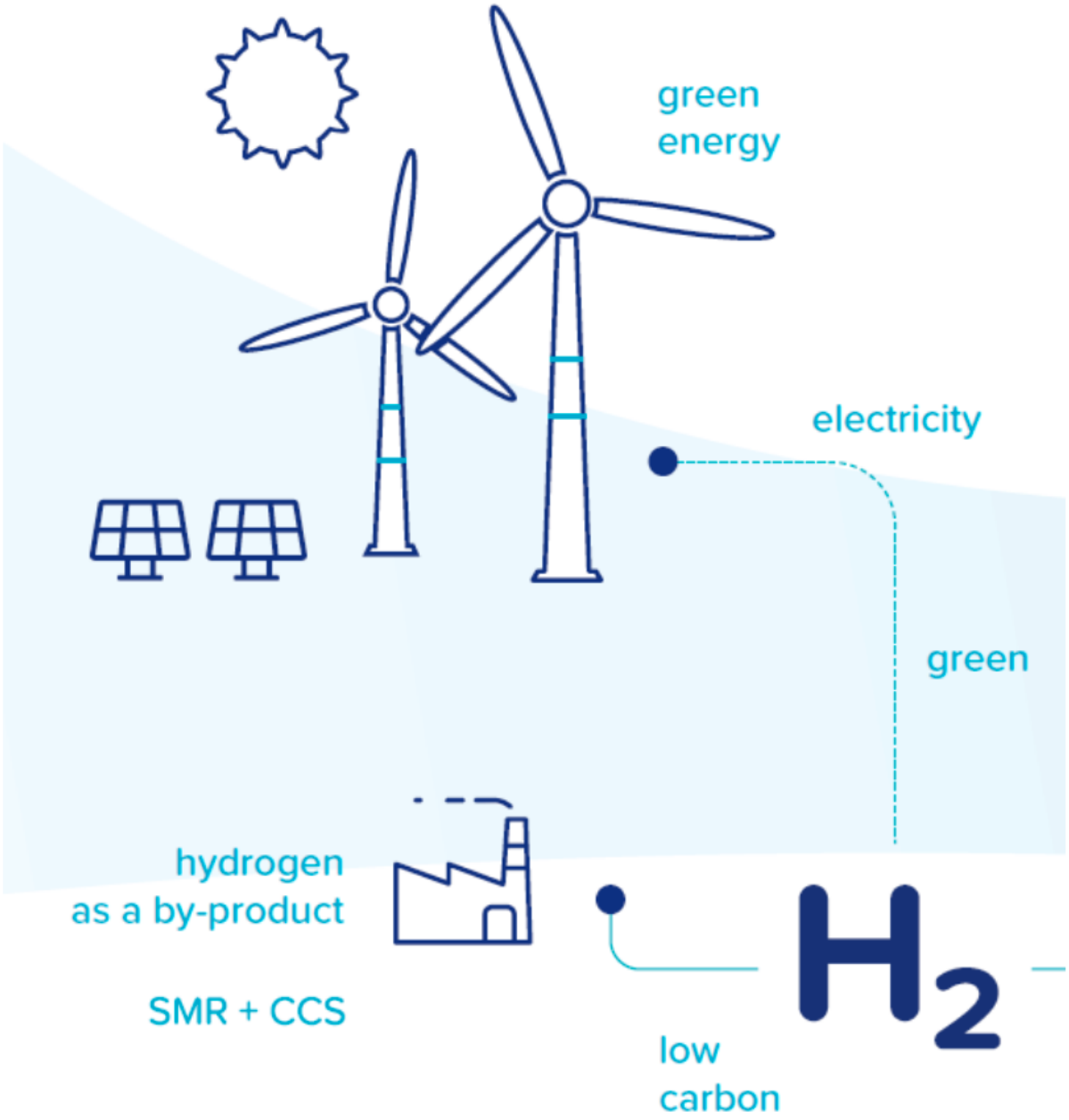

H2[hub]
wallonia
Academic research related to hydrogen in Wallonia
Status September 2023
BELGIAN HYDROGEN COUNCIL
BE-HyFE
HYDROGEN
H2

# Introduction

The objective of the present document is to present an inventory of all academic and research groups based in Wallonia and Brussels working on hydrogen topics. This inventory exercise has been already achieved by WaterstofNet for the Flemish level. This document is therefore a draft version. The final document will be a compilation of both documents in order to provide a complete overview of the Belgian strength in terms of hydrogen research activities. This will help gaining in visibility for the research, both in a national and an international perspective, as well as facilitate new initiatives in the field.

# Content

## Production, storage and transport of hydrogen



# ULiège: Chemistry for Sustainable Food and Environmental Systems Biomass and green technologies

University of Liège, Gembloux Agro-Bio Tech, GxABT Deparment

Process development

Production of H2

## General expertise of the research group

The laboratory of Biomass and Green Technologies from the University of Liege (Gembloux Agro-Bio Tech Campus) is engaged in research and education in the field of the chemistry of renewable resources and associated technologies.

The PI (Prof. A. Richel) is involved in more than 15 national and international projects related to the production of bioenergy and bioproducts, including the design of innovative pretreatment protocols for the cracking of lignocellulosic materials, the formulation of novel "biomass-energy" solutions (including biofuels and energy vectors) as well as the upgrade of lignin for high-added value applications.

## Specific hydrogen- related expertise & research topics

Production of hydrogen from renewable resources including mostly vegetal resources and organic waste: evaluation of the scale-up constraints, techno-economic analysis.
Application of hydrogen for biofuels production (e.g. synthetic fuels or drop-in fuels for road and air transportation): hydrotreatment, power-to-fuels, ammonia production, Fischer-Tropsch reaction, waste-to-fuels, etc. Conversion pathways, economics and prospects for transportation.

## Available equipment/tools:

Several reactors allowing the thermochemical conversion of several inflows into fuels in the presence of hydrogen. Online analytical devices allowing the in situ determination of the key constituents during the reaction.

## Participating in RW/B/EU funded projects with H2 related research:

ADV_BIO « Innovation technologique dans la production de biocarburants avancés applicables au territoire belge pour le transport routier et aérien et analyses technico-économique et environnementale » (2020-2025) Fonds de Transition Énergétique, SPF Energie.

## Main relevant publications

On the last two years


1. Martinez-Villarreal, S., Breitenstein, A., Nimmegeers, P., Perez Saura, P., Hai, B., Asomaning, J., Eslami, A.A., Billen, P., Van Passel, S., Bressler, D.C., Debecker, D.P., Remacle, C., Richel, A. Drop-in biofuels production from microalgae to hydrocarbons: Microalgal cultivation and harvesting, conversion pathways, economics and prospects for aviation (2022) Biomass and Bioenergy, 165, art. no. 106555, .
2. Berger, M., Radu, D., Detienne, G., Deschuyteneer, T., Richel, A., Ernst, D. Remote Renewable Hubs for Carbon-Neutral Synthetic Fuel Production (2021) Frontiers in Energy Research, 9, art. no. 671279, .
3. Lepage, T., Kammoun, M., Schmetz, Q., Richel, A. Biomass-to-hydrogen: A review of main routes production, processes evaluation and techno-economical assessment (2021) Biomass and Bioenergy, 144, art. no. 105920
4. Martinez-Villarreal, S., Kammoun, M., Richel, A. The critical role of hydrogen in the development of new biofuels (2023) Current opinion in Green and Sustainable Chemistry, 39, 100716


## Contact persons


### Prof. Aurore Richel

Professeur Ordinaire - Full Professor
Biomass and Green Technologies
University of Liege - Gembloux Agro-Bio Tech
Passage des Déportés, 2
B-5030 Gembloux, BELGIUM
Tel: +32.81.622.633
Tel: + 32.477.98.00.66
a.richel@uliege.be
www.chem4us.be

# UCLouvain: Institute of Condensed Matter and Nanosciences (IMCN)

University of Louvain

Materias discovery and characterization

Hydrogen storage

## General expertise of the research group

Research in the IMCN institute focuses on condensed matter and nanoscience from the atomic and molecular levels to real materials. This research concerns the synthesis, design, manipulation, implementation and modeling of (bio)molecules, (bio)surfaces and solid materials. The latter are characterized or simulated by means of advanced techniques, which are also sometimes developed as an inherent part of the research. The obtained compounds, materials or devices are then investigated for their functions, properties or reactivity, leading up to applications. Thematics in the frame of this general methodology, and resulting research projects conducted in the institute, lead to the study of molecules, materials, surfaces and interfaces, with a strong connotation of nanosciences, nanotechnologies and nanomaterials.

## Specific hydrogen-related expertise & research topics

The groups of Yaroslav Filinchuk and Sophie Hemans are respectively centered on bulk (3D) and surface (2D) materials. The former has a background in metal and complex hydrides and more recently on using hydrides as solid-state electrolytes in batteries. The latter is having expertise in designing surfaces by functionalization and in surface characterization. The common research activity of the two groups is focused on porous materials, used in catalysis and for gas storage and separation. In particular, storage of compressed hydrogen in metal-organic frameworks, known as MOFs.

## Available equipment/tools:

- Fritsch Pulverisette 7 ball mill (bought in 2012), equipped with steel and tungsten carbide vials. Three sorts of experiments are possible, allowing creating and optimizing synthetic routes: milling under argon in standard vials, milling under gas

pressures using gas lids and milling with pressure-temperature control. Second mill: Retsch S1 planetary ball mill with 250 cc agate vial. These are used, in particular, for synthesis of some MOFs.

- Two 4 cc autoclaves for 200 bar and an oven with temperature control;
- Edwards nEXT Turbo-molecular pump;
- Two complete Schlenk setups for wet synthesis of air-sensitive compounds;
- Two 4-hand gloveboxes, with integrated microscopes, a deep freezer and a vacuum oven;
- "Solvent-box" - a 2-hand plastic glovebox for wet synthesis under protective atmosphere;
- Diamond anvil cells for high-pressure experiments;
- 3D printer for producing plastic vials for ball-milling experiments;
- Two autoclaves for 200 bar and high temperatures, with magnetic stirring

Charactezization:

- Two MAR345 diffractometers with microfocusing Mo sources installed in summer 2020. The diffractometers are equipped with cryogenic gas blower (80-400 K), a hot air blower (RT-750 °C) and a manually-controlled gas rig with sample holders for experiments up to 200 bar.
- Three volumetric instruments for measuring Pressure-Composition-Temperature (PCT) diagrams and temperature programmed desorption under gas pressures. Allows for physi- and chemi-sorption experiments.
- TGA/DSC-MS integrated into an argon-filled glovebox, allowing to measure air-sensitive high energy materials under inert atmosphere.
- FTIR instrument with heatable ATR cell was integrated inside one of our gloveboxes in 2017.

Available within our institute, IMCN:

- transmission Raman, solution NMR and high resolution mass spectrometers. New generation of three NMR spectrometers is being purchased for the ASM platform and installed in 2023/2024. One of them will be able to operate with solid-state probe.
- Micromeritics ASAP 2020 Surface Area and Porosity Analyzer. A proposal for another porosity analyser with closed cycle helium cryostat (25-350 K) is submitted in parallel with this project for the EQP call, in collaboration with Prof. Sophie Hermans.

## Participating in RW/B/EU funded projects with H2 related research:

| | |
|---|---|
| FNRS equipment project: Hydride Research Infrastructure | Project running from 01/2013-12/2014 (call FNRS-EQP), with a total budget of 161 k€ (all for UCLouvain); allowed to install argon gloveboxes and high-pressure volumetric system for adsorption studies. |

| | |
|---|---|
| FNRS research project: Hydrides Under Practical Conditions | Project running from 07/2013-06/2017 (call FNRS-PDR), with a total budget of 303 k€ (all for UCLouvain); synthesis and characterization of H-rich hydrides; in situ diffraction studies of porous materials. |
| FNRS equipment project: High-energy XRD at UCL | Project running from 01/2019-12/2020 (call FNRS-EQP), with a total budget of 196 k€ (all for UCLouvain); allowed to install two high-energy X-ray sources allowing to study in situ light-weight materials like hydrides and MOFs. |
| FNRS research credit: Energy Storage in Al-based Systems | Project running from 01/2020-12/2021 (call FNRS-CdR), with a total budget of 59 k€ (all for UCLouvain); synthesis and characterization of H-rich materials. |
| Regional project ARC MicroBat: Solid-State Micro-Batteries with Nanowire Electrodes: from Materials to Integration | Project running from 09/2018-08/2023 awarded by the Fédération Wallonie Bruxelles (FWB) as an Actions de Recherche Concertées with a total budget of 897 k€ (all for UCLouvain - Profs. Y. Filinchuk (spokeperson), A. Vlad, G. Hautier, L. Piraux). Development of microbatteries, using hydride-based solid-state electrolytes. |

- Collaboration with Michael Hirscher (Max Planck Institute for Intelligent Systems, Stuttgart, Allemagne) on hydrogen storage in porous solids.
- Collaboration with Torben R. Jensen (University of Aarhus, Danemark) on the synthesis and the characterization of complex hydrides.
- Collaboration with Swiss-Norwegian Beam Lines, European Synchrotron Radiation Facility (ESRF, Grenoble, France) on structural studies of crystalline materials
- Tasks 32/40 expert (Hydrogen Implementing Agreement) of the International Energy Agency
- delegate to the ESRF council from BeNeSync consortium (Belgium, the Netherlands)
- chair of the FNRS contact group on synchrotron radiation
- elected as a member of the International Steering Committee (ISC) of the International Symposium on Metal Hydrogen Systems (MH series), mandate for 10 years
- Representative of UCL to the national accompanying committee "European sources for synchrotron radiation and neutrons" (NAC SRN), Belgian Science Policy Office BELSPO
- Co-chair of **MH2024** with Fermin Cuevas. The conference is usually attended by >400 participants
- Vice co-chair of the **Gordon Research Conference** (GRC) on Hydrogen-Metal in 2023, and co-chair of the GRC in 2025 with Rana Mohtadi

## Main relevant publications


- H. Oh, N. Tumanov, V. Ban, X. Li, B. Richter, M. Hudson, C. Brown, G. Iles, L. Daemen, D. Wallacher, R. Balderas-Xicohtencatl, A. Ramirez-Cuesta, Y. Cheng, M. Heere, M. Hirscher, T. Jensen, **Y. Filinchuk** *Ultra-dense hydrogen in small pore hydridic framework* accepted in Nature Chem. (2023) DOI: 10.21203/rs.3.rs-1177691/v1
- X. Li, Y. Yan, T.R. Jensen, **Y. Filinchuk**, I. Dovgaliuk, D. Chernyshov, L. He, Y. Li, H.W. Li *Magnesium borohydride $Mg(BH_4)_2$ for energy applications: A review* Journal of Materials Science & Technology 161 (2023) 170-179.
- T. Zhang, T. Steenhaut, M. Devillers, **Y. Filinchuk** *Release of Pure $H_2$ from $Na[BH_3(CH_3NH)BH_2(CH_3NH)BH_3]$ by Introduction of Methyl Substituents* Inorganics 11 (2023) 202.
- J. Wang, T. Steenhaut, H.W. Li, **Y. Filinchuk** *High Yield Autoclave Synthesis of pure $M_2B_{12}H_{12}$ (M = Na, K)* Inorg. Chem. 62 (2023) 2153-2160.
- T. Zhang, T. Steenhaut, X. Li, F. Devred, M. Devillers, **Y. Filinchuk** *Aluminum methylamidoborane complexes: mechanochemical synthesis, structure, stability and reactive hydride composites* Sustainable Energy Fuels 7 (2023)1119-1126.
- I.E. Golub, M. Heere, V. Gounaris, X. Li, T. Steenhaut, J. Wang, K. Robeyns, H.W. Li, I. Dovgaliuk, K. Ikeda, G. Hautier, **Y. Filinchuk** *Structural insight into the magnesium borohydride–ethylenediamine solid-state Mg-ion electrolyte system* Dalton Transactions 52 (2023) 2404-2411.
- T.H. Rupam, T. Steenhaut, M.L. Palash, **Y. Filinchuk**, S. Hermans, B.B. Saha *Thermochemical energy applications of green transition metal doped MIL–100 (Fe)* Chemical Engineering Journal 448 (2022) 137590.
- M. Reberc, M. Mazaj, J. Stare, M. Pockaj, G. Mali, X. Li, **Y. Filinchuk**, R. Cerny, A. Meden *Trinuclear Magnesium Imidazolate Borohydride Complex* Inorg. Chem. 61 (2022) 12708-12718.
- T. Steenhaut, S. Lacour, G. Barozzino-Consiglio, K. Robeyns, R. Crits, S. Hermans, **Y. Filinchuk** *Synthesis, Structure, and Thermal Stability of a Mesoporous Titanium(III) Amine-Containing MOF* Inorg. Chem. 61 (2022) 11084-11094.
- M. Benzaqui, M. Wahiduzzaman, H. Zhao, M. Rafiul Hasan, T. Steenhaut, A. Saad, J. Marrot, P. Normand, J.M. Grenèche, N. Heymans, G. De Weireld, A. Tissot, W. Shepard, **Y. Filinchuk**, S. Hermans, F. Carn, M. Manlankowska, C. Téllez, J. Coronas, G. Maurin, N. Steunou, C. *Serre A robust eco-compatible microporous iron coordination polymer for $CO_2$ capture* J. Mater. Chem. A 10 (2022) 8535-8545.

