from which they may originate, and more precisely the ones adapted for smart manufacturing applications. Such an approach is particularly interesting to define the bill of operations adapted to a given manufacturing process, but also to automatically generate the set of CAD models associated to the manufacturing steps. Indeed, being able to compare the CAD model at a given step to its manufactured and digitized counterpart is of major interest for control purposes and process optimization in the context of the Industry 4.0. The main idea relies in the use of reinforcement learning able to learn how to perform those complex tasks in a very efficient way, and without requiring large databases. Starting from state-of-the-art and

known geometric and manufacturing rules to be established with the environment, an autonomous agent will learn the different actions to be applied at the feature level to move towards the next steps, with a known final objective that is the point cloud used as input of the algorithm. This singularity will be exploited to define the reward function to be optimized step after step. The proposed framework will be implemented and validated on academic as well as industrial examples.

Required background of the student:
Computer science, machine learning, computer-aided design

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

1. Peuzin-Jubert M., Polette A., Nozais D., Mari J-L., Pernot J-P., Survey on the View Planning Problem for reverse engineering and automated control applications, Computer-Aided Design, vol. 141, 103094, 2021.
2. Shah G. A., Polette A., Pernot J-P., Giannini F., Monti M., Simulated annealing-based fitting of CAD models to point clouds of mechanical parts' assemblies, Engineering with Computers, vol. 37(4), pp. 2891-2909, 2021.
3. Hu S., Polette A., Pernot J-P., SMA-Net: Deep learning-based identification and fitting of CAD models from point clouds, Engineering with Computers, vol. 38, pp. 5467-5488, 2022.
4. Zhang C., Pinquié R., Polette A., Carasi G., De Charnace H., Pernot J-P., eCAD-Net: editable parametric CAD models reconstruction from dumb B-Rep models using deep neural networks, Computer-Aided Design, vol. 178, 2025.
5. Zhang C., Polette A., Pinquié R., Iida M., De Charnace H., Pernot J-P., Reinforcement Learning-Based Parametric CAD Models Reconstruction From 2D Orthographic Drawings, Computer-Aided Design, vol. 188, 2025.

ParisTech

TITLE: PRELIMINARY;CONCEPTUAL DESIGN OF MANUFACTURING SYSTEMS INTEGRATING HUMAN FACTORS WITH VIRTUAL REALITY

Topic number : ***2025_026***

Field : Design, Industrialization - Life and Health Science and Technology - Information and Communication Science and Technology

Subfield: Virtual Reality ; Human Factors ; Manufacturing System Deqsign

ParisTech School: Arts et Métiers
Research team : LCFC - Product and Manufacturing Design Team
Research team website: https://lcfc.ensam.eu/
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website: https://lcfc.ensam.eu/

Contact point for this topic: Alain ETIENNE - alain.etienne@ensam.eu

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Advisor 2: Alain ETIENNE - alain.etienne@ensam.eu
Advisor 3: Jelena PETRONIJEVIC - jelena.petronijevic@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Virtual reality is frequently used for the evaluation [3] and/or design of production systems when these systems are already substantially developed (layout choices, technical and geometric solutions have already been finalized). Consequently, aspects related to the users of these systems are often considered too late, and any potential corrections become costly in terms of rework or insufficient in terms of ergonomics and operator freedom of action. Renjie ZHANG's work demonstrates that virtual reality is an effective method for evaluating a workstation design regarding human factors [2]. Other works underlined as well that VR can be used for more conceptual immersion [1] [5]. The primary objective of this thesis is to integrate the use of virtual reality earlier in the design phase of a manufacturing system (or workstation) during the preliminary design stage, similar to product design methodology. Instead of modelling

a highly detailed and accurate representation of the workstation for immersive exploration, the goal is to utilize a set of simple primitives that the designer can strategically place spatially and temporally, to assess their suitability considering the task to be performed (and the actions involved) and human factors [4]. As soon as validated, this draft and light version of the system can then be developed and detailed, based on a set of areas.

Required background of the student:
Virtual Reality user and/or designer; Python programming; Product Design

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

1. [1] Haobo Wang, Frédéric Noël, Romain Pinquié. Exploring the Potential of Virtual Reality for Model-Based Systems Architecting. AFIS Congrès National 2025, Jan 2025, Paris, France. https://hal.science/hal-05192592v1

2. [2] Zhang, R., Petronijevic, J., Etienne, A. et al. Experiments design methodology for comparison of operators' behavior in immersive and real manufacturing environments and application to productivity. Int J Adv Manuf Technol 140, 1053–1071 (2025). https://doi.org/10.1007/s00170-025-16345-6

3. [3] Aurich, J. C., D. Ostermayer, and C. H. Wagenknecht. 2009. "Improvement of Manufacturing Processes with Virtual Reality-Based CIP Workshops." International Journal of Production Research 47 (19). doi:10.1080/00207540701816569.

4. [4] Vijayakumar, Vivek, Fabio Sgarbossa, W. Patrick Neumann, and Ahmad Sobhani. 2022. "Framework for Incorporating Human Factors into Production and Logistics Systems." International Journal of Production Research 60 (2). doi:10.1080/00207543.2021.1983225.

5. [5] Nguyen, Huyen, Charles Pontonnier, Simon Hilt, Thierry Duval, and Georges Dumont. 2017. "VR-Based Operating Modes and Metaphors for Collaborative Ergonomic Design of Industrial Workstations." Journal on Multimodal User Interfaces 11 (1). doi:10.1007/s12193-016-0231-x.

ParisTech

TITLE: MULTICOMPONENT TRANSFORMATIONS INVOLVING ACETYLENIC COMPOUNDS MEDIATED BY TRANSITION METAL COMPLEXES

Topic number : ***2025_027***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Organic synthesis, catalysis, transition metals

ParisTech School: Chimie ParisTech - PSL
Research team : Catalysis, Synthesis of Biomolecules and Sustainable Development Team (CSB2D)
Research team website: https://iclehs.fr/research/csb2d/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr

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Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Multicomponent reactions are pivotal transformations in organic chemistry since they allow the introduction of a large structural diversity in one-pot conditions. Our team has a long-standing expertise in the development of transition-metal-catalyzed [2+2+2] cycloadditions, which enables the construction of (hetero)aromatic cores using a variety of alkynes, diynes, nitriles or cyanamides promoted by the use of Ru, Pd or Cu catalysts. For example, in a past collaboration with GlaxoSmithKline (UK), we have started a broadly-based program dedicated to metal-catalyzed [2+2+2] cycloadditions of α,ω-diynes with different electrophiles. In a green chemistry context, the development of sustainable and low-cost catalysts of earth-abundant metals, able to promote such transformations is also particularly appealing and will be the aim of this research project. Using this library of new complexes, the

PhD student will then develop suitable cycloaddition conditions of transition metal-mediated processes leading to the obtention of nitrogen, oxygen and boron-containing heterocycles that are valuable building blocks of medicinal interest.

Required background of the student:
The applicant should have strong knowledge in both organic and organometallic synthetic chemistry. A good level in analytical techniques is required (NMR). A very good level in English is mandatory, both spoken and written. The candidate should have a Master's degree in molecular chemistry with a good experience in organic synthesis including working under inert atmosphere.

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

1. Parisot, W.; Haddad, M.; Phansavath, P.; Ratovelomanana-Vidal, V.; Lefèvre, G. Chem. Eur. J. 2025, 31, e202404574.

2. Parisot, W.; Haddad, M.; Phansavath, P.; Lefèvre, G.; Ratovelomanana-Vidal, V. Chem. Eur. J. 2024, 30, chem.202400096.

3. Parisot, W.; Huvelle, S.; Haddad, M.; Lefèvre, G.; Phansavath, P.; Ratovelomanana-Vidal, V. Org. Chem. Front. 2023, 10, 1309.

4. Robin, M., Bakas, N., Clisson, A., Chamoreau, L.-M., Haddad, M., Ratovelomanana-Vidal, V., Neidig, M. L., Lefèvre, G. ACS Catal. 2023, 13, 4882.

5. Huvelle, S.; Matton, P.; Tran, C.; Rager, M.-N.; Haddad, M.; Ratovelomanana-Vidal, V. Org. Lett. 2022, 24, 5126.

ParisTech

TITLE: ASYMMETRIC CATALYSIS TOWARD BIORELEVANT ARCHITECTURALLY NOVEL NATURAL AND UNNATURAL PRODUCTS

Topic number : ***2025_028***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Organic Chemistry, Catalysis, Synthesis of bioactive molecules

ParisTech School: Chimie ParisTech - PSL
Research team : Catalysis, Synthesis of Biomolecules and Sustainable Development (CSB2D Team)
Research team website: https://iclehs.fr/research/csb2d/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://www.chimieparistech.psl.eu/

Contact point for this topic: PHANSAVATH Phannarath

Advisor 1: Phannarath PHANSAVATH - phannarath.phansavath@chimieparistech.psl.eu
Advisor 2: Virginie VIDAL - virginie.vidal@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

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 transfer hydrogenation reactions (ATH) through dynamic kinetic resolution (DKR) to target scaffolds of biorelevant molecules of medicinal interest. The PhD research program aims at developing new catalytic asymmetric

approaches to address longstanding problems in the synthesis of chiral key intermediates to access natural products and pharmaceutical drugs.

Required background of the student:
The applicant should have strong knowledge in both organic and organometallic synthetic chemistry. A good level in analytical techniques is required (NMR). A very good level in English is mandatory, both spoken and written. The candidate should have a Master's degree in molecular chemistry with a good experience in organic synthesis including working under inert atmosphere.

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

1. M. Kosiuha, A. Karapetyan, O. Charron, C. Meyer, P. Phansavath, V. Ratovelomanana-Vidal. Synthesis 2025, 57, 2909.

2. L. Bacheley, R. Ravindra, G. Guillamot, P. Phansavath, V. Ratovelomanana-Vidal. Adv. Synth. Catal. 2024, 366, 1019.

3. L. Bacheley, R. Molina Betancourt, R. Ravindra, G. Guillamot, P. Phansavath, V. Ratovelomanana-Vidal Eur. J. Org. Chem. 2023, 26, e202300383 (VIP).

4. R. Molina-Betancourt, L. Bacheley, A. Karapetyan, G. Guillamot, P. Phansavath, V. Ratovelomanana-Vidal, ChemCatChem 2022, 14, e202200595.

5. “Asymmetric Hydrogenation and Transfer Hydrogenation”, Wiley-VCH Verlag GmbH, Weinheim, Germany, P. Phansavath, V. Ratovelomanana-Vidal, Eds, p 1-384, 2021.

ParisTech

TITLE: IRON-CATALYZED SYNTHESIS OF GROUP XIV HETEROCYCLES

Topic number : ***2025_029***

Field : Chemistry, Physical chemistry and Chemical Engineering

Subfield: Organometallic chemistry

ParisTech School: Chimie ParisTech - PSL
Research team : CSB2D - Catalysis, Synthesis of Biomolecules and Sustainable Development
Research team website: https://iclehs.fr/research/csb2d/
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr/

Contact point for this topic: guillaume.lefevre@chimieparistech.psl.eu

Advisor 1: Guillaume LEFEVRE - guillaume.lefevre@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Heterocycles containing an element from group XIV (E = Si, Ge) are of high interest in various fields of chemistry, including agrochemistry, non-usual material synthesis, but also in the pharmaceutical domain, as those compounds can be considered as heavier drug analogues of carbon-containing active scaffolds. Consequently, the development of general and efficient methods to access these frameworks has focused a considerable attention from synthetic chemists. In this project, we will use some recent redox-active iron complexes developed in the Host Team and successfully applied in alkyne hydroelementation reactions (see references below) to access those scaffolds. Mechanistic aspects of those transformations will also be investigated by operando techniques (paramagnetic NMR monitoring, Mössbauer or EPR spectroscopy – no background is requested from the candidate regarding those techniques).

