Hydrogen Research in Flanders

Overview of Hydrogen related activities at Flemish knowledge institutes





1 Introduction

Hydrogen is high on the EU agenda as one of the pillars of the climate policy and recognized as an essential building block to realize climate neutrality by 2050. Also, in Flanders & Belgium, hydrogen is a hot topic, with the 'Hydrogen vision' of the Flemish government as starting point for further development and roll-out of H_2 - technology in our region. In the industry the interest in hydrogen keeps on growing, which is clearly shown by the growth of the *Waterstof Industrie Cluster* (WIC), that has developed into a network of more than 170 members of which about 165 are located in Belgium.

Flanders boasts considerable expertise in the field of hydrogen, with a number of important technology players globally recognized for their products and expertise. However, to sustain our leading position and continue to play a role in this rapidly evolving ecosystem, it is important to bring our research competences to the required level to feed and support our industry.

In our Flemish knowledge institutes several research groups are active in hydrogen related domains that are very relevant for the further development and scaling up of the hydrogen technology. We have a large diversity in topics, covering the whole value chain and comprising both experimental research and modelling activities.

Given the large number of topics, distributed over many diverse groups, WaterstofNet – as a knowledge platform and facilitator for hydrogen in Flanders - has taken the initiative to make an overview of the relevant research groups in a comprehensive publication for Flanders.

The first catalogue 'Hydrogen Research in Flanders' was published in the beginning of 2022² and an annual updates were published afterwards. This catalogue provides an overview of the most relevant research groups, categorized by their focus area in the hydrogen value chain (production, storage, transport, use of hydrogen & general hydrogen topics) and the type of research (material or process development & modelling).

This new document is an update of last year's catalogue, retaining the same structure and content, while incorporating new data and topics. We hope this catalogue can be a practical guide for both research groups and industrial technology developers, facilitating the search for certain skills and expertise in the field. An interactive version of the research at the Flemish institutes, together with the research at the Walloon institutes was also brought together on the Belgian Hydrogen Council website³.

The ultimate goal of this overview is to stimulate collaboration among knowledge institutes and industrial partners, allowing for the identification of knowledge gaps and opportunities for new research topics.

The WaterstofNet team January 2025

¹ Mededeling aan de Vlaamse regering, Vlaamse Waterstofvisie "Europese koploper via duurzame innovatie" https://www.vario.be/nl/nieuws/vlaamse-waterstofvisie-%E2%80%98europese-koploper-duurzame-innovatie%E2%80%99

² https://www.waterstofnet.eu/en/knowledge-centre/publications

³ https://www.belgianhydrogencouncil.be/research



1.1. Content & structure

With the SRIA program, the European Union has proposed a research agenda that delineates various topics for hydrogen research, as shown in Figure 1.

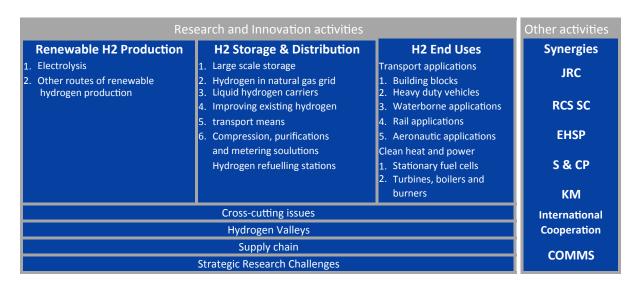


Figure 1: SRIA 2021 - 2027 EU. It divides the topics of hydrogen research.4

The most common method to produce green hydrogen involves the separation of water into hydrogen and oxygen via electrolysis using electricity from renewable energy sources like wind and solar energy. Numerous research institutions are active in further optimization of existing technologies such as Alkaline (AEL) and Proton Exchange Membrane (PEM) Electrolysis or exploring less conventional types of electrolysis such as Anion Exchange Membrane (AEM) or high temperature Solid Oxide (SO) Electrolysis. For instance, ELCAT (a research group from UAntwerpen) is committed to advancing flow electrolyzers encompassing all previously mentioned technologies, focussing on electrochemical reactor engineering and steering electrocatalysis away from the typical high-cost catalysts. Similarly, VITO possesses substantial expertise in the development and testing of both types. At the same time the VIVES University of Applied Science investigates further system optimization for integrating green hydrogen production into the energy landscape.