- Dovgaliuk I., Senkovska I., Li X., Dyadkin V., **Filinchuk Y.**, Chernyshov D. *Kinetic barriers and microscopic mechanisms of noble gas adsorption by nanoporous γ-$Mg(BH_4)_2$ obtained by means of sub-second X-ray diffraction* Angew. Chem. Int. Ed. 60 (2021) 5250-5256.
- Steenhaut T., **Filinchuk Y.**, Hermans S. *Aluminium-based MIL-100(Al) and MIL-101(Al) metal-organic frameworks, derivative materials and composites: synthesis, structure, properties and applications* J. Mater. Chem. A 9 (2021) 21483-21509.
- Le Ruyet R., Fleutot B., Berthelot R., Benabed Y., Hautier G., **Filinchuk Y.**, Janot R. *$Mg_3(BH_4)_4(NH_2)_2$ as inorganic solid electrolyte with high $Mg^{2+}$ ionic conductivity* ACS Appl. Energy Mater. 3 (2020**)** 6093-6097.
- Steenhaut T., Hermans S., **Filinchuk Y.** *Green synthesis of a large series of bimetallic MIL-100(Fe,M) MOFs* New J. Chem. 44 (2020) 3847-3855.
- Dovgaliuk I., Dyadkin V., Vander Donckt M., **Filinchuk Y.**, Chernyshov D. *Non-isothermal kinetics of Kr adsorption by nanoporous gamma-$Mg(BH_4)_2$ from in situ synchrotron powder diffraction* ACS Appl. Mater. Interfaces **12** (2020) 7710-7716.

Hirscher M., Yartys V.A., Baricco M., Bellosta von Colbe J., Blanchard D., Bowman R.C., Jr., Broom D.P., Buckley C.E., Chang F., Chen P., Cho Y.W., Crivello J.-C., Cuevas F., David W.I.F., de Jongh P.E., Denys R.V., Dornheim M., Felderhoff M., **Filinchuk Y.**, Froudakis G.E., Grant D.M., Gray E.M., Hauback B.C., He T., Humphries T.D., Jensen T.R., Kim S., Kojima Y., Latroche M., Li H.-W., Lototskyy M.V., Makepeace J.W., Møller K.T., Naheed L., Ngene P., Noréus D., Nygård M.M., Orimo S.-I., Paskevicius M., Pasquini L., Ravnsbæk D.B., Veronica Sofianos M., Udovic T.J., Vegge T., Walker G.S., Webb C.J., Weidenthaler C., Zlotea C. *Materials for hydrogen-based energy storage – past, recent progress and future outlook* J. Alloys Comp. 827 (2020) 153548. 39-page review


## Contact persons


**Prof. Yaroslav Filinchuk (yaroslav.filinchuk@uclouvain.be)**
**Prof. Sophie Hermans (sophie.hermans@uclouvain.be)**

# UCLouvain: Thermodynamics and fluid mechanics (TFL)

University of Louvain, Institute of Mechanics, Materials and Civil Engineering

Sustainable energy systems

Storage and use of H2

## General expertise of the research group

The **Sustainable Energy Systems research** team consists of Profs. H. Jeanmart and F. Contino.

**Prof. Hervé Jeanmart** works mainly on 3 energy-related themes: energy systems, biomass conversion and combustion. With his research team, he is studying the energy transition through the modelling of energy systems. In particular, his group is developing a tool for modelling energy systems in collaboration with EPFL, EnergyScope TD. Current work focuses on the multi-cell approach, agent-based optimisation and coupling with dispatch and economic models. Using EROI (Energy Return On Investment) as a metric, the group is studying the global potential of renewable energies in relation to energy accessibility and economic trajectories. At the component level, the research team is working on thermochemical conversion of biomass, primarily small-scale gasification, including close collaboration with Burkina Faso to develop a local technology. At a more fundamental level, the group is active in the combustion kinetics of oxygenated compounds and synthetic fuels. This includes an experimental approach to low-pressure burners, the study of combustion in HCCI engines and the development of kinetic models.

**Prof. Francesco Contino** works at both micro (cogeneration systems, heat storage, Carnot batteries, gas microturbines, hydrogen storage, etc.) and macro (region, country) levels to understand the key factors that will help us achieve a successful energy transition. In this context, he is developing new methods and making them affordable - in terms of computing costs - by developing efficient optimisers and rapid methods for quantifying uncertainty.
In the context of robust optimisation, he proposes alternatives that are less vulnerable to the uncertainties of the energy system's operating environment. Over the past ten years, he has used this technique to create robust designs for various energy systems, including gas

microturbines, solar photovoltaic systems with battery storage, hydrogen applications and other e-fuels. Finally, he is also interested in the concept of antifragility in optimisation under uncertainty, in order to take advantage of rare and major events (e.g. COVID, war in Ukraine), to improve the energy transition trajectory rather than suffer the consequences. He also integrates other disciplines into his research by studying the social practices associated with energy consumption and the impact of policies on the transition.

## Specific hydrogen- related expertise & research topics

- Experimental characterisation and modelling of cogeneration units (piston engines and gas turbines) powered by syngas, e-fuel (H2) and alternative fuels.
- Internal combustion engine characterisation of e-fuels (methane, methanol, ammonia, hydrogen).
- Robust Design Optimisation of e-fuel (ammonia & hydrogen) production systems, taking account uncertainties (essential in a context of fluctuating renewable production)
- Development of tools to model energy systems (whole-energy model) including uncertainties and the uncertain path towards a sustainable transition (EnergyScope);
- Optimisation of energy systems at different scales (consumer group, city, region, country) including detailed hour-by-hour energy storage using available and developing technologies.

## Available equipment/tools:

- Equipment to characterize combustion phenomena, with gas analysers, gas chromatography, mass spectrometer, etc.
- Low-pressure burners
- A 200 kW two-stage pilot gasifier (TGP)
- A drop-tube furnace for studying biomass conversion
- An HCCI test bench
- Cogeneration units
- Industrial compressor (delivering 1200 Nm3/h at 40bar)
- Several other research benches (ejector systems, syngas engines, etc.).
- Developer of EnergyScope TD

## Participating in RW/B/EU funded projects with H2 related research:

- **FLEXnCONFU** (EU H2020): to assess the role of ammonia as an energy carrier. The role of UCLouvain is to evaluate the impact of ammonia on the whole-energy system.
- **BEST** (ETF, SPF-FOD Belgium) https://best-energy.be : role of e-fuels for Belgium. The tasks here focus on different levels of the system from the micro scale to the macro scale.

- **METRIC** (FNRS): machine learning for reactive system simulations. The methodologies developed in METRIC will be applied to reactive systems (furnaces, engines, …) but will also give momentum to the current project.
- **BE_HyFE** (2021-2025) https://www.behyfe.be/, BE-HyFE is a Belgian academic collaboration project, funded by the federal Energy Transition Fund, bringing together all Belgian knowledge institutes to join forces in fundamental research on the topic of hydrogen.
- **FEDECOM** (EU HE 2022-2026) – Federated - system of systems- approach for flexible and interoperable energy communities

## Main relevant publications


- Rixhon X., Limpens G., Coppitters D., Jeanmart H., Contino F., *The Role of Electrofuels under Uncertainties for the Belgian Energy Transition*. Energies, Vol. 14, no.4027 (2021). doi:10.3390/en14134027.
- Contino F., Moret S., Limpens G., Jeanmart H., *Whole-energy system models: The advisors for the energy transition*. Progress in Energy and Combustion Science, Vol. 81, p. 100872 (2020). doi:10.1016/j.pecs.2020.100872
- Coppitters D., Verleysen K., De Paepe W., Contino F., *How can renewable hydrogen compete with diesel in public transport? Robust design optimization of a hydrogen refueling station under techno-economic and environmental uncertainty*. Applied Energy, Vol. 312, no., p. 118694 (2022). doi:10.1016/j.apenergy.2022.118694
- Lhuillier C., Brequigny P., Contino F., Mounaïm-Rousselle C., *Experimental study on ammonia/hydrogen/air combustion in spark ignition engine conditions*. Fuel, Vol. 269, no., p. 117448 (2020). doi:10.1016/j.fuel.2020.117448
- Coppitters D., De Paepe W., Contino F., *Robust design optimization and stochastic performance analysis of a grid-connected photovoltaic system with battery storage and hydrogen storage*. Energy, Vol. 213, no., p. 118798 (2020). doi:10.1016/j.energy.2020.118798
- Pochet M., Dias V., Moreau B., Foucher F., Jeanmart H., Contino F., *Experimental and numerical study, under LTC conditions, of ammonia ignition delay with and without hydrogen addition*. Combustion Institute Proceedings, 37, 621-629 (2019)


## Contact persons


**Francesco Contino,**
francesco.contino@uclouvain.be

**Hervé Jeanmart,**

herve.jeanmart@uclouvain.be

**Véronique Dias,**
veronique.dias@uclouvain.be

# UMons: Laboratory of Polymeric and Composite Materials (LPCM)

University of Mons, Faculty of Engineering and Architecture

Material developpment

Storage of H2

## General expertise of the research group

UMONS counts 7 faculties, 2 schools, 10 research institutes, 3 partner research centers, a dozen spin-off companies and operates on two campuses for nearly 8000 students and 90 research teams across 40 nationalities; strongly encourages interdisciplinarity both regionally and internationally and knowledge transfer. In Chemistry and Materials engineering holds the European label for "Research in Excellence", is 175th "publications most cited by peers", 170th "citation rate", 36th "publication rate in collaboration with other international institutions" and 1st/2d Belgian university/11 (U-Multirank 2018). The UMONS MATERIALS Institute offers research on synthesis and implementation methods, characterization and applications with end-of-life scenarios. As part of it, the LPCM (head: J.-M. Raquez) is internationally recognized in (i) polymer synthesis, (ii) polymer blends and (nano)materials, (iii) industry-relevant batch and continuous processes, (iv) polymer materials ecotoxicity and end-of-life. Knowledge is constantly transferred to Society via local and network-wide teaching/research and training, mobility and intersectoral exposure at all levels (students & professionals). LPCM EU projects count H2020-EJD, H2020-RISE, H2020-ERANET, FP-7, FP-6, and ERA-NET as well as National Programs.

## Specific hydrogen- related expertise & research topics

In the framework of the hydrogen-related expertise, LPCM is active in the design of polymeric composites with advanced properties for hydrogen storage. More specifically, innovative solutions will be addressed via the design of polymeric composites with key-features (fire-resistance, enhanced barrier properties, and so on.) using extrusion technologies and related techniques (plasma-based treatments).

## Available equipment/tools:

LPCM is equipped with the state-of-the-art equipements in the frame of polymeric composites as:Synthesis: ROP & RP equipments @ Lab-scale, 6 twin-screws extruders. 3D printing: SLA & FDM. Multi-scale characterization: 4 SEC, 1 automatic capillary viscosimeter; 1 automatic vapor phase osmometer/tonometer; 1 UV-VIS; 3 multinuclear NMR 600, 500 et 300 MHz; 2 FTIR; 2

viscosimeters; 1 Temperature-controlled tensiometer; 4 TGA (1 simultaneously coupled to a MS & FTIR); 4 DSC; 2 DMTA.

## Participating in RW/B/EU funded projects with H2 related research:

Industrial collaboration at national level & participation to Win4Excellence TiNTHyN

## Main relevant publications

Microwave Atmospheric Plasma : A versatile and Fast Way to Confer Antimicrobial Activity toward Direct Chitosan Immobilization onto Poly(lactic acid) Substrate, X. Carette, M. Herbin, P. Cabecas Segura, R. Wattiez, X. Noirfalise, C. Thai, P. Leclere, T. Godfroid, M. Boudifa, H. Kerdjoudj, O. Jolois, J.-M. Raquez, ACS Applied BioMaterials 2021, 4, p. 7445.
The micromechanics of graphene oxide and molybdenum disulfide in thermoplastic nanocomposites and the impact to the polymer-filler interphase, J. Cremonezzi, G. Pinto, R. Mincheva, R. Andrade, J.M. Raquez, G. Fechine, Composites Science and Technology 2023, 24320, Article number 110236.
Solid-State Modification of Poly(butylene terephthalate): Design of Process from Calorimetric Methods for catalyst Investigation to Reactive extrusion, C. Gerbehaye, K.V. Bernaerts, R. Mincheva, J.-M. Raquez, Eur. Polym. J. 2022, 166, P. 111010.

## Contact persons

**Prof. Jean-Marie RAQUEZ (jean-marie.raquez@umons.ac.be)**
**Prof. Rosica MINCHEVA (rosica.mincheva@umons.ac.be)**

# ULB – Chemistry of Surfaces, Interfaces and Nanomaterials (ChemSIN)

Synthesis of hydrogen by plasma, water electrolysis and plasma electrolysis ; fuel cells ; (electro)catalysis

Production of H2

## General expertise of the research group

ChemSIN (formerly Chani) is a research service of the Faculty of Sciences. It brings together 4 academics, 30 researchers, 4 technicians and 1 secretary. Research activities focus on the chemistry of atmospheric plasmas (F. Reniers), Catalysis (T. Visart), electrochemistry (T. Doneux) and nanoelectrochemistry (J. Ustarroz).