Required background of the student:
A strong background in organic chemistry and organometallic synthesis is required, as well as a high proficiency in English (written and oral).

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

1. Djebbar, F.; Chamoreau, L.-M.; Lefèvre, G. JACS Au 2025, 5, 2135-2147

2. G.-Simonian, N.; Féo, M.; Tanguy, C.; Troufflard, C.; Lefèvre, G. ACS Catal. 2024, 14, 12163-12172

3. Parisot, W.; Haddad, M.; Phansavath, P.; Lefèvre, G.; Ratovelomanana-Vidal, V. Chem. Eur. J. 2024, 30, chem.202400096

4. Wowk, V.; Bauer, A. K.; Radovic, A.; Chamoreau, L.-M.; Neidig, M. L.; Lefèvre, G. JACS Au 2024, 4, 2, 512-524

5. Féo, M.; Bakas, N. J.; Radovic, A.; Parisot, W.; Clisson, A.; Chamoreau, L.-M.; Haddad, M.; Ratovelomanana-Vidal, V.; Neidig, M. L.; Lefèvre, G. ACS Catal. 2023, 13, 4882–4893

ParisTech

TITLE: PEROVSKITE SOLAR CELLS BASED ON SELF-ASSEMBLED BURIED HOLE SELECTIVE CONTACT

Topic number : ***2025_030***

Field : Chemistry, Physical chemistry and Chemical Engineering - Energy, Processes - Physics, Optics

Subfield: Perovskite solar cells

ParisTech School: Chimie ParisTech - PSL
Research team : MPOE
Research team website:
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/en/chemistry-research-institute-of-paris/

Contact point for this topic: Thierry Pauporté E-mail: thierry.pauporte@chimieparistech.psl.eu

Advisor 1: Thierry Pauporté - thierry.pauporte@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Emerging photovoltaic technologies, particularly perovskite solar cells (PSCs), show great promise for efficiently delivering abundant and low-cost energy. However, emerging solar cells (composed of both organic and inorganic compounds and integrating multiple layers and materials) remain complex, time-consuming to fabricate, and difficult to optimize. For advanced solar cells to be widely deployed, it is essential to (i) simplify their fabrication processes and (ii) to develop dedicated tools and protocols that combine synthesis, device preparation, performance tests and aging tests to enable the rapid optimization of both active layers and their interfaces. The project is specifically designed to tackle these two key challenges in the case of PSCs. It will evolve "hole transport layer-free" (electron transport layer on the top), efficient, stable and

reproducible PSCs using additives in the perovskite precursors molecules able to produce a buried self-assembled monolayers (SAMs). The project targets to: (i) develop a fundamental understanding of the effect and behavior of SAM molecules in the perovskite layers and devices and comprehend the self-formation of buried selective contact; (ii) identify the molecular properties required for SAM molecules to be efficient; and (iii) develop treatments of the layers to improve their quality and their performances in solar cells.

Required background of the student:
Material science; Chemistry; Physics of semiconductors; Photovoltaics; Material characterization techniques (SEM, XRD, UV-Vis absorption…).

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

1. M. Cresp, M. Liu, M.-N. Rager, Th. Pauporté, 2D Ruddlesden-Popper versus 2D Dion-Jacobson Perovskites: Of the Importance of Determining the "True" Average n-Value of Annealed Layers. Adv. Funct. Mater., 15 (2025) 2413671. https://doi.org/10.1002/adfm.202413671

2. S. Yuan, D. Zheng, T. Zhang, Y. Wang, F. Qian, L. Wang, X. Li, H. Zheng, Z. Diao, P. Zhang, Th. Pauporté, S. Li, Scalable preparation of perovskite films with homogeneous structure via immobilizing strategy for high-performance solar modules. Nature Commun. 16 (2025) 2052. https://doi.org/10.1038/s41467-025-57303-w

3. Z. Li, M. Cresp, K. Vegso, P. Siffalovic, N. Mrkyvkova, Th. Pauporté, Quasi-2D Ruddlesden-Popper phase induced vertically oriented FA1-xMAxPbI3 for high-performance sequential perovskite solar cell. Chem. Eng. J., 505 (2025) 159121. https://doi.org/10.1016/j.cej.2024.159121

4. B. Zhang, H. Zeng, H. Yin, D. Zheng, Z. Wan, C. Jia, T. Stuyver, J. Luo, Th. Pauporté, Combining Machine Learning, Component Screening and Molecular Engineering for the Design of High-Performance and Stable Inverted Perovskite Solar Cells. Energy Environ. Sci., 17 (2024) 5532 – 5541. https://doi.org/10.1039/d4ee00635f

5. D. Zheng, F. Raffin, P. Volovitch, Th. Pauporté, Control of perovskite film crystallization and growth direction to target homogeneous monolithic structures. Nature Commun., 13 (2022) 6655. https://doi.org/10.1038/s41467-022-34332-3

ParisTech

TITLE: DESIGN OF A NEW COUNTER-ROTATING AXIAL TURBINE TO BE COUPLED WITH A PUMP AS TURBINE

Topic number : ***2025_031***

Field : Energy, Processes - Material science, Mechanics and Fluids

Subfield: turbomachinery, fluid mechanics, energy harvesting

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website: https://lifse.artsetmetiers.fr

Contact point for this topic: Capurso Tommaso
tommaso.capurso@ensam.eu

Advisor 1: Florent Ravelet - florent.ravelet@ensam.eu
Advisor 2: Tommaso Capurso - tommaso.capurso@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Hydraulic energy demonstrates to be one of the trustworthy solution to fight climate change. In the past, pumps as turbines (PaT) have been used in industry as a cheap solution to convert hydraulic energy in mechanical and electrical energy. Recently, they have found place in pumped storage systems and in water distribution networks to recover energy from pressurized flows in place of pressure reducing valves. However, since these machines are designed as pumps, when they are used as turbines, their BEP is shifted towards higher values of flow rate. This means that at the exit of the runner, there is a flow characterized by a tangential component (swirling flow). Namely, there is still energy that can be recovered. The idea is to design an axial turbomachinery, which rotates on the opposite direction of the first impeller with the aim to recover energy still present in the fluid guaranteeing an absolute tangential

velocity of the flow equal to zero. Numerical simulations will be performed to study the 3D flows exiting from the runner. This input will be used to design the axial turbine blades. The shape of the joined turbine draft tube will be designed to maximize the matching between the 2 turbines. The resulting configuration will allow to maximize the exploitation of hydraulic energy. Finally, the new turbomachinery will be tested to assess its performance.

Required background of the student:
Fluid dynamics, Turbomachinery, Computational fluid dynamics, good English communication skills

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

1. Capurso, T., Bergamini, L., Torresi, M. (2019). Design and CFD performance analysis of a novel impeller for double suction centrifugal pumps. Journal of Nuclear Engineering and Design. Vol. 341 Pages 155-166 Elsevier. https://doi.org/ 10.1016/j.nucengdes.2018.11.002.

2. Capurso, T., Stefanizzi, M., Pascazio, G., Ranaldo, S., Camporeale, S.M., Fortunato, B., Torresi, M. (2019). CFD analysis of the slip factor at the outlet of centripetal turbomachineries. Water. 11(3), 565. MDPI. https://doi.org/10.3390/w11030565

3. Martin Bourhis, Michaël Pereira, Florent Ravelet, Ivan Dobrev. Experimental Thermal and Fluid Science, 2022, 130, pp.110504. ⟨10.1016/j.expthermflusci.2021.110504⟩

4. Florent Ravelet, F. Bakir, C. Sarraf, J. Wang. Experimental Thermal and Fluid Science, 2018, 96, pp.101. 10.1016/j.expthermflusci.2018.03.004

5. Dehnavi, E., Danlos, A., Solis, M., Kebdani, M., Bakir, F. Study on the pump cavitation characteristic through novel independent rotation of inducer and centrifugal impeller in co-rotation and counter-rotation modes. Physics of Fluids, 2024, DOI 10.1063/5.0182731

ParisTech

TITLE: NUMERICAL AND EXPERIMENTAL ANALYSIS OF INSTABILITIES DOWNSTREAM OF UNDER-EXPANDED JETS

Topic number : ***2025_032***

Field : Energy, Processes - Material science, Mechanics and Fluids

Subfield: fluid mechanics, instability IKH

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website: https://lifse.artsetmetiers.fr

Contact point for this topic: Capurso Tommaso
tommaso.capurso@ensam.eu

Advisor 1: Michael Deligant - michael.deligant@ensam.eu
Advisor 2: Florent Ravelet - florent.ravelet@ensam.eu
Advisor 3: Tommaso Capurso - tommaso.capurso@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
In the field of fluid mechanics, under-expanded jets are still a challenge for the contemporary presence of high speed flow and pressure waves dynamics. The near-field of the jet development can be modeled by a potential flow, whereas in the far field, is subject to interaction between shear layers and turbulence transport and mixing. The project will be divided in two parts a numerical and an experimental one. In the first part, a high order, multi-species, density-based solver will be developed on the OpenFOAM framework to run Large Eddy Simulations. Different nozzle section shapes will be studied (rectangular, elliptic, triangular, star, etc.). The interaction of the jet with the near and the far-field will be investigated. Furthermore, the interaction between close jets will be carried out (Coanda effect). The nature and the development of instabilities like the Kelvin–Helmholtz will be analyzed and further

understandings on the interaction between turbulence and instability will be proposed. A test bench will be developed and equipped with a Background Oriented Schlieren (BOS) image process. An experimental campaign of gases with different molecular diffusion and weight will be performed . Finally, the impact of the Lewis number and the Soret effect on the instabilities and turbulent mixing will be investigated.

Required background of the student:
Fluid dynamics, Computational fluid dynamics, Numerical methods, good English communication skills

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

1. Anaclerio, G., Capurso, T., Torresi, M., (2023) Gas-dynamic and mixing analysis of under-expanded hydrogen jets: effect of the cross section shape. Journal of Fluid Mechanics
DOI:https://doi.org/10.1017/jfm.2023.603

2. Anaclerio, G., Torresi, M., Capurso, T. Direct injection strategies for H2 internal combustion engines under ultra-lean conditions: a numerical analysis. International Journal of Hydrogen Energy DOI: https://doi.org/10.1016/j.ijhydene.2025.04.224

3. Anaclerio, G., Capurso, T., Torresi, M., Camporeale, S.M., (2023). Numerical characterization of hydrogen under-expanded jets with a focus on Internal Combustion Engines applications. International Journal fo Engine Research

4. Anaclerio, G., Capurso, T., Torresi, M., Camporeale, S.M., (2022) Numerical characterization of hydrogen under-expanded jets: influence of the nozzle cross-section shape, IOP Publishing

5. Koulekpa, K.S. , Deligant, M., Elias-Birembaux, H., Rossi, F., Poulachon, G., Model for temperature evolution in CO2 jets by background oriented schlieren method for applications in cryogenic-assisted machining, CIRP AnnalsOpen source preview, 2025, 74(1), pp. 133–137

ParisTech

TITLE: DEVELOPMENT OF A NUMERICAL SOLVER FOR THE SIMULATION OF COMPRESSIBLE, MULTI-SPECIES, REACTING FLOWS (DNS, LES)

Topic number : ***2025_033***

Field : Energy, Processes - Material science, Mechanics and Fluids - Environment Science and Technology, Sustainable Development, Geosciences

Subfield: Numerical methods, Fluid dynamics, Computational fluid dynamics, good English communication skills

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website: https://lifse.artsetmetiers.fr

Contact point for this topic: Capurso Tommaso
tommaso.capurso@ensam.eu

Advisor 1: Sofiane Khelladi - sofiane.khelladi@ensam.eu
Advisor 2: Tommaso Capurso - tommaso.capurso@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Turbulent combustion is still a challenge due to the complex interaction between kinetics and turbulence at small scales. Nonetheless, new technologies open to new combustion processes and issues, for instance, venting gas and their reaction in a extremely hot environment, e.g., battery fire after thermal runaways, gas tank leakages etc. Thus, in this project, a new compressible solver will be developed on the OpenFOAM environment to perform both DNS and LES simulations of reacting flows (diffusive, partially-premixed and premixed flames). Specifically, less diffusive schemes than them already available will be implemented. Moreover, this implementation will account for high order schemes and

to solve flows with discontinuities at the same time. The solver will take into account Soret effect and an appropriate species diffusion modeling. Thermodiffusive instabilities, flame front wrinkling, its interaction with obstacles and emissions will be investigated. In a second phase, a Dynamically Thickened Flame LES Model for Premixed and Non-Premixed Turbulent Combustion will be implemented. Validation on flames available in the literature will be carried out.