These electrolysers rely on high-cost catalysts such as platinum (Pt), iridium (Ir) or ruthenium (Ru). The LADCA research group at UAntwerpen designs heterogeneous catalysts for in-situ hydrogen production while the COCOON group at UGent researches Atomic Layer Deposition (ALD) of electrocatalysts. COMOC at UGent is internationally renowned for developing amongst others, novel porous materials and heterogeneous catalysts. At the UHasselt, the DESINe research group delves into the intricacies of catalyst design and synthesis for hydrogen and oxygen evolution reactions within PEM electrolysers. Typically, these PEM electrolysis cells are integrated into stacks, forming what is known as a membrane electrode assembly (MEA). The group of Electrochemical Engineering at IMO-IMOMEC undertakes membrane electrode assembly (MEA) preparation, which are part of an electrolysis cell. They also

⁴ Strategic Research and Innovation Agenda https://www.clean-hydrogen.europa.eu/about-us/key-documents/strategic-research-and-innovation-agenda_en

optimize and conduct extensive research into the lifespan and polarization characteristics of PEM electrolysers. Moreover, Imec focuses on developments in solid electrolyte materials and membranes, aiming for reduced resistance, thickness and gas crossover. They strive to create new thin electrodes with substantial surface area and porosity, achieved through controlled and ordered nanostructures, ultimately enhancing ionic conductivity. This innovation aims to increase current density, thereby enabling thinner MEAs for improved electrolyser performance. The EELAB & Lemcko research groups at the UGent investigate integration aspects of the electrolyser with the electrical grid, i.e. flexibility and support for power generation grids, while the ELECTA group from KU Leuven is evaluating hydrogen as storage for the electrical distribution grid. Electrolysis also requires a large amount of water. The A-PECS research group at the UAntwerpen is looking for sustainable and alternative ways of water production technologies using non-critical raw materials.

Beyond water electrolysis, various alternative technologies exist to produce hydrogen. SolHyd, a spinoff of COK-KAT at KU Leuven produces innovative hydrogen panels that directly produce renewable hydrogen from air and solar energy using catalysts without noble metals. At the UAntwerpen, the research group PLASMANT actively explores the utilization of plasma to convert CH4 and NH3 into H₂. Also, COK-KAT from the KU Leuven, in collaboration with ElectrifHy and PLASMANT seeks innovative ways to crack green ammonia into hydrogen.

Another method involves photoelectrochemical splitting, wherein water is split using semiconductor materials converting solar energy into chemical energy (hydrogen). Both the research groups Materials for Energy Applications and DESINe at UHasselt investigate this technology. Moreover, these research groups explore photocatalytic water splitting using catalyst instead of semiconductors. Meanwhile the HyMaD and OOE research group at UHasselt are developing hybrid perovskite for application in photoelectrochemical cells. The LCT research group at UGent conducts primary research of hydrogen production, intertwining this focus with research of other e-fuels such as methanol, methane and ammonia.

Hydrogen, due to its nature, requires specific storage methods. It can either be stored in pressurized tanks or bonded with chemical substances such as ammonia or liquid organic hydrogen carriers (LOHC). The INCAT research group at UGent develops NaBH₄ as a carrier for hydrogen. The ElectrifHy research groups focus on designing dehydrogenation units and test rigs for these LOHCs. When a carrier is used to transport or store hydrogen, a separation method is required to extract the hydrogen from the carrier. Following this, through purification, highly pure hydrogen remains. This purification is one of the main focusses of the Chemical Engineering research group from the VUB, but also from the PaInT research group. The ARCLATH consortium (COK-KAT & NMRCoRe, KU Leuven; CMM & COMOC, UGent; LADCA & EMAT, UAntwerpen; Chemical Engineering, VUB) develops hydrogen storage solutions based on H₂ hydrates confined in porous materials. Also, the Centre for Molecular Modelling (CMM) at the UGent is designing materials for hydrogen storage.