The studies cover various aspects of the chemistry of surfaces and interfaces since they relate to the modification, characterization and study of the reactivity of surfaces.
These studies carried out at the solid-solution interface and at the solid-gas interface relate to the modification of surfaces (metals, metal electrodes and polymers) by chemical or electrochemical means, by self-assembly as well as by plasma techniques.

Thin films, organized monolayers and nanostructured surfaces can thus be produced and characterized. Characterizations involve the use of a wide range of advanced (nanoscale) electrochemical methods, spectroscopy, microscopy, as well as contact angles.

The surface properties are evaluated mainly in connection with the development of "intelligent" materials, biosensors and electrocatalysis (environmental electrochemistry, batteries, fuel cells, electrolysis), electrodialysis, biocompatibility, development of barrier layers, etc.

## Specific hydrogen- related expertise & research topics

- Synthesis of H2 by atmospheric plasma and plasma electrolysis (in solution)
- Development of new electrocatalysts for water electrolysis
- Assessment of H2 electrocatalyst activity and durability with high-throughput experimentation, (*in-situ*) correlative microscopy and machine learning
- new catalysts for the catalytic synthesis of hydrogen (steam reforming of methane and water gas shift)
- new catalysts (e.g. for the Haber-Bosch process or plasma catalysis ammonia)

- barrier layers to hydrogen diffusion, membranes or functionalization of bipolar plates for fuel cells, anti-corrosion layers for the storage and transport of ammonia

## Available equipment/tools:

- 15 atmospheric plasma reactors and torches, with generators going from continuous DC, AC to nanopulse
- 3 high-resolution scanning electrochemical microscopes (SECCM, SECM) and ~10 electrochemical workstations (including FRA, EQCM, RDE, RRDE)
- micro-XPS for surface analysis, infrared spectroscopy, raman spectroscopy, AFM
- (atmospheric) mass spectrometry, gas chromatography
- *in-situ* electrochemical TEM holder (to study *operando* degradation of electrocatalysts)

## Participating in RW/B/EU funded projects with H2 related research:

- Plasma-ChemSIN (F.Reniers) is member of the EoS (Excellence of science, joint B-FNRS/FWO program) "PlaSyntH2" dedicated to the synthesis of hydrogen by plasma
- Plasma-ChemSIN is member of the FEDER-RW Decarbowal portfolio (project SynfonHy) dedicated to have an electrified circular loop hydrogen - nitrogen - ammonia
- Plasma-ChemSIN ismember of the EoS Nitroplasm project (finishing dec.2023) dedicated to the fixation of nitrogen by plasma (to nitrogen oxides and ammonia).
- F. Reniers was member of the GAZTON project (Greenwin-RW project) dedicated to the conversion of CO2 (and CH4) by plasma to make useful molecules and hydrogen
- F. Reniers was member of the Hylife and Innopem projects (RW) dedicated to the development of membranes and catalysts for hydrogen fuel cells
- Nano-ChemSIN (J. Ustarroz) is member of the Innoviris funded research project NDIAMO dedicated to develop advanced electron diffraction techniques for electrochemical applications, including H2 synthesis by water electrolysis.
- J. Ustarroz holds an ARC-Consolidator grant (RENEGADE) to study, among other topics, the initial stages of electrocatalyst degradation by local electrochemistry and in-situ TEM.
- J. Ustarroz was the PI of the FNRS-MIS project (EdNANO) to develop a nano-electrochemical platform to measure the electrochemical response of single nanoparticles.
- Plasma-ChemSIN (F.Reniers) and Nano-ChemSIN (J Ustarroz) are partners of the Win4Excellence " TinTHyN" PhD portfolio submitted to the RW (sept.2023), dedicated to fund PhD thesis on hydrogen research.

## Main relevant publications


- CO2–CH4 conversion and syngas formation at atmospheric pressure using a multi-electrode dielectric barrier discharge, A Ozkan, T Dufour, G Arnoult, P De Keyzer, A Bogaerts, F Reniers, Journal of CO2 utilization 9, 74-81 (2015)

- Disproportionation of nitrogen induced by DC plasma-driven electrolysis in a nitrogen atmosphere , C. Pattyn, N. Maira, M. Buddhadasa, E. Vervloessem, S. Iséni, N. Roy, A. Remy, M-P Delplancke, N. De Geyter, F. Reniers Green Chemistry 24 (18), 7100-7112 (2022)
- Plasma-catalytic ammonia synthesis in a DBD plasma: role of microdischarges and their afterglows , K van 't Veer, Y Engelmann, F Reniers, A Bogaerts , The Journal of Physical Chemistry C 124 (42), 22871-22883 (2020)
- Fuel cell electrodes from organometallic platinum precursors: an easy atmospheric plasma approach, D Merche, T Dufour, J Baneton, G Caldarella, V Debaille, N Job, F. Reniers, Plasma processes and polymers 13 (1), 91-104 (2016)
- Synthesis of Membrane-Electrode Assembly for Fuel Cells by Means of (Sub)-Atmospheric Plasma Processes,D Merche, T Dufour, J Hubert, C Poleunis, S Yunus, A Delcorte, P. Bertrand, F. Reniers, Plasma processes and polymers 9 (11-12), 1144-1153 (2012)
- Electrochemical behavior of electrodeposited nanoporous Pt catalysts for the oxygen reduction reaction. B Geboes, J Ustarroz, K Sentosun, H Vanrompay, A Hubin, S Bals, T. Breugelmans. ACS Catalysis 6 (9), 5856-5864 (2016)
- Mobility and poisoning of mass-selected platinum nanoclusters during the oxygen reduction reaction. J Ustarroz, IM Ornelas, G Zhang, D Perry, M Kang, CL Bentley, M Walker, PR Unwin. ACS Catalysis 8 (8), 6775-6790 (2018)
- Electrodeposition of nanostructured catalysts for electrochemical energy conversion: Current trends and innovative strategies. MB Lopez, J Ustarroz. Current Opinion in Electrochemistry 27, 100688
- Estimating pitting descriptors of 316 L stainless steel by machine learning and statistical analysis LB Coelho, D Torres, V Vangrunderbeek, M Bernal, GM Paldino, G Bontempi, J. Ustarroz. npj Materials Degradation 7 (1), 82 (2023)


## Contact persons


**F. Reniers (francois.reniers@ulb.be)**
**J. Ustarroz (jon.ustarroz@ulb.be)**

# CENTEXBEL

Material development

Production/storage/ transport

## General expertise of the research group

Centexbel Expertise

- Technical textiles
- Composite reinforcements
- Surface treatment & Coatings
- Material testing
- Recycling
- Ecodesign

## Specific hydrogen- related expertise & research topics

Development of technical textile and composite materials and associated processes to meet the need for functionalized membranes and high-performance, lightweight and durable composite materials for the green hydrogen sector.

## Available equipment/tools:

- Textile & Composite prototyping: knitting, weaving, braiding, TFP, light RTM, nano fiber e-spinning
- Pilot lines for surface treatments and Coatings

Labs for physical and chemical tests

## Participating in RW/B/EU funded projects with H2 related research:

Projects in the field of technical textiles, composites and coating

- COMP2BLADES - Composite with complex architecture for wind turbine blades
- VIBRA - Virtual Braiding - composite modeling with braided structures

- COBRACOMP – Braided Composites to improve competitiveness
- AACOMA - Accelerate Advanced Composite MAnufacturing (Interreg EMR)
- MACOBIO – Biocomposites for structural applications
- CISUFLO – Solvolyse of composite materials

## Main relevant publications

## Contact persons

**Ing. Bernard PAQUET**, R&D manager « Technical Textiles and Composites »
Email : bp@centexbel.be

**PhD. Jun YIN,** Researcher « Technical Textiles and Composites »
Email : jy@centexbel.be

**Ing. Baptiste HERLIN,** Contact Textile Technology Platform, Researcher « TT & C »
Email : bhe@centexbel.be

# Use of hydrogen

# ULiège : Nanomaterials, Catalysis, Electrochemistry (NCE)

University of Liège, Faculty of Applied Sciences, Department of Chemical Engineering

Design of catalysts for low temperature fuel cells
Fuel cell materials characterization

Use of H2

## General expertise of the research group

The Nanomaterials, Catalysis, Electrochemistry (NCE) laboratory, which is part of the Research Unit in chemical Engineering of ULiège, has developed a wide expertise in the conception and set-up of devices linked to chemical engineering based on an integrated approach, from the preparation of materials and their extensive characterization to trials in prototype (continuous) reactors. The first part of the activities concerns the design and preparation of new materials with controlled pore texture at the nanoscale. The mastering of the synthesis process enables to perform scale-up studies. Activities about materials also deal with shaping or assembly for industrial applications. The second part of the activities concerns the building of test benches dedicated to the determination of the materials properties (activity of catalysts, performances of fuel cell or battery electrodes) and to the set-up of pilot devices for the production of a given material.

Since 2009, electrochemical engineering applications such as fuel cells constitute a major axis of the research at NCE, and is currently driven by its recognized expertise in the synthesis and study of carbon materials and catalysts. In all cases, the goal is to include new materials, often with specific nanostructuration, first in (composite) electrodes, then in full electrochemical devices. In addition, the competences in catalyst manufacturing and characterization acquired in the past in the framework of other applications is widely used here to combine the advantages of mastered pore texture and high metal dispersion. It is particularly critical in Proton Exchange Membrane fuel cells given that the cell performance is related to both the specific activity of the catalyst and the mass transport properties of the electrode.

In order to study fuel cells, the NCE laboratory has developed remarkable equipment for the manufacture and *in situ* characterization of Proton Exchange Membrane fuel cell components, among which fully automated house-built monocell and stack test benches, along with all the necessary equipment to manufacture electrodes and

Membrane-Electrodes Assemblies from their components; those operations are performed in a very reproducible manner which allows for very accurate characterization.

Thanks to several large-scale projects and related investments, the laboratory is able to cover the complete manufacture chain, from basis materials (including catalysts) to the complete cell that can be further integrated in a user system.

## Specific hydrogen- related expertise & research topics

- Research in the field of the constituent materials of PEM fuel cells (catalysts, membranes, bipolar plates), from their manufacturing to the study of their aging in representative conditions.
- Characterization of materials and assemblies for PEM fuel cells.
- Development of manufacturing techniques for PEM fuel cell components.
- Development of test-benches for the characterization of materials and cells, for mobile and stationary applications.

## Available equipment/tools:

- All the necessary equipment to manufacture and characterize carbon-supported metal and alloy catalysts, from the carbon synthesis to the metal deposition;
- Electrochemical characterization tools: 3-cell electrodes, rotating disk electrodes (RDEs), rotating ring disk electrodes (RRDEs), corrosion cells, dedicated (and adapted) potentiostats (4, among which 2 adapted for RRDEs);
- Tools for the manufacturing and characterization of Membrane-Electrodes Assemblies (MEAs – fuel cells) and electrodes: fully home-made (and versatile) automated spray-coater, one industrial spray-coater, two bar-coaters (one with heating platform), instrumented hot presses, high performance profilometer, cells for electrical and ionic conductivity measurements (adapted to composite electrodes made of ionic and electronic conductors like in fuel cell MEAs);
- Equipment for the measurement of contact resistance between layers of materials (under pressurization);
- Fully instrumented fuel cell test benches: 2 hydrogen/air 5 cm x 5 cm benches. A third test-bench will be acquired in 2024;
- One instrumented stack test bench, up to 10 kWel.

## Participating in RW/B/EU funded projects with H2 related research:

- 2012-2018: European project FCH-JU-2011-1 - SWARM ("Demonstration of Small 4-Wheel fuel cell passenger vehicle Applications in Regional and Municipal transport"). Collaboration between 20 European partners (public and private); Coordinator: PLANET (Planungsruppe Energie & Technik GbR, Germany). Total budget: €19,665,734 (EC contribution: €6,978,279) - ULiège-NCE budget: €330,420 (EC contribution: €216,630).

- 2014-2018: ENERGINSERE call – HYLIFE project (agreement no. 1410135): "Long-life materials for PEM hydrogen-air fuel cells". Promoter: N. Job (ULg-LGC), in partnership with ULB (Pr. F. Reniers), UNamur (Pr. J.-J. Pireaux), Materia Nova (M. Poelman) and INP-Grenoble (F. Maillard). Overall budget: €2,431,118.44. ULiège-NCE budget: €906,707.50.

- 2014-2017: IDS-FunMat project 2014/04, doctoral thesis under joint supervision ULg – INP-Grenoble. Promoters: N. Job, F. Maillard (INP-Grenoble): "Hollow nanoparticles for low cost, high activity and durability PEMFC electrocatalysts (HOLLOW)". Doctoral scholarship (3 years).

- 2014-2021: FEDER, "Multifunctional films" portfolio - INOXYPEM project: "Prototyping of coated steel bipolar plates for PEM fuel cells". Promoter: N. Job (ULg-LGC) in partnership with CRM-Group (A. Lafort), UNamur (J.-J. Pireaux), ULiège-LTAS (P. Duysinx), CENAERO (C. Goffaux). Overall budget: €1,831,257 - ULiège-NCE budget: €675,279.

- 2016-2019 : Walloon Region ENERGIE – HYSTACK (agreement n°1550260) : « Design of a fuel cell test bench for stacks up to 10 kW ». Budget : €396.037,65.

- 2018-2021 : F.R.S.-FNRS – HOLCAT (PDR/OL T.0247.18) : « Hollow PtCo catalysts supported on carbon xerogels for Proton Exchange Membrane fuel cell cathode ». Budget : €204.000.

- 2021-2026: Energy Transition Fund Project, ETF-BeHYFE – Belgian Hydrogen Fundamental Expertise. Structuring hydrogen research network in Belgium: funding of 16 collaborative doctoral theses across the entire hydrogen value chain. Coordinator: UGent. Participants: KULeuven, UC Louvain, UAntwerpen, UHasselt, VITO, IMEC, VKI, VUB, ULB, ULiège, UMons, WaterstofNet, TWEED. 1 thesis funded at NCE, 0.5 thesis funded at PEPs (UR ChemEng). Total budget: €4,507,809. ULiège-NCE budget: €324,300.

## Main relevant publications

Book chapters

M. Chatenet, N. Job, F. Maillard. Basics of PEMFC including the use of carbon-supported nanoparticles. *In*: New and Future Developments in Catalysis; Catalysis by Nanoparticles. S. Suib (Ed.), 1st edition, Elsevier, 2013, pp. 401-423, ISBN: 9780444538741.

F. Maillard, N. Job, M. Chatenet. Approaches to synthesize carbon-supported platinum-based electrocatalysts for proton-exchange membrane fuel cells. *In*: New and Future Developments in Catalysis. Batteries, Hydrogen Storage and Fuel Cells; S. Suib (Ed.), 1st edition, Elsevier, 2013, pp. 407-428, ISBN: 9780444538802.

N. Job. Carbon gels for electrochemical applications. *In*: Organic and carbon gels: from laboratory synthesis to applications, M. Aegerter, M. Prassas (Eds.), Series Advances in Sol-Gel Derived Materials and Technologies, Springer International Publishing, 2019, pp. 149 - 189. ISBN: 978-3-030-13897-4.