Required background of the student:
Numerical methods, Fluid dynamics, Computational fluid dynamics, good English communication skills

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

1. Capurso, T., Laera, D., Riber, E., Cuenot, B., (2023). NOx pathways in lean partially premixed swirling H2-air turbulent flame. Combustion and Flame https://doi.org/10.1016/j.combustflame.2022.11258

2. Deligant, M., Romero-Casado, C.-J., Nogueira, X., Bakir, F., Khelladi, S. Very high order finite volume solver for multi component two-phase flow with phase change using a posteriori Multi-dimensional Optimal Order Detection Computers and Fluids, 2025, 288, 106509

3. Nogueira, X., Ramos, L., Seijo, S., Khelladi, S., Ramírez, L. Data-driven Riemann solvers: A neural network approach and a hybrid solver, Physics of Fluids, 2025, 37(9), 096142

4. Anaclerio, G., Capurso, T., Torresi, M., Camporeale, S.M., (2023) Influence of the Injection Timing on the Mixture Formation Process in a Spark-Ignition Hydrogen Fuelled ICE, SAE 16th International Conference on Engines & Vehicles, DOI: https://doi.org/10.4271/2023-24-0079

5. Stefanizzi, M., Capurso, T., Torresi, M., Pascazio, G. (2021). Recent combustion strategies in gas turbines for propulsion and power generation toward a zero-emissions future: Fuels, burners, and combustion techniques. Energies. https://doi.org/10.3390/en14206694

ParisTech

TITLE: DEVELOPMENT OF A TWO-PHASE FLOW SOLVER FOR FLUIDS IN META-STABLE THERMODYNAMIC CONDITIONS

Topic number : ***2025_034***

Field : Energy, Processes - Material science, Mechanics and Fluids

Subfield: fluid mechanics, fluid machinery

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website: https://lifse.artsetmetiers.fr

Contact point for this topic: Capurso Tommaso
tommaso.capurso@ensam.eu

Advisor 1: Sofiane Khelladi - sofiane.khelladi@ensam.eu
Advisor 2: Florent Ravelet - florent.ravelet@ensam.eu
Advisor 3: Tommaso Capurso - tommaso.capurso@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Numerical simulations of two-phase flows are still a challenge. In the future, more applications will be subject to two-phase flows. For instance, fluids encountring large temperature gradients (boil-off, heat exchanger, etc.). A new solver will be developed in the OpenFOAM framework. Phase-change due to temperature rise (boiling) and pressure reduction (cavitation) will be taken into account. The thermodynaimic metastablility (discrepancies between pressure and temperature in vapor cavities) of thermo-sensitive fluids will be included. Moreover, the new solver will be developed with the aim to also perform numerical simulations of the two-phase flows subject to momentum exchange. Once the code assessed on venturi or ogive 3D obstacles, a new impeller geometry of a high speed turbomachinery will be developed with the aim to not suffer the presence of incoming two-phase flows and the development of cavitation (low

suction pressure). Impact of the void ratio on the dynamic of the bubbles on the machine will be performed. Evolution of the vapor pockets from bubble to agglomerates will be investigated. Numerical simulations will be validated with experiments carried out on the hydraulic test rig with a thermo-sensitive fluid.

Required background of the student:
Numerical methods, Fluid dynamics, Turbomachinery, Computational fluid dynamics, good English communication skills

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

1. Ait-Ali, T., Khelladi, S., Bakir, F.,Nogueira, X., Ramírez, L., A Diffuse Interface Model for Cavitation, Taking Into Account Capillary Forces, International Journal for Numerical Methods in Fluids, 2025, 97(3), pp. 395–408 DOI: 10.1002/fld.5350

2. Deligant, M., Romero-Casado, C.-J., Nogueira, X., Bakir, F., Khelladi, S. Very high order finite volume solver for multi component two-phase flow with phase change using a posteriori Multi-dimensional Optimal Order Detection Computers and Fluids, 2025, 288, 106509 DOI: 10.1016/j.compfluid.2024.106509

3. Capurso, T., Lorusso, M., Camporeale, S.M., Fortunato, B., Torresi, M. (2019) Implementation of a passive control system for limiting cavitation around hydrofoils. IOP Conf. Ser.: Earth Environ. Sci. 240 032025. https://doi.org/10.1088/1755-1315/240/3/032025.

4. Gentis, V., Pereira, M., Ravelet, F., ... Pora, L., Brun, G., Experimental Comparison of Hydrodynamic Behavior Under Partial Flowrates and Cavitation in Three Configurations of a Centrifugal Pump With Inducer and Impeller, Journal of Fluids EngineeringOpen source preview, 2025, 147(9), 091204 DOI: 10.1115/1.4068132

ParisTech

TITLE: INNOVATIVE AND SUSTAINABLE OSMOTIC PROCESSES

Topic number : ***2025_035***

Field : Chemistry, Physical chemistry and Chemical Engineering - Environment Science and Technology, Sustainable Development, Geosciences - Energy, Processes

Subfield: water treatment

ParisTech School: ESPCI Paris - PSL
Research team : MIE CBI
Research team website: https://www.mie.espci.fr/spip.php?rubrique2
Research lab: CBI - Chimie, Biologie et Innovation
Lab location: Paris
Lab website: https://www.cbi.espci.fr/accueil-22/

Contact point for this topic: annie.colin@espci.fr

Advisor 1: Annie COLIN - annie.colin@espci.fr
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Osmotic pumping systems use rectified flow to drive liquids through membranes without high mechanical pressure, offering a promising low-energy alternative for fluid transport. Yet, the physico-chemical mechanisms behind osmotic transport, molecular selectivity, and energy conversion remain only partly understood. This project develops a rigorous theoretical and mechanistic framework for osmotic pumping in nanoporous membranes, identifying the key parameters that control and optimize performance. Combining interfacial physico-chemistry, non-equilibrium thermodynamics, and membrane transport theory, it will model water and solute fluxes across a range of nanoporous materials—from biomimetic structures to functionalized polymer and hybrid membranes. The project will also establish an experimental platform to validate models and guide future studies. Ultimately, this work will advance fundamental understanding of osmotic processes and provide

predictive tools for designing efficient, low-energy membrane technologies.

Required background of the student:
physics flow mechanics, a taste for experimentation

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

1. Wu, N., Levant, M., Brahmi, Y., Tregouet, C., & Colin, A. (2024). Mitigating the influence of multivalent ions on power density performance in a single-membrane capacitive reverse electrodialysis cell. Scientific Reports, 14(1), 16984.

2. Xu, Z., Wu, N., Abdelghani-Idrissi, S., Trégouët, C., Perez-Carvajal, J., Colin, A., ... & Siria, A. (2025). Advanced Nanoscale Functionalities for Water and Energy Technologies. Advanced Physics Research, 2400195.

3. Wu, N., Derkenne, T., Tregouet, C., & Colin, A. (2023). Comparison of miniaturized mechanical and osmotic energy harvesting systems. Nano Energy, 118, 109004.

4. Derkenne, T., Colin, A., & Tregouet, C. (2024). Macroscopic Access Resistances Hinders the Measurement of Ion-Exchange-Membrane Performances for Electrodialysis Processes. ACS Applied Energy Materials, 7(15), 6621-6629.

5. Wu, N., Brahmi, Y., & Colin, A. (2023). A strategy for power density amelioration of capacitive reverse electrodialysis systems with a single membrane. Environmental Science & Technology, 57(40), 14973-14982.

ParisTech

TITLE: DURABILITY AND DEGRADATION MECHANISMS OF STRUCTURAL METALLIC IMPLANTS WITH AI INTEGRATION

Topic number : ***2025_036***

Field : Life and Health Science and Technology - Information and Communication Science and Technology

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team :
Research team website:
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/en/chemistry-research-institute-of-paris/

Contact point for this topic: Sun-Fan-fan.sun@chimieparistech.psl.eu

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Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Metallic implants such as cardiovascular stents, orthopedic and neurovascular devices operate under extreme mechanical, chemical, and electrochemical conditions inside the human body. Their long-term durability, surface stability, corrosion behavior, and damage mechanisms directly control implant safety and clinical performance. Despite major advances in metallic biomaterials, the coupled effects of mechanical loading, corrosion, surface coating, and biological environment remain insufficiently understood under realistic conditions. This PhD project is part of the ANR APEX-STENT national research program, dedicated to next-generation implantable devices and AI for health. The work will focus on: • Degradation and durability mechanisms of metallic implants in physiological environments • Surface and material evolution during service • Structure–surface–property relationships under combined

mechanical and electrochemical conditions • Integration of experimental data for AI-assisted health databases

Required background of the student:
Metallic Material science, Surface science, AI-related engineering

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

1. Recent advances in Fe-based bioresorbable stents: Materials design and biosafety
Y Zhang, C Roux, A Rouchaud, A Meddahi-Pellé, V Gueguen, ...
Bioactive Materials 31, 333-354

2. Mechanisms underlying enhanced strength-ductility combinations in TRIP/TWIP Ti-12Mo alloy engineered via isothermal omega precipitation
B Qian, SA Mantri, S Dasari, J Zhang, L Lilensten, F Sun, P Vermaut, ...
Acta Materialia 245, 118619

3. Superior high-temperature mechanical properties and microstructural features of LPBF-printed In625-based metal matrix composites
E Tekoglu, JS Bae, HA Kim, KH Lim, J Liu, TD Doležal, SY Kim, MA Alrizqi, ...
Materials Today 80, 297-307

4. New insights into the corrosion of orthopedic Ti-6Al-4V under cathodic polarization
A Sotniczuk, B Dou, C Xie, J Tang, D Kalita, W Chromiński, H Garbacz, ...
Corrosion Science 238, 112354

5. Strong and ductile beta Ti–18Zr–13Mo alloy with multimodal twinning
FP JY Zhang, F SUN, Z Chen, Y Yang, BL Shen, J Li
Materials Research Letters 7 (6)

ParisTech

TITLE: AUTOMATIC GUIDED CAD ASSEMBLY GENERATION WITH MECHANICAL CONSTRAINTS USING DEEP LEARNING

Topic number : ***2025_037***

Field : Design, Industrialization - Mathematics and their applications

Subfield: Geometric modeling

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LISPEN - Laboratoire d'ingénierie des systèmes physiques et numériques
Lab location: Aix-en-Provence
Lab website: https://lispen.artsetmetiers.fr/

Contact point for this topic: Pernot - Jean-Philippe - Jean-Philippe.Pernot@ensam.eu

Advisor 1: Jean-Philippe Pernot - Jean-Philippe.Pernot@ensam.eu
Advisor 2: Arnaud Polette - arnaud.polette@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
The aim of this thesis is to implement methods for generating complex mechanical assemblies using existing databases of mechanical parts. The goal is to generate assemblies by controlling the level of coherence of the assembly according to the need (functionality, imposed interfaces, types of parts, etc.), while guiding the generation using functions to maximise certain objectives (encompassing shape, aesthetics, type of assembly, etc.). The idea would be to use databases of existing assemblies whose types and interfaces between parts are known, in order to learn the assembly logic according to the type of part and the consistency of functionality between the different geometries. Several solutions can be explored, such as reinforcement learning, in order to build an agent that can iteratively build these assemblies part by part. A second solution to explore would be to use auto-encoders and/or graphs (eg. GCN, Graph

Convolutional Network). The first step will be to build a database (as the host laboratory has already carried out work on using this type of database, this part will be greatly facilitated by the existing databases), then to explore the automatic assembly methods, and to validate the operation of these methods on the databases built, by illustrating them with concrete uses in an industrial context.