Articles in international journals (selected)

F. L. Deschamps, J. G. Mahy, A.F. Léonard, N. Job. Rotating disk electrode measurements on low and high loading catalyst layers: Diffusion limitations and application to Pt catalysts supported on porous micrometric carbon xerogel particles designed for proton exchange membrane fuel cells. *Journal of Electroanalytical Chemistry* 933 (2023) 117279.

F. L. Deschamps, J. G. Mahy, A.F. Léonard, S.D. Lambert, A. Dewandre, B. Scheid, N. Job. A practical method to characterize PEMFC catalyst layer topography: application to two coating techniques and two catalyst supports. *Thin Solid Films* 695 (2020) 137751.

A. Zubiaur, N. Job. Streamlining of the synthesis process of Pt/carbon xerogel electrocatalysts with high Pt loading for the oxygen reduction reaction in proton exchange membrane fuel cells applications. *Applied Catalysis B* 225 (2018) 364-378.

P.Y. Olu, N. Job, M. Chatenet. Evaluation of anode (electro)catalytic materials for the direct borohydride fuel cell: methods and benchmarks. *Journal of Power Sources* 327 (2016) 235-257.

P.-Y. Olu, F. L. Deschamps, G. Caldarella, M. Chatenet, N. Job. Investigation of platinum and palladium as potential anodic catalysts for direct borohydride and ammonia-borane fuel cells. *Journal of Power Sources* 297 (2015) 492-503.

N. Job, S. D. Lambert, A. Zubiaur, C. Cao, J.-P. Pirard. Design of Pt/carbon xerogel catalysts for PEM fuel cells. *Catalysts* 5 (2015) 40-57.

A. Zubiaur, M. Chatenet, F. Maillard, S. Lambert, J.-P. Pirard, N. Job. Using the Multiple SEA method to synthesize Pt/Carbon xerogel electrocatalysts for PEMFC applications. *Fuel Cells* 14 (2014) 343-349.

N. Job, M. Chatenet, S. Berthon-Fabry, S. Hermans, F. Maillard. Efficient Pt/carbon electrocatalysts for Proton Exchange Membrane fuel cells: avoid chloride-based Pt salts! *Journal of Power Sources* 240 (2013) 294-305.

N. Job, S. Lambert, M. Chatenet, C.J. Gommes, F. Maillard, S. Berthon-Fabry, J.R. Regalbuto, J.-P. Pirard. Preparation of highly loaded Pt/carbon xerogel catalysts for PEM fuel cells by the Strong Electrostatic Adsorption method. *Catalysis Today* 150 (2010) 119-127.

N. Job, F. Maillard, J. Marie, S. Berthon-Fabry, J.-P. Pirard, M. Chatenet. Electrochemical characterization of Pt/carbon xerogel and Pt/carbon aerogel catalysts - first insights into the influence of the carbon texture on the Pt nanoparticles morphology and catalytic activity. *Journal of Materials Science* 44 (2009) 6591–6600.

N. Job, S. Berthon-Fabry, M. Chatenet, J. Marie, M. Brigaudet, J.-P. Pirard. Nanostructured carbons as catalyst supports for PEM fuel cell electrodes. *Topics in Catalysis* 52 (2009) 2117-2122.

N. Job, J. Marie, S. Lambert, S. Berthon-Fabry, P. Achard. Carbon xerogels as catalyst supports for PEM fuel cell cathode. *Energy Conversion and Management* 49 (2008) 2461-2470.

PhD thesis

P.-Y. Olu (2015), Study of the anode for the Direct Borohydride Fuel Cell, 201. Co-supervision with M. Chatenet (INP-Grenoble, France), IDS-FunMat program. https://hdl.handle.net/2268/188808

T. Asset (2017). Hollow nanoparticles for low cost, high activity and durability PEMFC electrocatalysts. Co-supervision with F. Maillard (INP-Grenoble, France), IDS-FunMat program. https://hdl.handle.net/2268/214971

A. Zubiaur (2017). Development of new catalysts for Proton Exchange Membrane Fuel Cells (PEMFCs). https://hdl.handle.net/2268/216303

F. Deschamps (2022). Mise au point de méthodes d'étude de catalyseurs supportés sur carbones nanostructurés pour piles à combustible à membrane échangeuse de protons. https://hdl.handle.net/2268/289356

## Contact persons

**Prof. Nathalie Job**
Université de Liège - UR Chemical Engineering
Nanomaterials, Catalysis, Electrochemistry (NCE)
Quartier Agora, B6a, Sart-Tilman
allée du 6 août, 11
4000 Liège
Belgium
Nathalie.Job@uliege.be
+32 4 366 3537

# ULiège : LTAS-MN2L – Non-Linear Computational Mechanics

University of Liège, Applied Science faculty, Aerospace et Mechanical Engineering

Numerical simulation of fluid-structure interactions e.g. transient effect in cryogenic valves and sloshing in tanks

Storage/ transport and use of H2

## General expertise of the research group

The MN2L research group aims at developing digital simulation software in mechanics, thermo-mechanics and fluid-structure interactions.

## Specific hydrogen- related expertise & research topics

Among the latest developments from the MN2L Laboratory, designing hydrogen tanks (liquid and gaseous) in composites and metals occupies a significant place.
Another important aspect of the digital simulation developments is the sloshing of fluids in the tanks, as well as the dynamic behavior of valves and hydrogen distribution circuits in cryogenic conditions. These latter aspects constitute very attractive problems of fluid-structure interactions where the flow of the fluid influences mechanical deformations and where geometric modifications, for example of a valve opening or closing, influence the flow.

## Available equipment/tools:

- Simulation software based on Finite Element Method and Particle Finite Element Method
- Computing power

## Participating in RW/B/EU funded projects with H2 related research:

Skywin-Hypster project. “HYPSTER- HYdrogen Propulsion System: Thermique Et Régulation”. Leader: Safran Aero Boosters (SAB). Other involved companies: BeBlue, GDTech, DardenneV2i, Sirris and VKI.

## Main relevant publications


M.L. CERQUAGLIA, G. DELIEGE, R. BOMAN, V. TERRAPON & J.P. PONTHOT (2017) **Free-slip boundary conditions for simulating free-surface incompressible flows through the Particle Finite Element Method.** *International Journal for Numerical Methods in Engineering,* Vol. 110, pp. 921-946.

M.L. CERQUAGLIA, G. DELIEGE, R. BOMAN & J.P. PONTHOT (2017) **The Particle Finite Element Method for the numerical simulation of bird strike.** *International Journal of Impact Engineering* 109 (2017) 1-13.

M.L. CERQUAGLIA, D. THOMAS, R. BOMAN, V. TERRAPON & J.P. PONTHOT (2019) **A fully partitioned Lagrangian framework for FSI problems characterized by free surfaces, large solid deformations and displacements, and strong added-mass effects.** *Computer Methods in Applied Mechanics and Engineering* 348 (2019) 409-442

B.J. BOBACH, R. BOMAN, D. CELENTANO, V. TERRAPON & J.P. PONTHOT (2021) **Simulation of the Marangoni Effect and Phase Change Using the Particle Finite Element Method.** *Applied Sciences, 11.* https://doi.org/10.3390/app112411893

FERNANDEZ, S. FEVRIER, M. LACROIX, R. BOMAN & J.P. PONTHOT (2022) **Generalized α-scheme in the PFEM for velocity-pressure and displacement-pressure formulations of the incompressible Navier-Stokes equations.** I*nternational Journal for Numerical Methods in Engineering*, Vol. 124/1, pp. 40-79

E. FERNANDEZ, S. FEVRIER, M. LACROIX, R. BOMAN, L. PAPELEUX & J.P. PONTHOT (2023) **A Particle Finite Element Method based on Level–Set functions.** Journal of Computational Physics 487 112187.


## Contact persons


**Prof. Jean-Philippe Ponthot**
jp.ponthot@uliege.be
http://metafor.ltas.ulg.ac.be/

# ULiège : Products, Environment, Processes (PEPs)

University of Liège, Applied Sciences faculty, Department of Chemical Engineering

Experimental and modeling study of chemical & energy processes

Focus on the use of H2 for CO2 capture and re-use applications (CCU)

## General expertise of the research group

The **PEPs group** (Products, Environment and Processes, about 40 researchers) is part of the Department of Chemical Engineering at ULiège. In the PEPs group we are active in the fields of (bio)chemical reaction engineering, thermal and mechanical unit operations, process simulation, low carbon energy systems, $CO_2$ capture and re-use, life cycle assessments (LCA) and sustainable development. The main objective of the research unit consists in optimizing performance and energy efficiency of processes in order to inflict minimal harm on the environment. This includes the corresponding fundamentals, especially mass and energy transfers and multi-phase fluid dynamics. A strength of our approach is to link the different scales in time and space:

- starting from microscopic and even molecular level
- having a strong focus on the equipment level in experiment as well as modelling
- reaching up to the simulation of entire processes
- evaluating the economic and environmental impacts for large-scale deployment

This allows us to reliably describe and optimize equipment performance based on physically sound modelling, which even includes extrapolation beyond the region of experiments. These tools permit a knowledge-based optimization of equipment design and operation parameters, as a basis for safe, sustainable and profitable scale-up of the processes. Indeed, the simulation of entire processes together with Life Cycle Assessment as eco-design support guide the optimization on the process level, where economic as well as environmental parameters are included in the evaluation. Experimental infrastructures are available for model development and validation, covering a wide range of applications. In addition, adequate chemical analysis

equipment is used to determine gas and liquid phase compositions. Moreover, the majority of our methods and applications are developed in cooperation or at least in close contact with industry, including essentially all major chemical companies and a variety of local and European SMEs.

## Specific hydrogen- related expertise & research topics

- Use of hydrogen for CO2 hydrogenation reactions, including power-to-fuel and power-to-kerosene.
- Process modeling and optimisation, including techno-economic assessment and process design
- Experimental design of pilot-scale benches for CO2 capture and re-use (CO2-to-kerosene)

## Available equipment/tools:

- Process modeling using Aspen One simulation tools, expertise available with following tools: Aspen Plus, Aspen dynamics, Aspen Custom Modeler…
- AEM electrolyser, capacity of 1.5 $Nm^3/h$
- Experimental test benches for CO2 hydrogenation reactions: reverse Water-Gas-Shift reaction, Fischer-Tropsch synthesis (under construction)

## Participating in RW/B/EU funded projects with H2 related research:

- PROCURA (2020-2025): Project funded by the Belgian Energy Transition Research, its objective is to propose a roadmap for Power-to-X and carbon capture & utilization technologies in Belgium. https://procurabelgium.be/en
- 2021-2025: TRILATE: Project funded by the Belgian Energy Transition Fund. The TRILATE project studies the energy transition towards low-carbon processes in industrial clusters located in Belgium, The Netherlands and Germany. The role of ULiège is to provide process models for innovative low-carbon technologies that will then be used in system studies and strategic planning. https://www.ugent.be/ea/emsme/en/research/eelab/ecm/trilate
- 2021-2025: Be-HyFE: BE-HyFE stands for Belgian Hydrogen Fundamental Expertise. The aim of the project is to create a Belgian homebase for academic hydrogen expertise by establishing a core group of 16 broadly trained and highly networked early-stage researchers who can, together with their extended academic peer-network, support the Belgian industry in finding both technological and societal solutions to essential hydrogen challenges. https://www.behyfe.be/

- 2023-2025: FEDER, Decarbowal, CirculaCO2: Experimental and modeling study of the challenges towards a circular economy of CO2
- 2022-2025: Neutral-Kero-Lime (Walloon region & European Green Deal) : The NKL (Neutral-Kero-Lime) project brings together major industrial and academic players in Wallonia with the objective of creating important technological parts for the e-kerosene, lime and energy industries. More specifically, the backbone of this project revolves around the production of e-kerosene within Fischer-Tropsch reactors powered by green hydrogen and CO2 captured at the lime kiln outlet.
- 2022-2026: Antoine Rouxhet, FRIA scholarship: Experimental and modelling study of a reverse water-gas shift reaction unit for integration in a Power-to-X process.
- 2021-2025: European Green Deal, Environment and Energy transition platforms, Wallonia-Bruxelles Federation: Funding of remarkable experimental infrastructure for the energy transition. https://nextgenbelgium.be/fr/projet/les-universit%C3%A9s-francophones-font-des-recherches-sur-la-transition-%C3%A9nerg%C3%A9tique

**Official participation in projects abroad, as an unfunded partner :**

**Informal collaborations :**

- Expert for the Future of gas panel: Le rôle des vecteurs énergétiques gazeux dans une Belgique climatiquement neutre, SPF Economie. https://economie.fgov.be/fr/publications/le-role-des-vecteurs

## Main relevant publications

orbi.uliege.be/profile?uid=p012581

## Contact persons

**Grégoire LEONARD**
**g.leonard@uliege.be**

UMONS
Université de Mons

# UMons: Thermal Engineering and Combustion Unit (TRMI)

Numerical and experimental studies

Use of H2

## General expertise of the research group

**TRMI is the laboratory that brings together all research and teaching activities of the UMONS around heat transfer, and combustion. By specializing our research activities on energy in buildings and industry, as well as its sustainable production, we contribute to tackling the engineering challenges of today and tomorrow: Towards sustainable energy for all!**
**More specifically, the expertise of the research group can be found in the modelling, designing, and experimental testing of novel small-scale, highly-flexible and efficient, carbon-clean solutions towards sustainable cogeneration in decentralized applications, with a particular focus on micro gas turbines.**

## Specific hydrogen- related expertise & research topics

- **hydrogen combustion in (micro) gas turbine combustors: numerical expertise and limited experimental expertise for hydrogen combustion in industrial micro gas turbine combustors, including flame studies, the impact of dilution, design of 100% hydrogen combustors, etc.**
- **impact of hydrogen utilization as fuel on (micro) gas turbine cycle performance: both numerical and experimental expertise on the performance assessment**
-

## Available equipment/tools:

- **3 micro gas turbines (3 kW, 20 kW and 100 kW) which are partially H2 capable (up to 23% for the 3 kW, at least 10% for the 100kW unit and to be determined for the 20 kW). Research activities currently include the design of H2 combustors for each of these turbines**
- **30kW flameless furnace**
- **fuel mixing station with a thermal capacity of up to 50kW**
- **validated cycle models of the micro gas turbines and large scale turbines**
- **numerical tool for assessing flame stability when switching to hydrogen and stabilizing through water injection or EGR dilutions.**

## Participating in RW/B/EU funded projects with H2 related research:

- BEST project (ETF SPF Economie)
- BE-HyFE project (ETF SPF Economie)
- Hydrogenate (FRNS project, partner ULB )

## Main relevant publications

full list available on: https://staff.umons.ac.be/ward.depaepe/pubsfr.html)


- Rigaud, J., De Paepe, W., & Laget, H. (07 October 2022). Thermodynamic Assessment of the Conversion of a Typical CCGT Power Plant to a Fully E-Fuel Fired Unit. "Journal of Engineering for Gas Turbines and Power, 144" (12), 121012 (11. doi:10.1115/1.4055713
- Mendoza morales, M. J., Verhaeghe, A., Bricteux, L., Blondeau, J., & De paepe, W. (28 September 2023). Is Blue Hydrogen a Better Alternative Than Post-Combustion Carbon Capture for Combined Cycle Gas Turbines? A Thermodynamic Point of View. "Proceedings of ASME Turbo Expo 2023: Turbomachinery Technical Conference and Exposition, 2". doi:10.1115/gt2023-101986
- Ferrarotti, M., De Paepe, W., & Parente, A. (21 August 2021). Reactive structures and NOx emissions of methane/hydrogen mixtures in flameless combustion. "International Journal of Hydrogen Energy, 46" (68), 34018-34045.
- Pappa, A., Bricteux, L., Bénard, P., & De Paepe, W. (26 February 2021). Can water dilution avoid flashback on a hydrogen enriched micro Gas Turbine combustion? - a Large Eddy Simulations study. "Journal of Engineering for Gas Turbines and Power, 143" (4), 041008.
- Devriese, C., Bastiaans, R., & De Paepe, W. (30 September 2020). Opportunities, Advances and Challenges of Hydrogen micro Gas Turbines. "Evolutions in Mechanical Engineering, 3" (2)


## Contact persons


Ward De Paepe, ward.depaepe@umons.ac.be (https://staff.umons.ac.be/ward.depaepe/)

# ULB - Aéro-Thermo-Mécanique (ATM)

Université Libre de Bruxelles, Faculty of Applied Sciences

Expertise and experiment studies

Use of hydrogen

## General expertise of the research group

The ATM department is active in the fields of mobility, green energy, cogeneration, aerodynamics, aeronautical engineering, aerospace engineering, thermodynamics, thermal engineering and applied mechanics. The ATM team has developed a broad know-how and undertakes research projects applying this know-how for theoretical matters, numerical simulations and also test benches and experimental investigations.

## Specific hydrogen-related expertise & research topics

- The use of hydrogen as a fuel for aeronautical and terrestrial applications with European projects such as Cryoplane, Enfica-FC or CHAT (aeronautics) and SWARM (land transport).
- Techno-economic analysis and safety assessment for STIB-MIVB future fleet of H2 buses, and technical implementation of this solution with the manufacturer Vanhool.
- Experience in H2 combustion in gas turbines (P. Hendrick) and furnaces, particularly with flameless combustion with very low NOx and oxycombustion (A. Parente), as well as with digital and experimental simulation activities with several test benches (up to 450 kW on the output shaft).
- Development of methodological and software tools enabling the deployment and management of a multi-energy EC integrating a hybrid solution of electric and hydrogen storage, in a collective self-consumption context.
- Involvement in Be-Hyfe through two theses : “Study of low-cost compressors for GH2 storage at high pressure” and “Safety of operations and logistics using GH2 and LH2”.
- Implementation of a University Certificate in Hydrogen application, a training program towards candidates with a higher-education degree in science and/or technology, who are or would like to be active in the hydrogen field.

## Available equipment/tools:

- ULB-PEMFC test bench, which evaluates the global efficiency of a PEMFC when operating as a µ-CHP system for households.
- Acquisition of Solenco PowerBox thanks to the Walloon recovery plan funding. It is a cogeneration unit consisting of a reversible PEM Fuel Cell. It produces electricity and heat from renewable electricity, and hydrogen in case of electrical production excess.

## Participating in RW/B/EU funded projects with H2 related research:

- Cryoplane (EC FP5)
- USE-HAAS (EC FP6)
- ENFICA-FC (EC FP6)
- SWARM (EC FCH JU)
- TeacHy (EC FCH JU)
- CHAT (EC FP7)
- BE-HyFE (ETF, SPF Economie)
- LOOP-FC (SPW)
- H2CoopStorage (SPW, EC Horizon 2020)
- Hefaistos (ETF)
- HyAcademy.eu - *to start on Jan 1st, 2024* (HORIZON-JTI-CLEANH2-2023-1)

## Main relevant publications

Garcia Arenas, J.; Hendrick, P.; Henneaux, P. Optimisation of Integrated Systems: The Potential of Power and Residential Heat Sectors Coupling in Decarbonisation Strategies. *Energies* **2022**, *15*, 2638. https://doi.org/10.3390/en15072638

## Contact persons

**P. Hendrick (patrick.hendrick@ulb.be)**
**A. Parente (alessandro.parente@ulb.be)**
**A. Coussement (axel.coussement@ulb.be)**

# Hydrogen general topics

# ULiège : MMS – Metallic Materials for Additive Manufacturing

University of Liège, Applied Science faculty, Aerospace et Mechanical Engineering

Relationships between the processing parameters, microstructures, mechanical and thermophysical properties of metallic materials.

Hydrogen general topics

## General expertise of the research group

The MMS research group aims at a better understanding of the relationships between the processing parameters, microstructures, mechanical (fatigue behaviour, wear resistance...) and thermophysical properties of metallic materials. In particular, the MMS laboratory is well equipped for the **study of microstructural changes** in metallic materials and for measuring thermophysical data up to high temperatures (**DSC** and **DTA** up to 1500°C, and Laser flash diffusivimeter up to 2000°C). In complement to these equipments, a **new quenching dilatometer equipped with a compression module** has recently been acquired (funding of 260.000 euros awarded by the Walloon Region and the European Funds for Regional Development under convention FEDER IAWATHA). This new equipment will be key to the identification of the laws determining the behaviour of materials under complex thermomechanical histories involving high heating/cooling rates that are typical of additive manufacturing processes.

Another major field of activity is the study of the **tribological behaviour** of materials from the nano- to the macro-scale thanks to the combination of a high temperature **"pin-on-disc" tribometer** and a **high temperature nano-indenter**. Furthermore, equipments for **corrosion testings** will be acquired in the near future (thanks to an "Equipment" subvention of 30.647 euros awarded by the Faculty of Applied Sciences (ULiège in June 2023).

The MMS laboratory is also well equipped for the **microstructural characterisation** of materials, including equipments for sample preparation - microcutter, automated grinder and polisher... – and several optical microscopes. The optical microscope Olympus BX60M, with its motorised platform, is particularly well suited for carrying out image analysis on large areas e.g. to assess the metallurgical health of AM components.

Over the last few years, the group has been studying very actively the **additive manufacturing of metallic materials** (e.g. Ti- and Al-based alloys, stainless or high speed steels and metal matrix composites). Additive processes are characterized by ultra-fast heating and cooling rates that result in strongly out-of-equilibrium microstructures (epitaxial solidification, high residual stresses, obtention of supersaturated solid solutions…). In particular, epitaxial solidification and its consequences in terms of anisotropic microstructures and usage properties, have been investigated in Ti-based alloys processed by both powder-bed (selective laser melting) and by direct powder-feed (laser cladding) processes. Previous or ongoing works of the MMS unit in the field of laser cladding include the processing of thick tool steel deposits and stainless steel matrix composites. Special attention has also been given to the effect of microstructural heterogeneities and of post-processing thermal treatments on the mechanical properties e.g. of LBPF AlSi10Mg parts. Until now, activities in the field of additive manufacturing have been carried out in collaboration with various partners (Sirris, AnyShape…) which provided the necessary samples and/or access to AM equipments. In order to further develop this line of work, the MMS Unit has recently acquired its own **laboratory-scale LPBF equipment**, i.e. an Aconity Mini LPBF printer that is operational since September 2022 and that is specifically dedicated to the investigation of new materials (fundings for this equipment were allocated by the Aerospace and Mechanical Engineering Department of the University of Liège, and on the MMS Laboratory own funds). Besides, a Pulverisette 6 **planetary mill, together with a sieving system** (Haver EML 200 Pure)**,** are already available in the MMS laboratory, that are suitable for powders mixing and preparation.

## Specific hydrogen- related expertise & research topics

Expertise concerning interactions between metallic materials and hydrogen, including hydrogen embrittlement phenomena, also in cryogenic conditions.
Failure diagnosis.

## Available equipment/tools:

See above, General expertise of the research group.

## Participating in RW/B/EU funded projects with H2 related research:

Skywin-Hypster project. “HYPSTER- HYdrogen Propulsion System: Thermique Et Régulation”. Leader: Safran Aero Boosters (SAB). Other involved companies: BeBlue, GDTech, DardenneV2i, Sirris and VKI.

## Main relevant publications

Numerous expertise reports (confidential)

## Contact persons

**Prof. Anne Mertens, Dr Jérôme T. Tchuindjang**
anne.mertens@uliege.be ; j.tchuindjang@uliege.be
https://orbi.uliege.be/ph-search?uid=u216524

# UCLouvain: Materials and Processes Engineering (IMAP)

University of Louvain, Institute of Mechanics, Materials and Civil Engineering

Material and process dvlpt, characterization & modelling

Hydrogen general topics

## General expertise of the research group

The researches of the IMAP pole aim at (1) improving the fundamental knowledge in the field of process engineering and inorganic materials. Application areas include in particular the effluent treatment, development of lightweight structural inorganic materials, process optimization, the study of the mechanical properties and the durability of inorganic materials, their manufacturing and shaping processes, the recycling and refining of metals, the processes of organic chemistry and petrochemistry, excluding polymers ; (2) creating an integrated research methodology to address the issue of sustainable development as described above, based on the expertise of all members of the pole in order to implement the life cycle engineering, and proposing strategies to select materials and processes.

## Specific hydrogen- related expertise & research topics

Prof. J. Proost's group focuses on the intensification of electrochemical processes, in particular the development of new reactors and electrodes for green hydrogen, green ammonia and green cement production.

Prof. P. Jacques' research activities concern among others (i) the study and the development of advanced metallic solutions (bulk, coatings, architectured structures), particularly for hydrogen storage and transport (also at cryogenic temperatures (down to 4K)); (ii) the characterisation, understanding and control of the interactions between hydrogen and metallic materials, particularly the hydrogen embrittlement phenomena; (iii) the analysis of the mechanical behaviour of metallic materials in presence of hydrogen.

Prof. De Wilde's group focuses on the (i) high-efficiency Steam Methane Reforming (SMR) with focus on the development of novel technologies for reduction of CO2 emissions, improved heat transfer and reduced pressure drop; (ii) auto-thermal chemical looping reforming and bi-reforming for facilitating CO2 capture with focus on reactor design and

catalyst selection and evaluation; (iii) chemical storage of clean power using green energy and focusing on novel technologies for methanation and transient operation and integrated CO2 capture and conversion; (iv) electrification of SMR with focus on high-efficiency reactors and electrical heat supply systems.

Prof. T. Pardoen's research concern the thermomechanical resistance of materials and systems used for the hydrogen production and storage, including novel concepts of structural laminated metal vessels.

## Available equipment/tools:

- Heat transfer-pressure drop rig for measurements with pellets or structured reactors used for hydrogen production - with 6-zone electrically heated furnace and detailed tube skin and gas temperature profile measurements and with air in wide flow rate range, up to commercially relevant.
- Kinetics testing lab for studying steam methane reforming and the inverse reaction, methanation - using specifically designed micro-packed bed reactor allowing studying intrinsic kinetics and on-line GC and MS.
- Kinetics testing lab with micro-electrobalance reactor to study catalyst deactivation and allowing transient measurements of catalyst weight and gas exit composition.
- Unique world class SMR pilot plant (safety certified) for hydrogen/syngas production with electrically heated furnace, electrical start-up boiler and recuperative steam generator - 4m tube length (30% of commercial), commercial tube diameter, 30% commercial capacity, max gas exit temperature of 870°C, max operating pressure of 28 barg - fully equipped with measurements of tube skin and gas temperature profiles, pressure drop, flow rates, and exit gas composition (on-line GC and MS) and with PLCs/logic - NG desulfurizer and on-line sulfur slip measurement.
- Fully certified pilote-scale 6kW alkaline water electrolyser, modularly designed for 4-32 cells using 300 cm2 electrodes
- Different single cell lab-scale water electrolysers in flow-through and flow-by mode, with electrode sizes ranging from 4-10 cm2, including high-resolution in-situ electrochemical diagnostics
- Processing (melting, casting, shaping, thermomechanical treatment, 3D printing) of metallic materials;
- Materials characterization tools (microscopy, tomography, thermal analysis, chemical analysis);
- Set-ups for mechanical testing (deformation and fracture) at temperature ranging from 4K to 1500K;

## Participating in RW/B/EU funded projects with H2 related research:

- EU project "NEXTAEC" : Materials for Next Generation Alkaline Electrolyzers. Project running from 04/2020-03/2024 under EU/H2020/NMBP (Call Industrial

Sustainability), with a total budget of 4.4 M€ (570 k€ for UCLouvain) ; Prof. J. Proost is WP leader for 3D electrode development and upscaling.

- EU Project "ENDURE" : Alkaline electrolysers with enhanced durability. Project running from 01/2024-12/2027 under EU-HORIZON-JTI-Clean Hydrogen Partnership, with a total budget of 2.5 M€ (450 k€ for UCLouvain) ; Prof. J. Proost is WP leader on design and fabrication of 3D structured laterally graded flow-engineered monolithic electrodes.
- EU project "KICStartH2" : Accelerating Hydrogen Uptake in Europe. Project running from 07/2022-06/2024 under the European Institute of Innovation and Technology (EIT) and its Knowledge and Innovation Communities (KICs), in particular the HEI Initiative on Innovation Capacity Building for Higher Education, with a total budget of 1.1 M€ (220 k€ for UCLouvain). Prof. J. Proost is WP leader on Dissemination Plan and Public Relations, and contributes directly to the Business Module Content Development.
- EU/Regional Walloon project "HeCO2" : Production of decarbonated hydrogen by water electrolysis. Project running from 07/2022-06/2026, partly funded also by the EU Recovery and Resilience Plan, with a total budget of 10 M€ (550 k€ for UCLouvain). Prof. J. Proost is WP leader on CFD modeling of single and multiphase flow on electrolyser cell and stack level.
- Belgian Federal Research project "MuSE" : Molecules at Sea. Project under the call Energy Transition Fund, running from 11/2023-10/2026 with a total budget of 1.7 M€ (300 k€ for UCLouvain). Prof. J. Proost is WP leader on hydrogen production from seawater electrolysis.
- Belgian Federal project “BE-HyFE” : Belgian Hydrogen Fundamental Expertise. 2 joint PhD UCLouvain – UGent (2021 – 2025) : “Controlling Hydrogen Embrittlement of High Strength Steels" (Prof. P. Jacques) and "Process implications of electrifying NH3 production" (Prof. J. Proost).
- Regional Walloon project "Faraday" : Integrated electrochemical reactor for the production of H2/O2/CO2 for CCU applications. Project under GreenWin call 31, running from 11/2021-10/2025 with a total budget of 4.0 M€ (490 k€ for UCLouvain). Prof. J. Proost is WP leader on the design and testing of a new electrolyzer-based process for cement clinker production.
- Project Win2Wal "Cryostress" (2021-2025, 1.400.000 Euro). “Compréhension et modélisation des comportements métallurgiques et mécaniques des aciers inoxydables pour le stockage de l'hydrogène liquéfié” (project with CRM and Aperam)
- ERC Advanced Grant HAPI (2023 - 2028) with the final objective to develop a new class of metal systems with extreme fracture toughness towards pressure vessel applications.
- FNRS PhD grant (Hannah Yang) (2022-2026). “Alloy design and assessment of the positive effect of hydrogen as an alloying element in austenitic steels”
- FNRS Research project grant (2022-2026). “Hydrogen embrittlement-activated toughening of architectured steels”
- Belgian Federal project “ReadHy” (Energy Transition Fund). “Development of an innovative testing method towards a better understanding of hydrogen-metal interactions to secure gaseous hydrogen transportation” (coll. CRM-UGent-UCLouvain).