Required background of the student:
Computer Science, Machine Learning, CAD assembly

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

1. Lucas Vergez, Arnaud Polette, Jean-Philippe Pernot. Automatic CAD Assemblies Generation by Linkage Graph Overlay for Machine Learning Applications. Computer-Aided Design and Applications, 2022, https://doi.org/10.14733/cadaps.2022.722-732 19(4), pp. 722–732

2. Lucas Vergez, Arnaud Polette, Jean-Philippe Pernot. Interface-Based Search and Automatic Reassembly of CAD Models for Database Expansion and Model Reuse, Computer Aided Design, 2023 (online publication), Volume 167, 103630 https://doi.org/10.1016/j.cad.2023.103630

3. Lucas Vergez, Arnaud Polette, Jean-Philippe Pernot. Multi-part kinematic constraint prediction for automatic generation of CAD model assemblies using graph convolutional networks. Computer-Aided Design, Volume 178, 2025, 103805, ISSN 0010-4485, https://doi.org/10.1016/j.cad.2024.103805.

ParisTech

TITLE: TUNING NANOCRYSTAL LUMINESCENCE WITH VO2 AND PEROVSKITE BASED NANOSTRUCTURED DEVICES

Topic number : ***2025_038***

Field : Physics, Optics - Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: ESPCI Paris - PSL
Research team : MNC group
Research team website: https://mnc.lpem.espci.fr/spip.php?rubrique8
Research lab: LPEM - Laboratoire Physique et d'études des matériaux
Lab location: Paris
Lab website: https://www.lpem.espci.fr/spip.php?rubrique4

Contact point for this topic: Aigouy-Lionel-lionel.aigouy@espci.fr

Advisor 1: Lionel Aigouy - lionel.aigouy@espci.fr
Advisor 2: Zhuoying Chen - zhuoying.chen@espci.fr
Advisor 3: Alexandre Zimmers - alexandre.zimmers@espci.fr
Advisor 4:

Short description of possible research topics for a PhD:
The control of nanocrystal luminescence emission is of interest both from a fundamental point of view and for various applications such as bio-imaging, light-emitting devices, nanoscale sensing, and quantum photonics. One approach to enhance or suppress luminescence consists in placing the nanocrystal in the vicinity of a nanostructure and monitoring the resulting emission changes. This can be achieved either by scanning a single nanocrystal across a nanostructured surface using an atomic force microscope tip, or by depositing multiple nanocrystals directly onto the nanostructures. The objective of this project is to modulate the optical response by inducing a phase transition in the material that hosts the nanostructures. For example, materials such as VO_2 or certain perovskites exhibit pronounced refractive-index variations at relatively low transition temperatures, which can drastically tune the luminescence emission of nearby nanocrystals. The project will involve exploring these

effects experimentally, through the fabrication and characterization of the structures, and numerically in collaboration with a partner group specialized in electromagnetic simulations.

Required background of the student:
The applicant should have a background in physics. He/she should be interested in learning and performing experiments in optics, materials fabrication, synthesis, characterization.

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

1. Mid-infrared optical valve based on VO2.

A. Garcia-Martin, R ; Alvaro, Z. Fang, A. Zimmers, Z. Chen, L. Aigouy.

Phys. Rev. Research 7, 023301 (2025).

2. Direct imaging of fluorescence enhancement in the gap between two gold nanodisks.

H.-J. Lin, H. Xiang, C. Xin, Z. Hu, L. Billot, P. Gredin, M. Mortier, Z. Chen, M.-U. González, A. García-Martín, L. Aigouy.

Applied Physics Letters 118, 161105 (2021)

3. Plasmon-enhanced photothermal sensing through coupled VO_2/Au nanodisks

Z. Fang, A. Zimmers, Z. Chen, L. Billot, A. García-Martín, L. Aigouy.

Surfaces and Interfaces 62, 106145 (2025)

4. Luminescence enhancement effects on nanostructured perovskite thin films for Er/Yb-doped solar cells.

Z. Hu, M.-U. Gonzalez, Z. Chen, P. Gredin, M. Mortier, A. Garcia-Martin, L. Aigouy.

Nanoscale Advances 4, 1786 (2022)

5. Tuning the Resistance of a VO2 Junction by Focused Laser Beam and Atomic Force Microscopy

Z. Fang, M. Alzate-Banguero, A.R. Rajapurohita, F. Simmons, E.W. Carlson, Z. Chen, L. Aigouy, A. Zimmers

Adv. Electron. Mater. 2025, 11, 2400249

ParisTech

TITLE: UNCERTAINTY-AWARE DIGITAL TWIN OF GREEN MANUFACTURING

Topic number : ***2025_039***

Field : Design, Industrialization - Mathematics and their applications - Information and Communication Science and Technology

Subfield:

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website: https://lcfc.ensam.eu

Contact point for this topic: ZHANG Tian tian.zhang@ensam.eu

Advisor 1: Lazhar HOMRI - lazhar.homri@ensam.eu
Advisor 2: Tian ZHANG - tian.zhang@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Industry 5.0 mandates the integration of sustainability objectives into manufacturing processes, giving rise to the systemic paradigm of green manufacturing. The characteristics of green manufacturing systems include requirements as reducing energy consumption, lowering scrap rates, and enhancing resource utilization, etc.. Incorporating these new criteria into models will inevitably increases the complexity level of model design, simulation, and analysis, thereby elevating uncertainty within production processes. Digital twins, as virtual replicas of the physical world, enable real-time monitoring, model updates, prediction, feedback, and control of production processes, opening new possibilities for exploring advanced control strategies for autonomous systems. Similarly, when using digital twin systems for prediction and decision-making, uncertainty is a critical factor that must be incorporated into the analysis. Failure to do so compromises the accuracy and credibility of the system's predictions. Therefore, the main objective of this research is to address

such uncertainty, specifically epistemic uncertainty, by developing an uncertainty-aware digital twins for green manufacturing systems, which has the capability to provide real-time feedback and production processes control.

Required background of the student:
Mech. Eng. or Ind. Eng. or Applied Math.

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

1. Diallo, A. R., Homri, L., Boeuf, T., Dantan, J. Y., & Bonnet, F. (2025). Quantifying and mitigating alarm fatigue caused by fault detection systems. Reliability Engineering & System Safety, 111890.

2. Diallo, A. R., Homri, L., & Dantan, J. Y. (2025). Reducing false alarms in fault detection: A comparative analysis between conformal prediction and classical methods applied to PCA and autoencoders. Journal of Process Control, 152, 103495.

3. Heddoub, A., Diallo, A. R., Homri, L., Dantan, J. Y., & Siadat, A. (2025). Uncertainty-Aware Fault Diagnosis with Conformal Prediction. IFAC-PapersOnLine, 59(10), 536-541.

4. Ciancio, V., Homri, L., Dantan, J. Y., & Siadat, A. (2024). Development of a flexible data management system, to implement predictive maintenance in the Industry 4.0 context. International Journal of Production Research, 62(6), 2255-2271.

5. Zhang, T., Homri, L., Dantan, J. Y., & Siadat, A. (2023). Models for reliability assessment of reconfigurable manufacturing system regarding configuration orders. Reliability Engineering & System Safety, 231, 109035.

ParisTech

TITLE: PHYSICS-INFORMED GENERATIVE AI FOR ACCURATE MESOSCALE MODELING OF POLYCRYSTALLINE MATERIALS

Topic number : ***2025_040***

Field : Material science, Mechanics and Fluids - Mathematics and their applications

Subfield: Mechanical Engineering

ParisTech School: Arts et Métiers
Research team : Méthodes Numériques, Instabilités et Vibrations (Numerical Methods, Instabilities and Vibrations)
Research team website:
Research lab: LEM3 - Laboratoire d'étude des microstructures et de mécanique des matériaux
Lab location: Metz
Lab website: https://lem3.univ-lorraine.fr

Contact point for this topic: Nguyen - Duc Vinh - duc-vinh.nguyen@ensam.eu

Advisor 1: Duc Vinh Nguyen - duc-vinh.nguyen@ensam.eu
Advisor 2: Mohamed Jebahi - mohamed.jebahi@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Accurate modeling of polycrystalline structures is essential for understanding and predicting the mechanical behavior of materials. Most microstructures used in numerical studies are generated synthetically using purely geometric or stochastic approaches, such as those based on Voronoi tessellations. While these approaches allow for rapid construction of idealized microstructures, they only capture a limited portion of the complexity observed in real materials. Physically-based generators considering, for example, statistical distributions of grain morphology, crystallographic texture (Dream.3D) or fabrication processes (SPPARKS), are able to give more physically credible microstructures. However, these methods still suffer from simplifying assumptions

affecting their ability to capture correlations between geometry and crystallographic texture. In many recent applications, the ability to generate realistic 3D microstructures from surface measurements, especially EBSD (Electron Backscatter Diffraction) maps, becomes highly needed. This is particularly true for mesoscale simulations of miniature samples, which are now widely used, and for which the individual influence of each grain cannot be ignored. In these simulations, reconstructing realistic 3D microstructures from 2D images enables more reliable validation, calibration, and enrichment of mesoscale models, and greatly expands the range of investigations when direct 3D characterization is impractical. In this context, recent advances in generative AI offer a major opportunity. Although application of this new paradigm to microstructure reconstruction remains very recent, several studies have demonstrated its potential to synthesize 3D microstructures from partial information. Nevertheless, existing AI-based tools are still limited to relatively simple grain morphology and do not account for realistic microstructure features such as crystallographic texture or misorientation, making them immature for practical applications. The proposed project aims to further leverage the potential of data-driven microstructure generators by developing an enriched generative framework, augmented by physics-based constraints, for rapid and realistic generation of 3D polycrystalline microstructures from surface observations. Incorporating physical and expert knowledge into the generative process will help to overcome the limitations of existing approaches, improve the mechanical and crystallographic consistency of the synthesized microstructures, and provide robust tools for advanced mesoscale simulations.

Required background of the student:
- Solid background in machine learning and material science
- Good programming skills (preferably in Python)
- Excellent English level

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

1. Nguyen, D.V., Jebahi, M., Chinesta, F. (2025). Wavelet-based enrichment for physics informed neural networks to approximate localized and heterogeneous solutions in solid mechanics. Submitted to Computer Methods in Applied Mechanics and Engineering.

2. Nguyen, D.V., Jebahi, M., Chinesta, F. (2024). Spatio-temporal physics-informed neural networks to solve boundary value problems for classical and gradient-enhanced continua. Mechanics of Materials. 198, 105141.

3. Nguyen, D.V., Jebahi, M., Chinesta, F. (2024). Identification of material parameters in low-data limit: application to gradient-enhanced continua. International Journal of Material Forming. 17, 10.
4. Jebahi M., Forest S. (2023). An alternative way to describe thermodynamically-consistent higher-order dissipation within strain gradient plasticity. Journal of the Mechanics and Physics of Solids, 170, 105103.
5. Cai L., Jebahi M., Abed-Meraim F. (2021). Strain localization modes within single crystals using finite deformation strain gradient crystal plasticity. Crystals, 11, 1235.

ParisTech

TITLE: DESIGN OF SUSTAINABLE RECONFIGURABLE MANUFACTURING SYSTEM THROUGH MODELING AND SIMULATION

Topic number : ***2025_041***

Field : Environment Science and Technology, Sustainable Development, Geosciences - Mathematics and their applications - Information and Communication Science and Technology

Subfield:

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Metz
Lab website: https://lcfc.ensam.eu

Contact point for this topic: ZHANG Tian tian.zhang@ensam.eu

Advisor 1: Lazhar HOMRI - lazhar.homri@ensam.eu
Advisor 2: Tian ZHANG - tian.zhang@ensam.eu
Advisor 3: Jelena PETRONIJEVIC - jelena.petronijevic@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Against a backdrop of increasingly volatile global market demand and growing sustainability requirements, the design of manufacturing systems now requires achieving both rapid responsiveness and reduced environmental impact. Traditional manufacturing systems suffer from poor scalability, inefficient energy utilization, and inadequate waste monitoring—clear limitations that prevent them from balancing economic and environmental dimensions. Sustainable Reconfigurable Manufacturing System (SRMS) offers modularity, scalability, and reconfigurability while accounting for energy consumption and waste. Consequently, integrating reconfigurability with sustainability goals represents a critical research direction aligned with contemporary demands. Despite its potential, SRMS design and operation exhibit greater complexity than traditional Reconfigurable Manufacturing

System (RMS). Academic research has yet to provide a systematic solution for combining or balancing these approaches. This study aims to analyze the SRMS design process using Anylogic-based modeling and simulation. Specific challenges include: 1. Balancing multiple objectives during design, primarily economic viability, sustainability, and operability. These objectives often conflict, making multi-objective optimization or decision-making methods crucial. 2. Analyzing the complexity of reconfigurable combinations. Reconfigurable systems inherently possess higher modeling and analysis complexity than most manufacturing system paradigms. Incorporating sustainability objectives further increases this complexity. Sustainable parameters, such as scrap rates and consumption statistics, must be integrated appropriately while ensuring algorithmic complexity remains within levels achievable for enterprise applications. 3. Dynamic modeling of sustainability metrics. Most sustainability indicators are not static but undergo real-time dynamic changes due to equipment aging, production batch variations, or operational adjustments. Capturing this temporal dynamism represents a critical research focus.

Required background of the student:
Mech. Eng. or Ind. Eng. or Applied Math.

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

1. Zhang, T., Homri, L., Dantan, J. Y., & Siadat, A. (2023). Models for reliability assessment of reconfigurable manufacturing system regarding configuration orders. Reliability Engineering & System Safety, 231, 109035.

2. Khan, A. S., Homri, L., Dantan, J. Y., & Siadat, A. (2022). An analysis of the theoretical and implementation aspects of process planning in a reconfigurable manufacturing system. The International Journal of Advanced Manufacturing Technology, 119(9), 5615-5646.

3. Zhang, T., Homri, L., Dantan, J. Y., & Siadat, A. (2022, December). Proposition of applying markov transfer state in reliability analysis of manufacturing system with different configuration orders. In 2022 IEEE International Conference on Industrial Engineering and Engineering Management (IEEM) (pp. 1583-1587). IEEE.

4. Heddoub, A., Diallo, A. R., Homri, L., Dantan, J. Y., & Siadat, A. (2025). Uncertainty-Aware Fault Diagnosis with Conformal Prediction. IFAC-PapersOnLine, 59(10), 536-541.

5. Zhang, T., Homri, L., Dantan, J. Y., & Siadat, A. (2021, August). Conceptual maps of reliability analysis applied in reconfigurable manufacturing system. In IFIP International Conference on Advances in Production Management Systems (pp. 136-145). Cham: Springer International Publishing.

ParisTech

TITLE: MECHANICS OF RED BLOOD CELLS MODULATED BY NANOPARTICLES

Topic number : ***2025_042***

Field : Physics, Optics - Chemistry, Physical chemistry and Chemical Engineering - Life and Health Science and Technology

Subfield: Biophysics, bioengineering

ParisTech School: Chimie ParisTech - PSL
Research team :
Research team website:
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/en/research-groups/2pm-group/

Contact point for this topic: Feng-Ching Tsai (in Physics of Cells and Cancer (UMR168), Institut Curie), feng-ching.tsai@curie.fr

Advisor 1: Min-Hui Li - min-hui.li@chimieparistech.psl.eu
Advisor 2: Feng-Ching Tsai - feng-ching.tsai@curie.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Plastic pollution has become one of the most pressing environmental challenges of our time, with millions of tons of waste entering the ecosystems annually. In the environment, plastics fragment into micro- and nano-sized particles that seriously threaten to both the environmental and human health. These plastic particles have been detected in water, food, and air. Recent studies show that nano- and microplastics can cross biological barrier and enter bloodstream. Notably, it has been shown that plastic particles can interact with red blood cells directly by adhering on the cell membranes, which causes morphological changes of the cells and impairing their physiological functions. Yet, the precise effects of plastic particles on the biophysical properties of the cell membranes remains poorly understood. Common plastics such as polystyrene (PS), polyethylene (PE), polypropylene (PP) and polyvinyl chloride (PVC) can

associate strongly with lipid bilayers. Molecular simulations predicted that these plastic particles alter membrane mechanical properties that are fundamental to maintain normal cell function. However, comprehensive experimental validation of these membrane-level effect is largely lacking. This project aims to develop a robust experimental framework to quantitatively assess nano-plastic-induced alternations in membrane mechanics using synthetic vesicles, RBC-derived vesicles, and intact RBCs. We will use lab synthesized plastic particles as well as environmentally obtained particles. We will perform quantitative characterization of membrane mechanics using micropipette aspiration and microfluidic devices to reveal changes in membrane elasticity, stability and overall mechanical behavior. By integrating results across model and biological systems, we anticipate our work to contribute to the mechanistic understanding of how plastic particles impact cellular functions.

Required background of the student:
The ideal applicant should have a sound foundation in biophysics and demonstrated experience working with microfluidic devices. He/She must be fluent in English, as it is the working language of the laboratory. Additional experience in biotechnology or polymer chemistry would be considered a strong asset.

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

1. (1) Tsai et al., Activated I-BAR IRSp53 clustering controls the formation of VASP-actin–based membrane protrusions. Sci. Adv. 8, eabp8677 (2022).

2. (2) Tsai et al., Encapsulation of active cytoskeletal protein networks in cell-sized liposomes. Langmuir 27, 10061–10071 (2011).

3. (3) Mabrouk et al., Bursting of sensitive polymersomes induced by curling. PNAS 106, 7294–7298 (2009).

4. (4) Ma et al., An Anaerobic Biomimetic Metal-Free AIE Polymersome Nanozyme as NADH Oxidase Mimic for Photocatalytic Tumor Suppression by Impairing Cancer Cell Energy Metabolism under Hypoxia. JACS 147, 26557–26572 (2025)

5. (5) Zhang et al., AIE Polymer Micelle/Vesicle Photocatalysts Combined with Native Enzymes for Aerobic Photobiocatalysis. JACS 145, 288-299 (2022).

ParisTech

TITLE: MECHANOCHEMICAL SYNTHESIS OF SINGLE ATOM CATALYSTS AND APPLICATION IN SUSTAINABLE SYNTHESIS OF FINE CHEMICALS - BATCH VS CONTINUOUS FLOW

Topic number : ***2025_043***

Field : Chemistry, Physical chemistry and Chemical Engineering - Environment Science and Technology, Sustainable Development, Geosciences - Life and Health Science and Technology

Subfield: Flow Chemistry

ParisTech School: Chimie ParisTech - PSL
Research team : SCiFLOW
Research team website: https://www.lenresearch.com
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr

Contact point for this topic: Len - Christophe - christophe.len@chimieparistech.psl.eu

Advisor 1: Christophe LEN - christophe.len@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Recent advances in green chemistry and sustainable development have included heterogeneous catalysis,1 and alternative technologies such as continuous flow and ball milling.2 In heterogeneous catalysis, the size of the metal particles has a significant impact on catalytic performance. Smaller particles, with more weakly coordinated atoms, improve activity, but are confronted with size inhomogeneity and aggregation problems. To overcome these drawbacks, mechanochemical synthesis of single atom catalysts (SACs) has become a hot area of research in sub-nanoscale fabrication and heterogeneous catalysis.3-5 However, it should be noted that SACs have never been synthesised in a continuous mechanochemical flow. In this project, we envisage to produce novel non-noble metal SACS

(such as Fe, Ni, Co, Mn, Cu, Sn, and Zn) based on biomass support (such as humin, sporopollenin, biochar) in mechanochemistry using either ball mill (batch reactor) or Impact Continuous Heated Mechanochemical equipment – ICHEM (flow reactor). The SACs obtained will be tested in heterogeneous catalysis on model reactions mastered in the laboratory for the synthesis of molecules with a high industrial impact.

Required background of the student:

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

1. M.E. Medina Ruiz, R. Maderuelo-Solera, C.P. Jimenez-Gomez, R. Moreno-Tost, I. Malpartida, C. Garcia-Sancho, J.A. Cecilia, C. Len, J.M. Merida-Robles, P. Maireles-Torres. Supported palladium catalysts for the selective hydrogenation of furfural with polymethylhydrosiloxane. ACS Sustainable Chem. Eng. 2024 12, 14910-14920.

2. C. Len, V. Duhan, W. Ouyang, R. Nguyen, B. Lochab. Mechanochemistry and oleochemistry: a green combination for the production of high-value small chemicals. Front. Chem. 2023, 11, 1306182.

3. J. Lan, P. Yu, Z. Tao, Y. Niu, C. Len, W. Yang. Single-atomic cobalt catalyst for the efficient aerobic oxidation of monosaccharides to sugars acids by controleed hydroxyl radicals genaration at ambient temperature. Green Carbon 2025, in press.

4. S.K. Kaiser, Z. Chen, D.F. Akl, S. Mitchell, J. Perez-Ramirez. Single-atom catalysts across the Periodic Table. Chem. Rev. 2020, 120, 11703-11809.

5. V.B. Saptal, V. Ruta, M.A. Bajada, G. Vile. Single-Atom catalysis in organic synthesis. Angew. Chem. Int. Ed. 2023, 62, e202219306.

ParisTech

TITLE: CHEMICAL RECYCLING OF PLASTIC WASTE COMBINING A UNIQUE CATALYTIC SYSTEM AND CONTINUOUS FLOW MICROWAVE IRRADIATION

Topic number : ***2025_044***

Field : Chemistry, Physical chemistry and Chemical Engineering - Environment Science and Technology, Sustainable Development, Geosciences - Energy, Processes

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team : SCiFLOW
Research team website: https://www.lenresearch.com
Research lab: I-CLEHS - Institute of chemistry for life and health
Lab location: Paris
Lab website: https://iclehs.fr

Contact point for this topic: LEN - Christophe - christophe.len@chimieparistech.psl.eu

Advisor 1: Christophe LEN - christophe.len@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
The daily use of plastics generates an enormous amount of waste that has a considerable impact on the environment and on living species at the end of the plastics' life cycle. Indeed, approximately 300 million tons of plastic are produced worldwide each year, and only a small fraction—less than 9%—is recycled; 12% is incinerated, while the remaining 79% leads to severe contamination issues. In parallel, the decarbonization of all activity sectors has become critically important, and hydrogen is expected to play a key role in decarbonizing hard-to-electrify sectors, as well as serving as a carbon-free feedstock for the production of chemicals and fuels.1-3 To address the major challenge of producing H_2 at a competitive cost while achieving deep decarbonization, we aim to develop an innovative process that combines a catalytic system with continuous-

flow microwave (MW) irradiation to selectively produce high-purity clean hydrogen and valuable decarbonized chemical products (solid carbon), thereby simultaneously contributing to plastic depollution and climate change mitigation.