## Main relevant publications


- A. Dechany, K. Van Geem and J. Proost, "*Process implications of electrifying ammonia production*", Current Opinion in Chemical Engineering (I.F. 6,6) 40 (2023) 100955
- F. Rocha, R. Delmelle, C. Georgiadis and J. Proost, "*Electrochemical performance enhancement of 3-D printed electrodes tailored for enhanced gas evacuation during alkaline water electrolysis*", Advanced Energy Materials (I.F. 29,7) 10 (2022) 107648
- F. Rocha, R. Delmelle, C. Georgiadis and J. Proost, "*Effect of pore size and electrolyte flow rate on the bubble removal efficiency of 3D pure Ni foam electrodes during alkaline water electrolysis*", Journal of Environmental Chemical Engineering (I.F. 7,7), 10 (2022) 107648
- F. Rocha, Q. de Radiguès, G. Thunis and J. Proost, "*Pulsed water electrolysis : a review*", Electrochimica Acta (I.F. 6,9), 377 (2021) 138052
- F. Rocha and J. Proost, "*Discriminating between the effect of pulse width and duty cycle on the hydrogen generation performance of 3-D electrodes during pulsed water electrolysis*", International Journal of Hydrogen Energy (I.F. 7,1), 46 (2021) 28925-28935
- J. Proost, "*Critical assessment of the production scale required for fossil parity of green electrolytic hydrogen*", International Journal of Hydrogen Energy (I.F. 7,1), 45 (2020) 17067-17075
- A. Delvaux, G. Lumbeeck, H. Idrissi and J. Proost, "*Effect of microstructure and internal stress on hydrogen absorption into Ni thin film electrodes during alkaline water electrolysis*", Electrochimica Acta (I.F. 6,9) 340, 135970 (2020)
- Z. Chehade, C. Mansilla, P. Lucchese, S. Hilliard and J. Proost, "*Review and analysis of demonstration projects on Power-to-X pathways in the world*", International Journal of Hydrogen Energy (I.F. 7,1) 44 (2019) 27637-2765
- J. Proost and A. Delvaux, "*In-situ monitoring of hydrogen absorption into Ni thin film electrodes during alkaline water electrolysis*", Electrochimica Acta (I.F. 6,9) 322, 134752 (2019)
- J. Proost, "*State-of-the art CAPEX data for water electrolysers, and their impact on renewable hydrogen price settings*", International Journal of Hydrogen Energy (I.F. 7,1) 44 (2019) 4406-4413
- R. Poulain, A. Klein and J. Proost, "*Electro-catalytic properties of (100), (110) and (111) oriented NiO thin films towards the oxygen evolution reaction*", Journal of Physical Chemistry C (I.F. 3,7) 122 (2018) 22252–22263

- A. Delvaux, Q. Van Overmeere, R. Poulain, and J. Proost, "*Enhanced oxygen evolution from (de-)alloyed nickel thin film electrodes*", Journal of the Electrochemical Society (I.F. 4,3)164 (2017) F1196-F1203
- Q. de Radiguès, P.-Y. Sévar, R. Santoro, F. Van Wonterghem and J. Proost, "*Electrochemical characterization of mass transport in porous electrodes*", Industrial & Engineering Chemistry Research (I.F. 4,3) 51 (2012) 14229–14235

Catalyst-enhanced autothermal chemical looping reforming: Intrinsic SMR kinetics and numerical simulation
Z He, F Minette, J De Wilde
Energy Conversion and Management 293, 117525, 2023

Structured catalyst reactor system for steam methane reforming
S Ratan, W Blasko, W Spieker, F Minette, J De Wilde
PTQ Magazine, 2023

Structured ZoneFlow™-Bayonet steam reforming reactor for reduced firing and steam export: pressure drop and heat transfer modelling and evaluation of the reactor performance
F Minette, LC de Almeida, J Feinstein, J De Wilde
Chemical Engineering Journal Advances 10, 100258, 2022

Numerical simulation of commercial scale autothermal chemical looping reforming and bi-reforming for syngas production
Z He, J De Wilde
Chemical Engineering Journal 417, 128088, 2021

Pressure drop and heat transfer of ZoneFlowTM structured catalytic reactors and reference pellets for Steam Methane Reforming
F Minette, LC de Almeida, S Ratan, J De Wilde
Chemical Engineering Journal 417, 128080, 2021

Multi-scale modeling and simulation of low-pressure methane bi-reforming using structured catalytic reactors
F Minette, J De Wilde
Chemical Engineering Journal 407, 127218, 2021

Intrinsic kinetics of steam methane reforming on a thin, nanostructured and adherent Ni coating
F Minette, M Lugo-Pimentel, D Modroukas, AW Davis, R Gill, MJ Castaldi, J De Wilde
Applied Catalysis B: Environmental 238, 184-197, 2018

Antoine Hilhorst, Pascal J. Jacques, Thomas Pardoen, Towards the best strength, ductility, and toughness combination: High entropy alloys are excellent, stainless steels are exceptional, Acta Materialia 260 (2023) 119280

M. Mandy, C. Georges, T. Sturel, P. Drillet, P.J. Jacques, On the analysis of the simultaneous uptake and desorption of different isotopes of gaseous hydrogen by advanced high strength steels, Scripta Materialia 161 (2019) 84–87

Hilhorst, A., Pardoen, T., Jacques, P.J., Optimization of the essential work of fracture method for characterization of the fracture resistance of metallic sheets, Engineering Fracture Mechanics, 2022, 268, 108442

## Contact persons

**Prof. Joris Proost (joris.proost@uclouvain.be)**
**Prof. Pascal Jacques (pascal.jacques@uclouvain.be)**
**Prof. Juray DE WILDE ( juray.dewilde@uclouvain.be )**

# UCLouvain: Heterogeneous catalysis

University of Louvain, Institute of Condensed Matter and Nanosciences

Material and process dvlpt, characterization & modellin

Hydrogen general topics

## General expertise of the research group

The **group of heterogeneous catalysis** is led by Profs. Damien Debecker and Eric Gaigneaux.

**Prof. Damien Debecker** works mainly on the development of heterogeneous catalysts and biocatalysts, using innovative preparation routes. Strategies to do so involve sol-gel chemistry, enzyme immobilization and encapsulation, spray processing, surface grafting, impregnation, etc. Targeted applications include the greener synthesis of high value chemicals through chemo-enzymatic cascade reactions, the upgrading of biomass and bio-based chemicals (alcohols, sugars, aromatics, short acids, triglycerides), and carbon capture and utilization. In this latter field, the focus is on the hydrogenation of $CO_2$ using green hydrogen, to obtain either methane or methanol. Beyond the catalytic reaction itself, the group investigates the chemical process as a whole, focusing also on *in situ* product separation/purification, carbon capture, biomass pre-treatments, enzyme selection, scale-up, transfer from batch to flow processes, assessment of new processes through sustainability metrics, etc.

The main scientific interests of **Prof. Eric Gaigneaux** are the preparation, scaling up and shaping of heterogeneous catalysts while controlling their morphology at the atomic and nanoscopic scales, their physicochemical characterization under operational *in situ*/*operando* conditions, and their applications in the production of bio- and e-fuels, abatement of air and water pollutants, transformation of hydrocarbons and (biomass derived) alcohols to more valuable molecules via selective oxidation / ammoxidation / dehydration / oxidative dehydrogenation / deoxydehydration, storage of hydrogen via the hydrogenation of nitrogen to ammonia and decomposition of the later, and (biomass related) fine chemistry with a

particular interest for epoxidation, Friedel-Crafts reactions and the valorization of (unsaturated) fatty acids.

## Specific hydrogen- related expertise & research topics

- Development (formulation, scaling up and shaping) of metal-based heterogeneous catalysts for the hydrogenation reactions of $CO_2$ (e.g. methanation) and of $N_2$ (to $NH_3$) used as a mean to store $H_2$ in the form of chemical energy vectors ($CH_4$, $CH_3OH$, $NH_3$, also called e-fuels).
- Experimental measurement of catalyst performance in the hydrogenation reactions of $CO_2$ and $N_2$ allowing kinetic and mechanistic studies on hydrogenation reactions
- Characterization of hydrogenation catalysts through various physico-chemical tools, to highlight the properties that decisively govern catalytic performance and unravel the structure-activity relationships in the perspective of further catalyst development
- Development of heterogeneous catalysts dedicated to the production of $H_2$ through ethanol dry reforming
- Development of dual function materials for the combined capture and hydrogenation of $CO_2$
- Development of catalysts dedicated to the enhancement of the hydrogenation of $N_2$ to $NH_3$ under plasma conditions
- Development of catalysts for the decomposition of $NH_3$, and the related production of $H_2$

## Available equipment/tools:

- Equipment to measure catalytic performance (continuous flow catalytic microreactors equipped with online gas chromatography and/or mass spectroscopy, batch catalytic microreactors with offline gas chromatography)
- Equipment for the preparation, scaling-up, shaping and regeneration of heterogeneous catalysts (precipitation/impregnation flasks, rotavapors, calcination furnaces, spray driers, pressurized autoclaves, plasma reactors, ball miller, pelletization etc.)
- Equipment (or access to) for the characterization of heterogenous catalysts: advanced spectroscopies (Raman, UV-Vis, IR, XPS, SIMS), microscopies (SEM, TEM), temperature-programmed-oxidation/reduction/desorption/etc experiments, textural measurements (specific surface area and porosity), chemisorption, thermogravimetry, X-ray diffraction, etc.

  Several techniques (UV-Vis, IR, Raman, XRD and soon XPS) are performed *in situ* / *operando* with the catalysts analyzed under realistic conditions (temperature, flow, pressure) of their use.

## Participating in RW/B/EU funded projects with H2 related research:

- **HEAT** (FSR 2023-2025) High Entropy Alloys for Thermocatalytic hydrogenation of $CO_2$
- **$CO_2$-spark** (FNRS – CR Dr. P. Hongmanorom 2022-2025) Spark ablation technology for the design of efficient $CO_2$ methanation catalysts
- **Recovery plan** (2023): acquisition of equipment to support research in the framework of the Energy Transition: XPS with high-pressure introduction and pretreatment chamber, hydrogenation reactors, IR spectrometer, temperature-programmed reactor.
- **2 CSC fellowships** (Y. Zhao and F. Yang) on $CO_2$ methanation and on the dry reforming of ethanol
- **NanoCat$CO_2$** (2020-2025) Joined research program between UCLouvain, ETH Zürich and Chulalongkorn University on the understanding of interfacial effects in $CO_2$ methanation catalysts
- **CATALYSTNH3SYNTHESIS** (H2020-Marie S Curie Action, 2019-2020): Synthetically Tuned Atomic Ordering and Electronic Properties of Nano-Intermetallic Compounds for the Ammonia Synthesis
- **Industrial project** (confidential, 2019-2024): formulation, scaling-up and shaping of novel catalysts for the production of ammonia via the hydrogenation of $N_2$
- **FEDER Synfonhy** (2023-2025): formulation and shaping of catalysts to enhance the chemical storage of $H_2$ in ammonia under plasma conditions, and the decomposition of the later

## Main relevant publications


- *Effect of the size and distribution of supported Ru nanoparticles on their activity in ammonia synthesis under mild reaction conditions*
  C. Fernández, C. Sassoye, C. Sanchez, D.P. Debecker, P. Ruiz*
  Applied Catalysis A: General, 474 (2014) 194-202
- *Insights in the mechanism of deposition and growth of RuO2 colloidal nanoparticles over alumina. Implications on the activity for ammonia synthesis*
  Camila Alejandra Fernández, Capucine Sassoye, Nicolas Flores, Néstor Escalona, Eric M Gaigneaux, Clément Sanchez and Patricio Ruiz
  Applied Catalysis A, 502 (2015) 48-56.
- *Disclosing the synergistic mechanism in the catalytic activity of different-sized Ru nanoparticles for ammonia synthesis at mild reaction conditions*
  Camila Fernández, Chiara Pezzotta, Eric M. Gaigneaux, Nicolas Bion, Daniel Duprez and Patricio Ruiz
  Catalysis Today, 251 (2015) 88-95.
- *$CO_2$ hydrogenation with shape-controlled Pd nanoparticles embedded in mesoporous silica: Elucidating stability and selectivity issues*
  J. Martins, N. Batail, S. Silva, S. Rafik-Clement, A. Karelovic, D.P. Debecker, A. Chaumonnot, D. Uzio*
  Catalysis Communications, 58 (2015) 11-15
- *The Active State of Supported Ruthenium Oxide Nanoparticles during Carbon Dioxide Methanation*

Sophie Carenco*, Capucine Sassoye, Marco Faustini, Pierre Eloy, Damien P. Debecker, Hendrik Bluhm, Miquel Salmeron
Journal of Physical Chemistry C, 120 (2016) 15354−15361

- *Selective $CO_2$ methanation on Ru/$TiO_2$ catalyst: unravelling the decisive role of the $TiO_2$ support crystal structure*
  Ara Kim, Clément Sanchez, Gilles Patriarche, Ovidiu Ersen, Simona Moldovan, Andreas Wisnet, Capucine Sassoye, Damien P. Debecker*
  Catalysis Science & Technology, 6 (2016) 8117-8128
- *Kinetics of hydrogen adsorption and mobility on Ru nanoparticles supported on alumina: Effects on the catalytic mechanism of ammonia synthesis*
  Camila Alejandra Fernández, Nicolas Bion, Eric M. Gaigneaux, Daniel Duprez and Patricio Ruiz
  Journal of Catalysis, 344 (2016) 16-28.
- *The inhibitor role of NH3 on its synthesis process at low temperature, over Ru catalytic nanoparticles*
  Charles Leterme, Camila Fernández, Pierre Eloy, Eric M. Gaigneaux and Patricio Ruiz
  Catalysis Today, 286 (2017) 85-100.
- *$CO_2$ methanation on Ru/$TiO_2$ catalysts: on the effect of mixing anatase and rutile $TiO_2$ supports*
  Ara Kim, Damien P. Debecker,* François Devred, Vincent Dubois, Clément Sanchez, Capucine Sassoye*
  Applied Catalysis B: Environmental, 220 (2018) 615-625
- *Combining $CO_2$ capture and catalytic conversion to methane*
  Paulina Melo Bravo, Damien P. Debecker*
  Waste Disposal & Sustainable Energy, 1 (2019) 53-65
- *Mesoporous $TiO_2$ Support Materials for Ru-Based $CO_2$ Methanation Catalysts*
  Ara Kim, Clément Sanchez, Bernard Haye, Cédric Boissière, Capucine Sassoye,* Damien P. Debecker*
  ACS Applied Nano Materials, 2 (2019) 3220-3230
- *$CO_2$ hydrogenation to methanol with Ga‐ and Zn‐doped mesoporous Cu/SiO2 catalysts prepared by the aerosol‐assisted sol‐gel process*
  Charlie Paris, Alejandro Karelovic,* Raydel Manrique, Solène Le Bras, François Devred, Vit Vykoukal, Ales Styskalik, Pierre Eloy, Damien P. Debecker*
  ChemSusChem, 13 (2020) 6409-6417
- *Recent Advances in Heterogeneous Catalyst for Ammonia Synthesis*
  Vijaykumar Marakatti and Eric Gaigneaux
  ChemCatChem, 12 (2020) 5838-5857.
- *Abiotic Transformation of H2 and CO2 into Methane on a Natural Chromitite Rock*
  Patricio Ruiz, Camila Fernández, Elena Ifandi, Pierre Eloy, Isaac Meza-Trujillo, François Devred, Eric M. Gaigneaux, and Basilios Tsikouras
  ACS Earth and Space Chemistry, 5 (2021) 1695–1708.
- *Can $CO_2$ and Renewable Carbon Be Primary Resources for Sustainable Fuels and Chemicals?*
  M. M. Faruque Hasan, Liane M. Rossi, Damien P. Debecker, Kevin C. Leonard, Zhenxing Li, Banothile C. E. Makhubela, Chuan Zhao, Arjan Kleij
  ACS Sustainable Chem. Eng., 9 (2021) 12427–12430
- *Immobilization of carbonic anhydrase in an hydrophobic poly(ionic liquid): a new functional solid for $CO_2$ capture*
  Christian Molina Fernández, Ariane Péters, Damien P. Debecker, Patricia Luis*
  Biochemical Engineering Journal, 187 (2022) 108639