Required background of the student:

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

1. M. Qiu, B. Du, X. Chen, J. Meng, D. Hu, Y. Sun, C. W. Tsang, C.S.K. Lin, C. Len, C. Liang. Ni/Nb2O5 as a noble-metal free catalyst for the chemical upcycling of waste polyolefin plastics. Chem. Eng. J. 2025, 520, 166381.

2. Y. Wang, R.H. Bai, Q. Liu, Q.X. Tang, C.H. Xie, A. Richel, C. Len, J.X. Cui, C.R. Yan, W.Q. He. Degradation of biodegradable plastic films in soil: microplastics formation and soil microbial community dynamics. J. Hazard Mater. 2025, 492, 138250.

3. Q. Liu, S. Martinez-Villarreal, S. Wang, N.N. Thanh Tien, M. Kammoun, Q. De Roover, C. Len, A. Richel. The role of plastic chemical recycling processes in a circular economy context. Chem. Eng. J. 2024, 498, 155227.

ParisTech

TITLE: FATIGUE DAMAGE MECHANISMS IN SLM-FABRICATED H13 TOOLING UNDER NON-PROPORTIONAL THERMOMECHANICAL LOADING

Topic number : ***2025_045***

Field : Material science, Mechanics and Fluids - Energy, Processes - Design, Industrialization

Subfield:

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés
Lab location: Châlons-en-Champagne
Lab website: https://www.msmp.eu/

Contact point for this topic: Nan KANG, nan.kang@ensam.eu

Advisor 1: Nan KANG - nan.kang@ensam.eu
Advisor 2: Mohamed EL MANSORI - mohamed.elmansori@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Selective Laser Melting (SLM) gives new opportunities for die-casting molds because it allows cooling channels to be created in shapes that traditional machining cannot achieve. However, the real working conditions of die-casting molds are very complex, in which the mold experiences high-pressure metal injection and very fast temperature changes. In this project, the hybrid fatigue behavior of H13 steel molds made by SLM was investigated with focus on the high carbon content induced cracks sensibility and residual stress. The combination of finite element simulations with mechanical characterization will be employed to reveal the damage mechanism under Non-Proportional Thermomechanical Loading. In addition, AI-based optimization methods will be used to improve fatigue-life prediction and to help design better SLM process parameters and cooling-channel system.

Required background of the student:
1. Candidates should have a master's degree in the field of materials science;
2. A background in additive manufacturing will be a clear advantage;
3. Candidates should be able to work in a multidisciplinary environment and be fluent in English (both oral and written)

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

1. Z Qin, N Kang*, M El Mansori, Mechanical homogeneity induced by bainitic transformation in laser powder bed Fused H13 steel at Ultra-High substrate preheating temperatures, Materials & Design, 253 (2025) 113961.

2. Qin Z, Kang N*, El MansoriI M., Surface condition driven fatigue performance of laser powder bed fusion H13 steel, Journal of Materials Research and Technology, 33 (2024) 6767-6779.

3. J Xie, RN Raoelison, N Kang*, PE Mazeran, M Rachik, Study on the in situ strengthening and toughening mechanism of H13 tool steel/WC-12Co composite using laser-based directed energy deposition, Composites Part B: Engineering 266, 111011

ParisTech

TITLE: DESIGN AND FABRICATION OF FUNCTIONALLY GRADED COPPER/H13 STEEL BI-METALLIC LATTICE COMPOSITES

Topic number : ***2025_046***

Field : Material science, Mechanics and Fluids - Energy, Processes - Design, Industrialization

Subfield: Additive Manufacturing

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: MSMP - Laboratoire Mécanique, Surface, Matériaux et Procédés
Lab location: Châlons-en-Champagne
Lab website: https://www.msmp.eu/

Contact point for this topic: Nan KANG, nan.kang@ensam.eu

Advisor 1: Mohamed EL MANSORI - mohamed.elmansori@ensam.eu
Advisor 2: Rajendran Sri Harini - sri-harini.rajendran@ensam.eu
Advisor 3: Nan KANG - nan.kang@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
H13 hot-work tool steel is widely used for die-casting and hot-forming due to its strength, toughness, and wear resistance at high temperatures. However, its low thermal conductivity (18 $W \cdot m^{-1} \cdot K^{-1}$) limits heat dissipation, increasing energy use, tool wear, scrap rate, and production costs. Improving thermal management could extend die life from 80,000 to 120,000 cycles and reduce scrap from 5% to 3%, lowering unit costs by up to 10%. Copper, with a high thermal conductivity of 402 $W \cdot m^{-1} \cdot K^{-1}$, offers an effective solution. A copper lining in cooling channels can increase cooling efficiency by around 12%. While traditional steel–copper bonding methods allow only simple geometries, additive manufacturing now enables more complex composite designs. Yet the mismatch between Cu and H13 remains a challenge. This project proposes designing optimized Cu/H13 lattice composites using machine-learning-based

models and fabricating them via additive manufacturing combined with advanced casting. The study will analyse microstructure, thermal response, and mechanical performance and develop AI-driven models to link processing, architecture, and properties for accelerated design of high-performance tooling materials.

Required background of the student:

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

1. M. Osman, P. Wanjara, J. Gholipour, F. Bernier, M. Molavi-Zarandi, M. Brochu, H13 tool steel-copper composite fabricated by laser powder bed fusion and melt infiltration for high thermal conductivity tooling applications, Materials Today Communications,Volume 49,2025,114221.

2. H. J. Roos, M. Lagler, L. Quintana, The Future of Structural Components in HPDC, Buhler whitepaper, Uzwil, Switzerland.

3. S-S. Shin, S-K. Lee, D-K. Kim, B. Lee, Enhanced cooling channel efficiency of high-pressure die-casting molds with pure copper linings in cooling channels via explosive bonding, Journal of Materials Processing Technology, Volume 297, 2021, 117235.

4. 4. Y.H. Cho, D. Choi, K. Jeong, Y. Kim, M. Park, S. Lee, H. Choi, I-S. Choi, S-G. Kang, H.N. Han, Copper lattice-embedded steel composite: One-step fabrication and its thermal and mechanical properties, Journal of Materials Research and Technology, Volume 37, 2025, Pages 89-101.

ParisTech

TITLE: MULTISENSORY PERCEPTION OF HEMODYNAMIC INSTABILITIES IN A VIRTUAL HUMAN ARTERIES

Topic number : ***2025_047***

Field : Information and Communication Science and Technology - Material science, Mechanics and Fluids - Life and Health Science and Technology

Subfield:

ParisTech School: Arts et Métiers
Research team : Cardiovascular technologies and blood flows (Technologies Cardiovasculaires et Ecoulements Sanguins)
Research team website: https://lifse.artsetmetiers.fr/
Research lab: LIFSE - Laboratoire Ingénierie des Fluides Systèmes Energétiques
Lab location: Paris
Lab website: https://lifse.artsetmetiers.fr/

Contact point for this topic: GARBAYA Samir Email: samir.garbaya@ensam.eu

Advisor 1: Samir Garbaya - samir.garbaya@ensam.com
Advisor 2: Farid BAKIR - Farid.BAKIR@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Arterial stenosis, the narrowing of brain or cardiovascular arteries, disrupts normal blood flow and can lead to stroke or heart attack. As the vessel constricts, blood is forced through a tighter passage, creating turbulence and unstable flow patterns. These disturbed hemodynamics increase mechanical stresses on the arterial wall. Clinical studies indicate that severe stenosis is strongly associated with recurrent stroke [1, 2, 3], in part because turbulent flow can initiate arterial damage and contribute to wall weakening or rupture when the resulting stresses exceed the vessel's structural strength. Dynamic 3D visualization of fluids such as blood flow in the arteries and tiny vessels [4, 5], high-fidelity

representation models and augmented perception are promising for the exploration/understanding of critical pathological situations. Additionally, blood flow in human body is inherent to physico-chemical properties specific to each patient. Hence, personalized models of blood flow in arteries are necessary for the accuracy and efficiency of prediction and medical decision making. This PhD project will focus on the development of real-time multisensory interaction of blood flow instabilities in human arteries using computational fluid dynamics (CFD), interactive computer graphics, haptic and auditory (sonification) feedback. The objective is to identify the risk associated with blood flow instabilities based on augmented perception of the hydrodynamics and interactions in stenosed arteries of personalized patient. The research work includes geometric data acquisition, 3D modelling of human body organs and dynamic visualization of fluid flow and its interactions with deformable shapes/surfaces. A novel approach of multisensory interaction in virtual environment integrating sound and haptic feedbacks will be developed to assist in the identification of pathological risks and the optimization of the therapy.

Required background of the student:
Applicants must have completed a Master of Engineering in a discipline related to Mechanical Engineering/Computer Science with good skills in Computational Fluid Dynamics (CFD), programming in C# and Python, 3D Computer Graphics and Modelling, Virtual/Augmented Reality. Basic knowledge of human anatomy and motivation to apply research to neurology will be appreciated.

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

1. Huang, L., Garbaya, S. & Khelladi, S. Haptic interaction with fluids in virtual environment: an analytical review. Virtual Reality 29, 62 (2025). https://doi.org/10.1007/s10055-025-01120-5

2. Koskas L, et al. Experimental Study of the Influence of Mechanical and Hemodynamic Parameters on Abdominal Aortic Aneurysmal Growth. Journal of Vascular Surgery (J Vasc Surg). 2025. doi: 10.1016/j.jvs.2025

3. M. Boumrah, S. Garbaya, and A. Radgui, “Real-Time Visual Analytics for Remote Monitoring of Patient’s Health,” WSCG’2023 -. International Conference in Central Europe on Computer Graphics, Visualization and Computer Vision’2023, Prague, Czech Republic

4. N. Abbasnezhad, M. Shirinbayan, S. Champmartin, F. Bakir, "Analyzing the impact of pulsatile flow on drug release from a single strut of a drug-

eluting stent",Journal of Biomechanics, Volume 146,2023,111425,ISSN 0021-9290,https://doi.org/10.1016/j.jbiomech.2022.111425
5. Abbasnezhad N., Specklin M., Bakir F., Leprince P., Danial P. “Hemodynamic Evaluation of a Centrifugal Left Atrial Decompression Pump for Heart Failure with Preserved Ejection Fraction.” Bioengineering, 2023, 10(3): 366. doi: 10.3390/bioengineering10030366

ParisTech

TITLE: INTERACTION OF BACTERIA WITH 3D MICROTOPOGRAPHIES GENERATED BY TWO-PHOTON POLYMERIZATION

Topic number : ***2025_048***

Field : Chemistry, Physical chemistry and Chemical Engineering - Material science, Mechanics and Fluids - Life and Health Science and Technology

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team : Processes, Plasmas, Microsystems Team
Research team website: https://www.ircp.cnrs.fr/equipes-recherche-ircp/equipe-2pm/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/

Contact point for this topic: vincent.semetey@chimieparistech.psl.eu

Advisor 1: Vincent SEMETEY - vincent.semetey@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
This PhD project aims to investigate how microscale and nanoscale surface architectures fabricated by two-photon polymerization (2PP) influence bacterial adhesion, colonization, and early biofilm formation. Using 3D-printed topographies with precisely controlled feature sizes, geometries and chemistries, the candidate will study species-specific responses of both Gram-positive and Gram-negative bacteria under controlled environmental conditions. Advanced imaging techniques (confocal microscopy, SEM) and quantitative biointerface assays will be used to correlate structural parameters with bacterial behavior. The project will also explore mechanistic hypotheses related to physical confinement, surface energy modulation, and mechanosensing. Ultimately, the work seeks to establish design principles for anti-adhesive

or pro-adhesive microstructures relevant to biomedical devices, biosensors, and engineered living materials.

Required background of the student:
A suitable background includes a Master's degree in chemistry, polymer science, materials science, or bioengineering.

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

1. [59] "Quantifying cell traction forces at the single-fiber scale in 3D: An approach based on deformable photopolymerized fiber arrays" Ucla P., Lê-Chesnais J., Ver Hulst H., Ju X.M., Calvente I., Nematollahi E., Leconte L., Salamero J., Bonnet I., Monnot C., Moreau, H.D., Landoulsi J., Semetey V.*, Coscoy S.* PNAS 2025, 122, e2507677122. DOI:10.1073/pnas.2507677122

2. "Dual role of marine bacteria Pseudoalteromonas NCIMB 2021 in corrosion of mild steel in artificial seawater" Jaume J., Mercier D., Seyeux A., Semetey V., Zanna S., Marcus P. Corrosion Science 2025, 255, 113076. DOI:10.1016/j.corsci.2025.113076

3. "Microtopographies control the development of basal protrusions in epithelial sheets." Coscoy S., Baiz S., Octon J., Rhoné B., Perquis L., Tseng Q., Amblard F., Semetey V.* Biointerphases 2018, 13, 041003. DOI: 10.1116/1.5024601

4. "Preventing biofilm formation and associated occlusion by biomimetic glycocalyx-like polymer in central venous catheters" Chauhan A., Bernardin A., Mussard W., Kriegel I., Estève M., Ghigo J. M., Beloin C., Semetey V.* The Journal of Infectious Diseases. 2014, 210, 1347-56.

5. "Facile and Efficient Control of Bioadhesion on Poly(dimethylsiloxane) by using a Biomimetic Approach" Mussard W., Kebir N., Kriegel I., Estève M., Semetey V.* Angewandte Chemie Int. Ed. Engl. 2011, 50, 10871-10874.

ParisTech

TITLE: ACOUSTIC TRIGGERING OF GRANULAR AVALANCHES

Topic number : ***2025_049***

Field : Physics, Optics - Material science, Mechanics and Fluids

Subfield: Applied Physics, Physical Acoustics

ParisTech School: ESPCI Paris - PSL
Research team :
Research team website:
Research lab: Institut Langevin
Lab location: Paris
Lab website: https://www.institut-langevin.espci.fr

Contact point for this topic: xiaoping.jia@espci.fr

Advisor 1: Xiaoping Jia - xiaoping.jia@espci.fr
Advisor 2: Arnaud Tourin - arnaud.tourin@espci.fr
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Unstable slopes in mountainous, costal or volcanic area are subject to different forcings acting on different time scales, leading the slopes to fall down and generate landslides or rockfalls. Our recent work on rockfalls in the crater Dolomieu of Piton de la Fournaise (Reunion Island) showed that the small seismicity related to the ascent of magma in the fragmented edifice may accumulate and trigger rockfalls, even though the magnitude of these volcano-tectonic events is much smaller than the standard triggering thresholds reported in the literature [1] . We also showed that the response of the slope to seismicity and rainfall is strongly related to its stability state, i.e., its distance to the failure, as observed in lab-experiments on granular slopes [2]. In this PhD, we seek to further investigate these effects by studying the spatio-temporal evolution of rockfalls and quantifying the correlation between the rockfalls themselves as well as between rockfalls, rainfall and seismicity, in collaboration with Prof. Anne Mangeney from Institut de Physique de Globe de Paris (IPGP). In parallel with the field studies carried out by our

colleagues from IPGP, we will be conducting laboratory-scale experiments at the Institut Langevin, in line with our previous work on the ultrasonic triggering of granular avalanches [2,3]. This work aims at providing a better understanding of the seismic triggering of landslides and earthquakes [4].

Required background of the student:
The applicant should have a master's degree, engineering diploma or equivalent, with a solid background in physics, and if possible, skills in acoustics or/and geophysics. He/She should be motivated by a multidisciplinary work at the interface between several disciplines.

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

1. V. Durand et al., Repetitive small seismicity coupled with rainfall can trigger large slope instabilities on metastable volcanic edifices, Commun. Earth Environ. 4, 383 (2023)

2. [2] J. Léopoldès, X. Jia, A. Tourin, and A. Mangeney, Triggering granular avalanches with ultrasound, Phys. Rev. E 102, 042901(2020)

3. [3] H. Martin et al., Ultrasound-induced dense granular flows: a two-time scale modeling", J. Fluid Mech. 1004 (2025)

4. [4] P. Johnson and X. Jia, Nonlinear dynamics, granular media and dynamic earthquake triggering, Nature 437, 871 (2005)

ParisTech

TITLE: REACTION MECHANISMS GOVERNING THE INTERFACIAL STABILITY OF SILICON ELECTRODES IN SI–AIR BATTERIES USING AQUEOUS AND NONAQUEOUS ELECTROLYTES

Topic number : ***2025_050***

Field : Chemistry, Physical chemistry and Chemical Engineering - Energy, Processes - Material science, Mechanics and Fluids

Subfield: electrochemistry, surface science, batteries

ParisTech School: Chimie ParisTech - PSL
Research team : Physical Chemistry Group
Research team website: https://www.linkedin.com/in/jolanta-swiatowska-1898b86?originalSubdomain=fr
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/

Contact point for this topic: Swiatowska Jolanta
jolanta.swiatowska@chimieparistech.psl.eu

Advisor 1: Jolanta Swiatowska - jolanta.swiatowska@chimieparistech.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
This research project aims to decipher the reaction mechanisms that control the interfacial stability of silicon electrodes in Si–air batteries operating in aqueous and nonaqueous electrolytes. The study will evaluate KOH-based systems, ionic liquids, water–ionic liquid mixtures, and selected organic electrolytes to identify formulations that enhance Si stability while reducing corrosion and structural degradation. Both pure silicon and doped silicon electrodes will be investigated to explore how material composition influences interfacial behavior and expands the usable electrochemical window of various electrolytes. Advanced electrochemical analysis and surface-characterization techniques will be

used to map degradation pathways, passivation-layer formation, and reaction intermediates. The overarching objective is to improve our fundamental understanding of Si/electrolyte interactions and to guide the development of next-generation, greener, and more sustainable Si-air energy-conversion systems.

Required background of the student:
- Strong background in electrochemistry, including electrochemical kinetics, electrode processes, and corrosion phenomena.
- Knowledge of materials science (batteries, fuel cells...).
- Experience with electrochemical techniques, such as voltammetry, impedance spectroscopy, galvanostatic cycling, and corrosion testing.
- Basic understanding of electrolytes, including aqueous, organic, ionic-liquid systems, and interfacial chemistry.
- Good written and oral communication skills in English.

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

1. Y. Zhou, X. Lu, G. Lin, F. Wang, J. Światowska, Towards high-performance aqueous Mg batteries: Insights into corrosion mitigation through material and electrolyte design, Corros. Sci. 253 (5) (2025) 113016. DOI: 10.1016/j.corsci.2025.113016

2. G. Lin, Y. Zhou, S. Zanna, A. Seyeux, P. Marcus, J. Światowska, Mg Anode Interface Engineering in KNO3 Electrolyte with Sodium 5-Sulfosalicylate as an Additive for Enhanced Performance of Mg-Air Batteries, Journal of Magnesium and Alloys 12 (9)(2024) 3646-3660. DOI: 10.1016/j.jma.2024.09.007

3. Y. Zhou, J.-T. Li, S. Zanna, A. Seyeux, P. Marcus, J. Światowska, Probing Mg anode interfacial and corrosion properties using an organic/inorganic hybrid electrolyte, Applied Surface Science 614(6) (2023) 156070. DOI: 10.1016/j.apsusc.2022.156070

4. Z.-Y. Wu, L. Deng, J.-T. Li, S. Zanna, A. Seyeux; L. Huang; S.-G. Sun, P. Marcus, J. Światowska, Solid Electrolyte Interphase Layer Formation on the Si-Based Electrodes with and without Binder

5. E. Roex, A. Aqil, J. Światowska, C. Malherbe, F. Boschini, R. Cloots, A. Mahmoud, Self-standing V2O5/Polydopamine/CNT film as high-performance cathode material for advanced zinc-ion batteries, J of Power Sources, 616, (2024) 235104. DOI: 10.1016/j.jpowsour.2024.235104

ParisTech

TITLE: TOWARDS AN INTEGRATIVE MULTI-LEVEL FRAMEWORK FOR SUPPLY CHAIN RISK MANAGEMENT

Topic number : ***2025_051***

Field : Design, Industrialization - Economics, Management and Social Sciences

Subfield: Supply chain management - Risk management

ParisTech School: Arts et Métiers
Research team :
Research team website:
Research lab: LCFC - Laboratoire de conception, fabrication, commande
Lab location: Paris
Lab website: https://lcfc.ensam.eu/lcfc-accueil-119817.kjsp

Contact point for this topic: Lassagne - Marc - marc.lassagne@ensam.eu

Advisor 1: Ali Siadat - ali.siadat@ensam.eu
Advisor 2: Marc Lassagne - marc.lassagne@ensam.eu
Advisor 3: Jihan Rajeh - jihan.rajeh@ensam.eu
Advisor 4:

Short description of possible research topics for a PhD:
Global supply chains are essential for business competitiveness yet increasingly vulnerable in today's VUCA (Volatile, Uncertain, Complex, Ambiguous) environment, as evidenced by recent disruptions. They face mounting requirements for traceability, environmental compliance, economic performance, and agility, while becoming more complex due to the diversity of actors involved, actors who must cooperate effectively despite competing interests. Despite the importance of these topics, their integration remains limited, primarily because of the absence of a comprehensive conceptual framework. Moreover, current research in supply chain risk management, which aims at addressing these issues, largely focuses on disruption prevention and recovery, without addressing the strategic trade-offs between risks and opportunities. This raises at least two scientific challenges: - How can environmental,

economic, social, and governance (ESG) criteria be systematically integrated into supply chain management? - What multi-level operational tools and decision-support systems, possibly AI-driven, can enable this integrated approach under uncertainty? The PhD may rely on a combination of quantitative modelling (e.g., stochastic optimization, simulation, multi-agent models), qualitative approaches (case studies, interviews with supply chain stakeholders), and data-driven methods. Mixed-methods designs will be encouraged to bridge theoretical modeling with empirical validation, and the candidate may also explore emerging technologies such as digital twins, traceability systems, or explainable AI. This doctoral research seeks to resolve the fundamental tension between agility and resilience in modern supply chains, while promoting collaborative governance models that enhance trust and transparency. Expected contributions include the development of an integrated conceptual framework combining ESG, risk, and performance dimensions; the proposal of new indicators or evaluation metrics for resilient and sustainable supply chains; and the design of an operational decision-support tool tailored to uncertain and complex environments. The work will contribute to the development of robust theoretical models and practical frameworks for managing the risk associated with complex, global supply chains in uncertain environments. Candidates will engage in cutting-edge research with strong academic and industrial relevance, in order to achieve sustainable supply chain management.

Required background of the student:
Master in industrial engineering, with a concentration in supply chain management or risk management.