- *Highly Active and Stable Co (Co3O4)_Sm2O3 Nano-crystallites Derived from Sm2Co7 and SmCo5 Intermetallic Compounds in NH3 Synthesis and CO2 Conversion*
  Marakatti, Vijaykumar; Ronda-Lloret, Maria; Krajčí, Marian; Joseph, Boby; Marini, Carlo; Delgado, Juan; Devred, François; Shiju, N. Raveendran; Gaigneaux, Eric
  Catalysis Science & Technology, 12 (2022) 686-706.
- *Patent on ammonia synthesis with industrial partner*

Y. Yyyyy, X. Xxxxx, V. Smeets, E. Gaigneaux.
EP xxxxxxxx.x, filled on xx/xx/2022

- *$CO_2$ Methanation with Ru@MIL-101 Nanoparticles Fixated on Silica Nanofibrous Veils as structured Catalytic Carrier*
  Eva Loccufier, Geert Watson, Yingrui Zhao, Maria Meledina, Robbe Denis, Parviz Gohari Derakhshandeh, Pascal Van Der Voort, Karen Leus, Damien P. Debecker,* Klaartje De Buysser, Karen De Clerck*
  Applied Catalysis B: Environmental, 320 (2023) 121972
- *$CO_2$ Methanation over Cobalt Nanoparticles Embedded in ZIF-L-Derived Porous Carbon*
  Nadia Gholampour, Yingrui Zhao, François Devred, Capucine Sassoye, Sandra Casale, Damien P. Debecker*
  ChemCatChem, 15 (2023) e202201338
- *$CO_2$ methanation with high-loading mesoporous Ni/$SiO_2$ catalysts: toward high specific activity and new mechanistic insights*
  Yingrui Zhao, Valentina Girelli, Ovidiu Ersen, Damien P. Debecker,*
  Journal of Catalysis, 426 (2023) 283-293
- *Solvent-free preparation of Ru/Al2O3 catalysts for $CO_2$ methanation: an example of frugal innovation*
  Ryma Haddad, Yingrui Zhao, Antoine Miche, Ferdaous Benromdhane, Nivedita Sudheer, Ovidiu Ersen, François Devred, François Ribot, Capucine Sassoye, Clement Sanchez, Damien P. Debecker, Corinne Chaneac,* Cédric Boissière*
  Chemistry of Materials, 35 (2023) 8248–8260

## Contact persons

**Damien Debecker,**
damien.debecker@uclouvain.be

**Eric Gaigneaux,**
eric.gaigneaux@uclouvain.be

# UNamur : Laboratoire d'analyse par Réactions Nucléaires (LARN)

University of Namur, Faculty of Science, Physics Department

Experimental studies

Hydrogen general topics

## General expertise of the research group

The research and teaching activities fold up around (1) Materials sciences, (2) Ion-Matter interactions and (3) Life sciences.

LARN is a research laboratory at UNamur, comprising 28 individuals (3 Professors, 5 post-docs, 13 PhDs, 3 Engineers, 3 technicians, 1 secretary), divided into two research areas: Materials Science and Biophysics, the latter not being related to this project.

LARN has extensive expertise in the deposition of high-performance thin films by vacuum method (physical vapor deposition). Over the past ten years, numerous projects (FEDER, SPW, M-ERANET, etc.) have enabled the development of unique know-how in the deposition of thin films via low-pressure plasma, using state-of-the-art equipment (vacuum deposition chamber, high-specificity plasma generator, characterization methods). Understanding the growth modes and physico-chemical properties of films, with the aim of maximizing the performance of these surfaces, is at the core of LARN's research activities. The targeted applications encompass the fields of engineering, optics, the medical sector, and the mechanical sector. These aspects are developed both experimentally with exceptional equipment and through simulation, thanks to the development of the NASCAM calculation code. This code allows for the determination of the growth and properties of films deposited by Monte Carlo method and is used by research centers as well as industries (approximately 700 licenses). In 2017, the spin-off Innovative Coating Solutions S.A. has been created based on the experience of the laboratory.

LARN also benefits from access to the SIAM platform (Synthesis, Irradiation, and Materials Analysis), which has state-of-the-art characterization equipment and recognized scientific expertise in materials analysis. Among its range of characterization techniques, we will particularly mention ion beam analyses, which have the unique ability to quantify the hydrogen concentration profile in materials without requiring sample destruction. Since its

establishment in September 2016, the SIAM platform's objectives are to support research within UNamur on one hand, and to offer its expertise in materials characterization to the industrial world on the other hand. The scientific staff of the platform is thus involved in daily interactions with both young scientists in their research and experienced industrial partners dealing with various challenges

The study of ion-matter interactions is the second topic in fundamental and applied research. Nuclear reactions which occur in the heart of stars (in the CNO cycle for instance) are the same as those used for materials analysis. Not only the efficient nuclear reactions mesure sections involved in astrophysics but also the knowledge about incident ions stopping section are of interest for materials analysis. Moreover, nuclear and atomic analysis techniques are improved and tested daily to better answer the growing needs of research and industry for surfaces and interfaces characterization.

Finally, the laboratory puts all the acquired knowledge in the two aforementioned topics to the service of life sciences. The multidisciplinary team studies cell response to photon or particle irradiation theoretically as well as experimentally.

## Specific hydrogen- related expertise & research topics

The laboratory has several activities related to hydrogen technologies:

LARN and SIAM have been at the forefront of an industrial project aimed at evaluating the degradation of mechanical performance in various metallic materials subjected to very high hydrogen fluxes. This SMART project itself followed another project funded by the company IBA to study the performance of lithium targets under very high hydrogen fluxes. In both cases, the UNamur particle accelerator (LARN/SIAM) is used to implant hydrogen into the material being characterized. This ion implantation technique allows for precise control over the quantity and depth at which hydrogen is introduced into the material. Furthermore, this technique enables the achievement of hydrogen concentrations in materials much more rapidly than through more conventional methods (e.g., exposing the material to a high-pressure and/or high-temperature hydrogen atmosphere).

The same particle accelerator is then used to perform ion beam analyses to determine the concentration profile of the implanted hydrogen. Since this analysis is non-destructive, it can be repeated after various sample treatments (e.g., temperature changes, corrosion, mechanical stresses), allowing the study of how hydrogen behaves in a given material based on its environmental conditions.

Regarding coating activities, LARN was involved in the development of coating for bipolar plates of fuel cells and electrolyzers in funded projects (INOXYPEM project), but also directly in relation with renowned actors (Siemens Energy, Borit, ZBT). The development of new plasma product/process in relation to energy production and storage is at the heart of LARN activities, in addition to the scaling and validation of new plasma couples/processes developed by Unamur in relation to energy production and storage.

## Available equipment/tools:

Available tools at LARN and platforms of UNamur:

- 5 plasma deposition chambers with different types of discharges (DC, HiPIMS, RF, Bipolar, etc.), enabling deposits through PVD and PECVD (Physical Vapor Deposition and Plasma Enhancement Chemical Vapor Deposition) methods, including plasma diagnostic techniques (probes, emission spectroscopy, in-situ stress measurement, etc.).
- Mechanical characterization equipment (nanoindenter, tribometer, profilometer, Rockwell).
- ALTAÏS accelerator for ion implantation and ion beam analysis, including hydrogen quantification.
- 2 XPS spectrometers with ion or cluster profiling capabilities.
- ToF-SIMS spectrometer.
- Access to X-ray Diffraction (DRX), Scanning Electron Microscopy (SEM), SEM Energy Dispersive Spectroscopy (EDS), Transmission Electron Microscopy (TEM), and TEM-EDS measurements at UNamur.

This extensive range of equipment and capabilities at LARN and SIAM enables comprehensive research and analysis in various material science and characterization fields, making them valuable resources for both scientific research and industrial applications.

## Participating in RW/B/EU funded projects with H2 related research:

INOXYPEM FEDER
Plasmanode (M-eranet) (energy/production storage)
Win4Ex TiNTHyN

Submitted project (not granted):
Win²Wal PLASCOLYZE
FTE COP-E
FEDER StorHywall

## Main relevant publications

E. Haye, F. Deschamps, G. Caldarella, M.-L. Piedboeuf, A. Lafort, H. Cornil, J.-F. Colomer, J.-J. Pireaux, N. Job, Formable chromium nitride coatings for proton exchange membrane fuel cell stainless steel bipolar plates, International Journal of Hydrogen Energy. 45 (2020) 15358–15365. https://doi.org/10.1016/j.ijhydene.2020.03.248.

S. Lucas, E. HAYE, J.-J. Pireaux, Tunable multifunctional carbon-based coatings, WO2022084519A1, 2022. https://patents.google.com/patent/WO2022084519A1/en (accessed August 18, 2022).

A. Costa, F. Ferreira, J.L. Colaux, et al., "Effect of hydrogen incorporation on the mechanical properties of DLC films deposited by HiPIMS in DOMS mode", Surface and Coatings Technology (2023) 129980. https://doi.org/10.1016/j.surfcoat.2023.129980

M. Michiels, A. Hemberg, T. Godfroid, et al., "On the relationship between the plasma characteristics, the microstructure and the optical properties of reactively sputtered TiO2 thin films", Journal of Physics D: Applied Physics 54 (2021). DOI: 10.1088/1361-6463/ac118e

-

## Contact persons

**Stéphane Lucas, stephane.lucas@unamur.be**
**Emile Haye, emile.haye@unamur.be**
**Julien Colaux, julien.colaux@unamur.be**

# UNamur: Laboratory Computational Modeling of Functional Materials (LCMFM)

University of Namur, Faculty of Science, Chemistry Department

Modelling

Hydrogen general topics

## General expertise of the research group

The research activities within the LCMFM are focused on the theoretical description of the structural and opto-electronic properties of p-conjugated organic materials in the bulk, organic/organic as well as excitation dynamics and transport properties. The LCMFM benefit from the full access to the computing facilities from the “Consortium des Équipements de Calcul Intensif” (CÉCI), a consortium of high-performance computing centers of the Universities from the French Community of Belgium supported by the F.R.S-FNRS and the Walloon Region and the Tier-1 CENAERO supercomputer of the Fédération Wallonie-Bruxelles which are entirely used for theoretical calculations in Chemistry and Physics.

## Specific hydrogen- related expertise & research topics

TiNTHyN: Recherche collaborative d'excellence dans la filière de l'hydrogène, structurée autour du plan d’actions de l’IIS e- WallonHY et les défis scientifiques et industriels associés

## Available equipment/tools:

- The access to the CÉCI and Tier-1 Cenaero allows to access to 30000 CPUs and GPUs to carry out our calculations

## Participating in RW/B/EU funded projects with H2 related research:

Not relevant

## Main relevant publications

Not relevant

## Contact persons

**Yoann Olivier (yoann.olivier@unamur.be)**

UMONS
Université de Mons

# UMons: Thermodynamics and Mathematical Physics Unit (TRMO)

Modelling and experimental studies

Hydrogen general topic

## General expertise of the research group

**In the field of Sustainable Industrial Processes, the phenomenon of solid-gas/vapour sorption is one of the main themes of R&D activities (thermodynamic and kinetic measurements, modelling of phenomena at the microscopic and macroscopic levels, process modelling, life cycle assessment (LCA), techno-economic analyses, development of experimental devices). The various applications concerned are the storage of natural gas, the design of CO2 capture processes, the separation of compounds from air, the purification of gases, the characterization of porous solids as well as catalytic conversion for e-fuels production.**

**In the field of Energy, the Thermodynamics and Mathematical Physics Lab is active in the modelling of complex energy systems at the scale of a district and in the study of specific energy technologies: heat storage, compression and sorption heat pumps (experimental studies, prototyping, development of simulation tools, measurement of on-site performance).**

## Specific hydrogen- related expertise & research topics

- **The Thermodynamics laboratory is active in 3D modelling of alkaline electrolysers at various scales. In particular, the modelling of a three-phase electrolyser for the decarbonation of calcium carbonate to simultaneously produce quicklime and hydrogen.**
- **The Laboratory other activity relates to the use of hydrogen: catalytic hydrogenation of $CO_2$ to produce e-fuels. Research activities involve both the modelling of conversion units (conversion to $H_2$ to methanol, $H_2$ to methane) and laboratory-scale experimental pilots ($H_2$ to methanol and $H_2$ to paraffin) for testing catalysts and determining the parameters of reaction kinetic models.**
- **Life cycle analysis are carried out on all processes**
-

## Available equipment/tools:

- Adsoption Lab : Devices for characterizing Gas sorption mechanism into porous solids
- Prototypes for CO2 capture
- prototype for catalytic conversion for e-fuel production
- Solar simulator
- Heat storage prototypes
- Simulation tools for:
    - Industrial process simulation
    - Buildings Energy Demand
    - Energy systems simulations
-

## Participating in RW/B/EU funded projects with H2 related research:

RW/ Greenwin : Integrated reactor for the production of $H_2/O_2/CO_2$ for CCU applications
As part of the objectives to reduce $CO_2$ emissions, the lime sector is faced with the difficulty of reducing both the CO2 emissions generated by combustion and, above all, the emissions linked to the transformation of limestone into lime. Combustion emissions can be reduced by using renewable energy. In addition to sequestration, the transformation of $CO_2$ into chemical compounds by reaction with hydrogen from the electrolysis of water is a promising way of avoiding industrial $CO_2$ emissions linked to the process.
The aim of the project, is to address these two challenges:

- Electrification of the lime manufacturing process, which generates a concentrated flow of $CO_2$.
- The production of hydrogen by electrolysis of water, which combined with $CO_2$ will provide the reaction mix ($H_2/CO_2$) needed to convert $CO_2$ into chemical products
-

## Main relevant publications

Coppitters, D., Costa, A., Chauvy, R., Dubois, L., De paepe, W., Thomas, D., De weireld, G., & Contino, F. (July 2023). Energy, Exergy, Economic and Environmental (4E) analysis of integrated direct air capture and CO2 methanation under uncertainty. "Fuel, 344", 127969. doi:10.1016/j.fuel.2023.127969
Energy, Exergy, Economic and Environmental (4E) analysis of integrated direct air capture and CO.pdf (955kb)