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

1. Rajeh, J, Amari, S, Addouche, SA, Letouzey A, Desforges X, Medjaher K (2025). Performance evaluation and reconfiguration of supply chains based on discrete event systems formalisms. Optimization and Engineering. https://doi.org/10.1007/s11081-025-09994-9

2. Magnani F, Siadat A, Caillaud E, Gaudichau E (2024), « Defining lean experts' roles and behavioral competencies during lean adoption: a case study of Groupe PSA", The TQM Journal, 2024, https://doi.org/10.1108/TQM-01-2023-0011

3. Petronijevic J, Etienne A, Siadat A, «Process-product risk propagation in a product development: from framework to simulator", International Journal of Product Lifecycle Management, 2023, https://doi.org/10.1504/IJPLM.2023.133602

4. Riemens J, Lemieux A-A, Lassagne M, Lamouri S (2023), Apprehending traceability implementation in support of sustainable value chains: A novel analysis framework for the fashion industry, Journal of Cleaner Production, Vo. 414, 2023, 13750, https://doi.org/10.1016/j.jclepro.2023.137501
5. Nagashima M, Wehrle FT, Kerbache L, Lassagne M (2015), Impacts of adaptive collaboration on demand forecasting accuracy of different product categories throughout the product life cycle. Supply Chain Management: An International Journal, Vol. 20 No. 4 pp. 415–433, https://doi.org/10.1108/SCM-03-2014-0088

ParisTech

TITLE: NEW PHENOMENA IN ACTIVE COLLOIDS IN 3D

Topic number : ***2025_052***

Field : Physics, Optics - Chemistry, Physical chemistry and Chemical Engineering - Material science, Mechanics and Fluids

Subfield: Soft Matter

ParisTech School: ESPCI Paris - PSL
Research team : Royall
Research team website: https://paddyroyall.github.io/padrus/index.html
Research lab: GULLIVER - Voyages expérimentaux et théoriques en matière molle
Lab location: Paris
Lab website: https://www.gulliver.espci.fr/

Contact point for this topic: paddy.royall@espci.psl.eu

Advisor 1: Christopher Royall - paddy.royall@espci.psl.eu
Advisor 2:
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Active matter is one of the most exciting fields in condensed matter physics. Much of the excitement comes from the discovery of new phenomena, and the connection to biological systems. While modelling biological systems – such as fish – enables insight into new domains of physics, quantitative understanding from first principles is challenging to put it mildly. Imagine a physical system with behaviour similar to biological systems and yet whose properties can be predicted in a well-controlled manner: such a system is active colloids. These micron-sized particles exhibit a unique combination of thermal motion (so they follow statistical mechanics) and activity (so they exhibit new phenomena). We have discovered a variety of new and unexpected phenomena in the active colloids, from hydrodynamic coupling akin to excited states in molecules, novel active polymerisation. We have recently developed the first 3d active colloidal system (see figure) which we can study both in

experiment and with computer simulation. This project aims to explore this system, from the role of activity in crystal nucleation and self-assembly to investigation of new phenomena such as phonon-like waves (which usually do not exist in colloidal systems).

Required background of the student:
Masters/Batchelors in Physics or Chemistry or related discipine

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

1. Sakai N. Skipper K, Moore FJ, Russo J and Royall CP, "Active Dipolar Colloids in Three Dimensions: Non– Equilibrium Structure and Re-entrant Dynamics", Soft Matter 21, 5204 (2025).

2. Chao X, Skipper K, Royall CP, Henkes S, Liverpool TB, "Traveling strings of active dipolar colloids", Phys. Rev. Lett. 134 018302 (2025).

3. Royall CP, Charbonneau P, Dijkstra M, Russo J, Smallenburg F, Speck T and Valeriani C, "Colloidal Hard Spheres: Triumphs, Challenges and Mysteries", Rev. Mod. Phys. 96 045003 (2024)

4. Zampetaki A, Yang, Y, Loewen, H and Royall CP, "Dynamical Order and Many-Body Correlations in Zebrafish show that Three is a Crowd" Nature Commun, 15 2591 (2024)

ParisTech

TITLE: PLASMA-ASSISTED ENGINEERING OF FUNCTIONAL SURFACES FOR BIOLOGICAL INTERFACES

Topic number : ***2025_053***

Field : Chemistry, Physical chemistry and Chemical Engineering - Material science, Mechanics and Fluids - Life and Health Science and Technology

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team : Processes, Plasmas, Microsystems Team
Research team website: https://www.ircp.cnrs.fr/equipes-recherche-ircp/equipe-2pm/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/

Contact point for this topic: vincent.semetey@chimieparistech.psl.eu; cedric.guyon@chimieparistech.psl.eu

Advisor 1: Vincent SEMETEY - vincent.semetey@chimieparistech.psl.eu
Advisor 2: Cédric GUYON - cedric.guyon@chimieparistech.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
This PhD project aims to develop innovative plasma-based strategies to tailor material surfaces for advanced biological applications. Using low-temperature plasma processes, the candidate will design and control surface chemical functionalities, nanoscale roughness, and crosslinking to modulate biomolecular adsorption, cell adhesion, and antimicrobial behavior. A central focus will be the development of bioinspired and stimuli-responsive coatings enabling selective interactions with proteins, mammalian cells, or microorganisms. Comprehensive characterization (XPS, FTIR, AFM, contact angle, fluorescence microscopy) will be coupled with biological assays to establish precise structure–function relationships. The project ultimately seeks to propose plasma-enabled

surface platforms for diagnostics, tissue engineering, and biointerfaces with tunable biological responses.

Required background of the student:

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

1. “Investigation of 3-aminopropyltrimethoxysilane for direct deposition of thin films containing primary amine groups by open-air plasma jets” Morand G., Guyon C., Chevallier P., Saget M., Semetey V., Mantovani D., Tatoulian M. Plasma Processes and Polymers 2022, 19, 2200047.

2. ”Quantifying cell traction forces at the single-fiber scale in 3D: An approach based on deformable photopolymerized fiber arrays” Ucla P., Lê-Chesnais J., Ver Hulst H., Ju X.M., Calvente I., Nematollahi E., Leconte L., Salamero J., Bonnet I., Monnot C., Moreau, H.D., Landoulsi J., Semetey V.*, Coscoy S.* PNAS 2025, 122, e2507677122.

3. “Efficient one-step passivation of biomedical polyurethane using transurethanisation” Rhone B., Galtayries A., Semetey V.* Macromol Biosci. 2023, e2300168.

4. “A Versatile Approach to Design on Demand Self-Assembled Monlayer on Glass using Thiolene Chemistry” Oberleitner B., Dellinger A., Déforet M., Galtayries A., Castanet A.-S., Semetey V.* Chemical Communications 2013, 49, 1615 - 1617.

ParisTech

TITLE: DEVELOPMENT OF SUSTAINABLE ELECTRONIC MATERIALS VIA ADDITIVE MANUFACTURING AND CONDUCTIVE ORGANIC POLYMERS

Topic number : ***2025_054***

Field : Material science, Mechanics and Fluids - Chemistry, Physical chemistry and Chemical Engineering

Subfield:

ParisTech School: Chimie ParisTech - PSL
Research team : Processes, Plasmas, Microsystems Team
Research team website: https://www.ircp.cnrs.fr/equipes-recherche-ircp/equipe-2pm/
Research lab: IRCP - Institut de Recherche de Chimie de Paris
Lab location: Paris
Lab website: https://www.ircp.cnrs.fr/

Contact point for this topic: vincent.semetey@chimieparistech.psl.eu; karim.inal@minesparis.psl.eu

Advisor 1: Vincent SEMETEY - vincent.semetey@chimieparistech.psl.eu
Advisor 2: Karim INAL - karim.inal@minesparis.psl.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
This project aims to design and fabricate next-generation sustainable electronic materials using additive manufacturing (AM) and conductive organic polymers. The candidate will explore bio-based or recyclable polymer matrices combined with intrinsically conductive polymers (e.g., PEDOT derivatives) to create environmentally responsible functional inks. Using advanced 3D printing techniques, the work will focus on optimizing printability, electrical performance, and long-term stability of printed architectures. Structural, thermal, and electronic characterization will be carried out to understand structure–property relationships and degradation pathways. The project will also investigate strategies for end-of-life recyclability and low-energy processing. Ultimately, this research aims to establish design rules for high-performance, low-impact

electronic components suited for sensors, flexible circuits, and emerging green technologies.

Required background of the student:
Master's degree in Materials Science, Polymer Chemistry, Chemical Engineering, or related field

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

1. "Advanced approach for phosphor recovery and characterization of LED components" Wehbie M., Delannoy S., Sun F., Minier M., Semetey V.* Dalton Transactions 2025, 54, 14926-149362025

2. "Advanced granulometric characterization of shredded waste printed circuit boards for sampling" Barthet A., Chauris H., Romary T., Semetey V., Chautru E., Waste management 2024, 187, pp.296-305.

3. "Characterization of end-of-life LED lamps: Evaluation of reuse, repair and recycling potential" Wehbie M., SemeteyV.* Waste Management 2022, 141, 202-207.

4. "Recycling Polyurethanes through Transcarbamoylation ", Zhao L.; Semetey V.* ACS Omega 2021, 6, 4175-4183.

ParisTech

TITLE: FRAMEWORK FOR THE ECO-DESIGN OF CHINESE ELECTRICAL AND ELECTRONIC EQUIPMENT WITH THE VALUE RETENTION REQUIREMENTS OF THE EUROPEAN UNION MARKET.

Topic number : ***2025_055***

Field : Design, Industrialization - Environment Science and Technology, Sustainable Development, Geosciences

Subfield: Early Design, Creativity, Innovation, Tools, Physical / Intermediary Objects / Stakeholders

ParisTech School: Arts et Métiers
Research team : Dr. José Hidalgo Crespo, Maître de Conférences - Dr. Nicolas Maranzana, Maître de Conférences, HdR
Research team website: https://lcpi.ensam.eu/equipe-114312.kjsp?RH=6600224935547&RF=6600147557471
Research lab: LCPI - Laboratoire conception de produits et innovation
Lab location: Paris
Lab website: https://lcpi.ensam.eu/cpi-page-accueil-112719.kjsp

Contact point for this topic: José Hidalgo jose-armando.hidalgo_crespo@ensam.eu

Advisor 1: Nicolas Maranzana - nicolas.maranzana@ensam.eu
Advisor 2: José Hidalgo - jose-armando.hidalgo_crespo@ensam.eu
Advisor 3:
Advisor 4:

Short description of possible research topics for a PhD:
Eco-design of Chinese EEE with EU value retention challenges

Required background of the student:
Engineer, Designer
Innovation Enthusiast
Motivation to coordinate actions with chinese and french stakeholders
Life cycle assessment notions

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

1. Micheaux, H., & Aggeri, F. (2021). Eco-modulation as a driver for eco-design: A dynamic view of the French collective EPR scheme. Journal of Cleaner Production, 289, 125714. https://doi.org/10.1016/j.jclepro.2020.125714

2. Hidalgo-Crespo, J., Riel, A., Golinska-Dawson, P., Peeters, J. R., Werner-Lewandowska, K., & Duflou, J. R. (2024). Facilitating circularity: challenges and design guidelines of Product-as-a-Service (PaaS) business model offers for electrical and electronic equipment. Procedia CIRP, 128, 567–572. https://doi.org/10.1016/j.procir.2024.03.037

3. Luu, D.-N., Gachet, H., Maier, C.-J., Maranzana, N., & Aoussat, A. (2022). Eco-design and medicine: Opportunities to implement eco-design in the pharmaceutical R&D process. Journal of Cleaner Production, 365, 132785. https://doi.org/10.1016/j.jclepro.2022.132785

4. Li, J., & Sarkis, J. (2021). Product eco-design practice in green supply chain management: a China-global examination of research. Nankai Business Review International, 13(1), 124–153. https://doi.org/10.1108/nbri-02-2021-0006