Henrotin, A., Heymans, N.* , Nandi, S., Nouar, F., Mouchaham, G., Serre, C., & De Weireld, G. (2022). Simulations on Industrial Scale CO2 Capture Vacuum Pressure Swing Adsorption Using Mil-160(Al). "SSRN Electronic Journal". doi:10.2139/ssrn.4283741
SSRN-id4283741.pdf (978kb)

Benzaqui, M., Wahiduzzaman, M., Zhao, H., Hasan, M. R., Steenhaut, T., Saad, A., Marrot, J., Normand, P., Grenèche, J.-M., Heymans, N., De Weireld, G., Tissot, A., Shepard, W., Filinchuk, Y., Hermans, S., Carn, F., Manlankowska, M., Téllez, C., Coronas, J., & Serre, C. (2022). A robust eco-compatible microporous iron coordination polymer for CO2 capture. "Journal of Materials Chemistry A".
TA-ART-12-2021-010385-NSteunou-highlighted_article.pdf (1068kb)

Chauvy, R., Dubois, L., Thomas, D., & De Weireld, G. (07 December 2021). Environmental impacts of the production of synthetic natural gas from industrial carbon dioxide. "Sustainable Production and Consumption, 30", 301-315. doi:https://doi.org/10.1016/j.spc.2021.12.004
Chauvy-Env-Impacts-With-SI-2021.pdf (3110kb)

## Contact persons

Guy De Weireld, guy.deweireld@umons.ac.be

# ULB – Transfers, Interfaces and Processes (TIPs)

Université Libre de Bruxelles, Faculty of Applied Sciences, Fluid Physics

Theoretical, numerical and experimental methods

Hydrogen general topics

## General expertise of the research group

At the TIPs (Transfers, Interfaces and Processes) Department of ULB, the main goal of the ongoing research is to develop new theoretical, numerical and experimental methods allowing to understand and predict the behavior of multiphase systems, and to design or optimize industrial processes dedicated to the transformation of matter (mineral, organic or biological) and energy. There are essentially six main research themes: mixing, gas-liquid mass transfer,dynamics of interfaces and their instabilities, wetting, porous media, heat transfer and phase change (evaporation, crystallization, ...). The Department is made of two complementary research units: the Fluid Physics Unit and the Chemical Engineering Unit. The Fluid Physics Unit collaborates with a number of scientific and industrial partners in Belgium, Europe, USA, Israel and Canada, in the frame of several networks funded by the European Commission or by the
European Space Agency, and also thanks to support at National level (BELSPO, FNRS, Brussels and Walloon Regions). The team investigates mostly fundamental and/or generic questions, i.e. common to several natural or industrial processes. Studied problems most often involve notions of nonlinear dynamics, physical chemistry (equilibrium and non-equilibrium), statistical mechanics

## Specific hydrogen- related expertise & research topics

The research of Professors Benoit Haut, Pierre Lambert and Benoit Scheid at the TIPs laboratory focuses in particular on gas-liquid flows within industrial processes, with a multi-scale approach ranging from the single bubble (formation, dynamics) to the complete process, but also on problems of coatings and additive manufacturing on small scales. This project, offering a new application framework, will strengthen the expertise of TIPs in these areas, in particular by focusing on the relationship between formation of bubbles by

electrochemical reaction and structure/coating of the electrode, or on the dynamics of a swarm of bubbles in complex structures or environments.

## Available equipment/tools:

The used tools are either theoretical (stability analyses, scaling laws, asymptotic techniques, ...), numerical (commercial or 'home-made' software), or experimental (fluid behavior visualization by interferometry, Schlieren, infrared thermography, ...).

## Participating in RW/B/EU funded projects with H2 related research:

- ESA projects (with additional funding from BELSPO) related to fluid physics:
- Non Inflammatory NO Change (NINOC): collaboration with Karolinska-Institutet (Sweden)
- Microgravity effects on partial phase separation and structure formation in thin films – solvent effects on a model system for organic optoelectronics (DIPCOM-2): collaboration with Karlstad University (Sweden)
- European Network on boiling-related research in microgravity (MAP and PRODEX Heat transfer)
- European Network on evaporation-related research (MAP and PRODEX Evaporation)
- Topical Team Bioprocesses and Bioreactors in Space
- The last three projects bring together more than 30 partners in around ten countries (Germany, Belgium, Spain, France, Greece, Italy, Portugal, Poland, Switzerland

## Main relevant publications

Text

## Contact persons

**Benoit Haut**
**Pierre Lambert**
**Benoit Scheid**

CENAERO

Digital twins and AI

Hydrogen general topics

## General expertise of the research group

In terms of cutting-edge skills, Cenaero develops cutting-edge R&D expertise in: 1. Multi-physics simulation (fluid, thermal, mechanics, etc.) 2. Expert systems (optimization) and machine learning 3. Numerical methods and software engineering 4 High Performance Computing (HPC) infrastructure operation.
Cenaero is active in applied research and development in digital simulation, optimization, data exploitation.

## Specific hydrogen- related expertise & research topics

The development of digital twins, based on physical models and the use of AI, is part of the center's strategy to improve the design and/or operations of manufacturing systems and processes. Cenaero is historically anchored in the transport sector and has also diversified into sectors such as energy, particularly around the development of the energies of the future.
In the field of hydrogen, Cenaero will position itself on

- optimization of hydrogen production processes (electrolysis, etc.) or use (fuel cell, gas turbine);
- virtual design as well as lifespan prediction of critical components linked to storage and transport (composite tanks, valves, functionalized electrodes, heat exchangers)
- optimization of energy conversion systems and planification including the hydrogen vector in either energy community (stationary) or mobile applications

## Available equipment/tools:

- Key Enabling Technology : High Performance Computer LUCIA (www.tier1.cenaero.be)

## Participating in RW/B/EU funded projects with H2 related research:

- H2COOPSTORAGE (Eranet funding; ending in 2023): H2 Coopstorage aims to develop methodological and software tools enabling the deployment and management of a multi-energy EC integrating a hybrid solution of electric and hydrogen storage, in a collective self-consumption context.
  https://h2coopstorage.eu/

## Main relevant publications

Text

- List

## Contact persons

**Cécile Goffaux, cecile.goffaux@cenaero.be**
**David Dumas, david.dumas@cenaero.be**

# CERTECH

Environment security

Hydrogen general topics

## General expertise of the research group

The research & development strategy of Certech is based on the synergies of three major themes, namely: environment, polymer materials technology, chemistry & industrial processes supported by an analytical & technological services platform.

## Specific hydrogen- related expertise & research topics

Certech contributes to research and innovation activities addressing environmentally friendly technologies and allowing to support a sustainable economic development. These activities integrate the following topics:

- Integration at a local level of mixed renewable electricity sourcing (for domestic or industrial exploitations) through the production of hydrogen or via storage in batteries.
- Reduction of the hydrogen storage costs via solid storage in porous materials, namely the Metal-Organic Frameworks (MOF). These MOF must be relevant from technical and regulatory aspects. The porous solids are developed in specific reactors, to increase their production while reducing the costs and environmental impact of the syntheses.

## Available equipment/tools:

- 
- Characterization / quantification of hydrogen in a gas mixture.
- Micro-reactors for sorption of gas on solid materials.
- Micro-reactors for sorption of hydrogen (*in development*).
- Intensified continuous reactor for solids adsorbent synthesis.
- Autoclaves for hydrothermal synthesis.

## Participating in RW/B/EU funded projects with H2 related research:

- INTERESTS project – DGO4 Wallonia
- H2Be Project – Fonds de Transition Energétique (FTE)

## Main relevant publications

Text

- *Continuous flow hydrothermal synthesis of zeolite LTA in intensified reactor. Experimental and multiphysics CFD modeling approach,* S. Ahmad, L. B. Mustapha, S. Calvo, F. Collignon, A. E. Fernandes, D. Toye, Chemical Engineering and Processing - Process Intensification 2023, 189, 109399.
  https://doi.org/10.1016/j.cep.2023.109399

- *Continuous, Greener Synthesis of Metal-Organic Frameworks*, Olivia Deresteau, François Collignon, Dominique Lalande, Lilia Ben Mustapha, EuroMOF 2019, 27- 30 October 2019 - Maison de la Chimie, Paris, France

## Contact persons

**info@certech.be**
**François Collignon**
**Benoît Kartheuser**

# CRM group

Metallic Materials: products, processes and applications development

Production – Transport and uses of Hydrdrogen

## General expertise of the research group

CRM Group's activities are centered on the production, transformation, coating and use of metallic materials. Since 1948, CRM Group offers R&D and technology solutions focusing on the development of innovative processes and products that create value for their industrial partners.

CRM Group has set up a Strategic Platform related to energy transition. This platform brings together its activities in the field of the development of renewable energies, storage, hydrogen, decarbonization of industrial processes, CO2 capture and alternative fuels. CRM Group has a strong expertise in the field of applied electrochemistry, material synthesis and characterization, innovative solutions and device development, pilot and prototypes– for various applications sectors and industrial processes.

## Specific hydrogen- related expertise & research topics

- Hydrogen production by electrolysis (low temperature)
  - From lab to pilot scale;
  - Lab & Pilot electrolyser (AEL);
  - Material development for electrodes and membranes;
  - Electrochemical optimization;
  - Equipment optimization
- Transport and storage
  - Tests in real conditions:
    - Dedicated equipments for tubes (ReadHY project);
    - Dedicated equipments for Materials (MaterHYum project under evaluation);
  - Leak detection - fugitive emissions;
  - Pipelines for distribution and transport (impact of welds and loadings)
- Thermal desorption analysis
  - Methodology and expertise;
  - Thermal Desorption Analysis coupled with mass spectrometry for hydrogen and deuterium

- Building equipments;
- ISO17025 (BELAC 267-TEST) certification for (zinc coated/) steel characterization

- Metal embrittlement due to hydrogen :
  - Hydrogen measurements (total and diffusible);
  - Mechanical properties;
  - Links to production parameters;
  - Welding;
  - Mitigation strategies through:
    - barrier coatings,
    - grade modifications,
    - process parameters,
    - …
- Use of hydrogen
  - Fuel cells: coating for metal bipolar plates, prototyping
  - Industrial processes :
    - Reduction of oxides;
    - impact of combustion;
    - As protective atmospheres;
    - …

## Available equipment/tools:

- Total Hydrogen content by combustion;
- Diffusible Hydrogen content by thermal conductivity and mass spectrometry;
- Hydrogen charging by electrochemical and thermal means
- Delayed fracture (under tension or bending)
- Lab & pilot electrolyser (AEL) and related electrochemical measurements
- Metal forming and forging including hydroforming press for bipolar plates prototyping
- Coating technologies (PVD, evaporation, liquid spray, thermal spray, cold spray, electro-coatings, serigraphy…) and pilot lines (roll to roll and robotized 3D coating)
- Material characterizations (Metallography, Chemistry, Surface analysis, Mechanical properties);
- Thermomechanical treatment, heat treatments, under hydrogen heat treatments, reactive annealing;
- Corrosion evaluation, testing and mitigation strategies;

To come:

- Dynamic Tube Rupture Test (ReadHy project)
- Tensile fatigue test (500 bars H2), autoclaves (700 bars), permeation (1000 bars) and autoclaves for long term exposures (MaterHYum project under evaluation)

## Participating in RW/B/EU funded projects with H2 related research:

- RFCS HPPM (2016) Methodology of hydrogen measurement in coated steels;
- Feder project INOXYPEM (2014-2020): Development and fabrication at pilot scale of coated stainless steel bipolar plates;
- RFCS CRYSTAL (2021): reduce the hydrogen embrittlement risk in high-strength steel parts for the advanced High Strength Steels;
- CWality Hydeal (2021): improvement of alkaline electrolyzer cells;
- PNRR HeCO2-electrolyzer (2022): decarbonated hydrogen generation by electrolysis;
- COODEVIIS MaterHYum (submitted): Setting up a new service offering and prototype test benches to characterize and certify materials and components in the hydrogen value chain under real-life conditions;
- IIS (e-WallonHY, 2023): activities linked to the management of IIS e-WallonHY on the development of the value chain of green hydrogen in Wallonia and the drafting of European projects;
- ETF ReadHY (2023): Development of an innovative testing method towards a better understanding of hydrogen-metal interactions to secure gaseous hydrogen transportation;
- ILZRO (2023): Hydrogen uptake control in galvanizing process (US)

## Main relevant publications

Papers


- F.Duminica, X. Vanden Eynde, M. Mandy, et al., Investigation of PVD thin films as hydrogen barriers in aluminized press hardened steels (PHS), Surface & Coatings Technology (2018), https://doi.org/10.1016/ j.surfcoat.2020.12594
- Krid, Mohamed and Mandy, Mélodie and Grigorieva, Raisa and Sturel, Thierry and Drillet, Pascal and Jacques, Pascal, A Better Understanding of Hydrogen Trapping and Diffusion in Aluminized Press-Hardenable Steels. (2023) Available at SSRN: https://ssrn.com/abstract=4525368 or http://dx.doi.org/10.2139/ssrn.4525368
- M Mandy, X Vanden Eynde, F Duminica, C Georges, M Larnicol, R Grigorieva (AM), T Sturel (AM), P Drillet (AM) Prevention of hydrogen uptake in Al-Si coated 22MnB5 steel using physical vapour deposition coatings *CHS² - 8th International Conference on Hot Sheet Metal forming of High Performance steel, 30 May-2 June 2022, Barcelona*
- Krid Mohamed (UCLouvain), Mandy Mélodie, Sturel Thierry (AM), Grigorieva Raisa (AM), Drillet Pascal (AM), Jacques Pascal J. (UCLouvain) A better understanding of hydrogen absorption - desorption from Al-Si coated high strength steels during hot stamping process *4th International Conference on Metals & Hydrogen, 11-13 Oct 2022, Ghent*
- Mélodie Mandy, Cédric Georges et Sturel, Thierry (AM) ; Drillet, Pascal (AM) ; Jacques, Pascal J. (UCLouvain) On the right use of deuterium to characterize hydrogen uptake mechanisms in bare 22MnB5 steel *4th International Conference on Metals & Hydrogen, 11-13 Oct 2022, Ghent*

- Mélodie Mandy, Florin Duminica, Xavier Vanden Eynde, Cédric Georges, Grigorieva R. (AM), Sturel Thierry (AM), Drillet Pascal (AM) PVD-deposited barriers to reduce hydrogen uptake during hot stamping of Al-Si coated 22MnB5 steel *4th International Conference on Metals & Hydrogen, 11-13 Oct 2022, Ghent*

Patent

- EP3633068 (CARBON STEEL SHEET COATED WITH A BARRIER COATING)
- EP3604606 (COATING FOR REDUCING THE CONTACT RESISTANCE OF A PASSIVE METAL SUBSTRATE PRIOR TO APPLICATION OF A CONDUCTIVE LAYER PROVIDING CORROSION RESISTANCE)

## Contact persons

**Catherine Archambeau, unit manager Advanced & Smart Surface Solutions, IIS e-WallonHY coordinator, catherine.archambeau@crmgroup.be**
**Xavier Vanden Eynde, unit manager Material Characterization; xavier.vandeneynde@crmgroup.be**
**Maïwenn Larnicol,activity manager Hydrogen & Electrochemistry Maiwenn.larnicol@crmgroup.be**