An alternative involves storing hydrogen as a gas in underground rock salt caverns, explored by the research groups New Materials/iR at KU Leuven or in underground porous rock layers (e.g. aquifers), as studied by PProGRess at UGent.

When opting for the pressurized tanks, designing pressurized vessels becomes essential. The MMS research group at the UGent studies the vessel design, stress calculation and Non-Destructive Testing (NDT) of thick-walled composites. The LMSD & CMG research groups at the KU Leuven focus on cylindrical components and dome-like end caps, investigating low- and high-pressure vessels for storage in liquid and gaseous state respectively. Von Karman Institute for Fluid dynamics applies its expertise in computational fluid dynamics to liquid hydrogen transport and application. In addition to technical aspects, ensuring the safety of hydrogen storage requires comprehensive exploration, an area investigated by the FLOW research group at VUB.



Hydrogen as a fuel offers three different pathways. The first involves its utilization in internal combustion engines, an area of expertise of the FLOW research group at the VUB. They investigate the combustion dynamics of H₂ and H₂-based carriers, such as ammonia. Similarly, the LowCarb research group at KU Leuven utilizes experimental and numerical methods to characterize alternative fuel combustion. Additionally, VIVES possesses expertise in internal combustion engines and specializes in dual fuel technology, particularly in diesel-hydrogen systems. The UGent based research group Transport Technology (TT) has extensive experimental and numerical expertise in internal combustion engines: it has been investigating hydrogen engines since 1992 and methanol engines since 2009, both in single fuel as dual fuel configurations.

The second option involves employing fuel cells, which is an additional area of expertise of VIVES. They investigate the use of these fuel cells in an integrated system. VITO contributes to the development and testing of these fuel cells. On the other hand, the Chemical Engineering group at VUB performs computational fluid dynamics (CFD) modelling to optimize the flow field design within fuel cells. Moreover, the MMS group at UGent specializes in designing and simulating fuel cell stacks, contributing to advancing fuel cell technology. The Precision Manufacturing group at Sirris investigates ultrashort pulsed laser texturing which can potentially increase the specific surface area of fuel cell electrodes, thereby increase the efficiency. Lastly, the TME (M-group) division at KU Leuven examines hybrid drone propulsion systems with fuel cells.

A third pathway would be using hydrogen as both fuel and feedstock in energy-intensive industries where full electrification is not feasible anymore as they effectively need to substitute fossil fuels as feedstocks with hydrogen in their production routes. One of the research focuses of the ESIM research group is to investigate the future potential demand for renewable hydrogen in energyintensive industrial sectors in North-West Europe following the emission reduction targets based on EU fit for 55 or Renewable Energy Directive.

Beyond technological considerations, the economic facets of hydrogen implementation are equally pivotal. Several research groups such as EVERGi from VUB and ESIM from KU Leuven concentrate on modelling, designing and optimizing techno-economic solutions. They delve into the intricate balance between technology and economics in various hydrogen-related applications, while also assessing European and national policies related to hydrogen. More specific for ESIM, they are focussing on analysing and designing a cost-effective and feasible future renewable hydrogen infrastructure encompassing production options, transmission networks and storage units in both Belgium and neighbouring countries. This involves identifying potential hydrogen hubs, supply zones, offshore corridors, demand areas, and storage locations. Moreover, VITO and KU Leuven developed various techno-economic models, which aid in assessing and strategizing the economic viability and potential of different hydrogen technologies. Similarly, the STEN research group at UGent also assessed e-fuels with an LCA while also investigating the resource footprint and efficiency. The LCT research group at UGent utilizes its knowledge of catalysts, kinetics, reactor and process design to evaluate the economic aspects of hydrogen and other e-fuels. The geopolitical aspects of hydrogen are an area of expertise for the Ghent Institute for International and European Studies, while the Centre for Sustainable Development at UGent conducts political analysis and socio-technical evaluation. The Centre of Environmental & energy law at UGent are specialized in certification of hydrogen and green molecules.



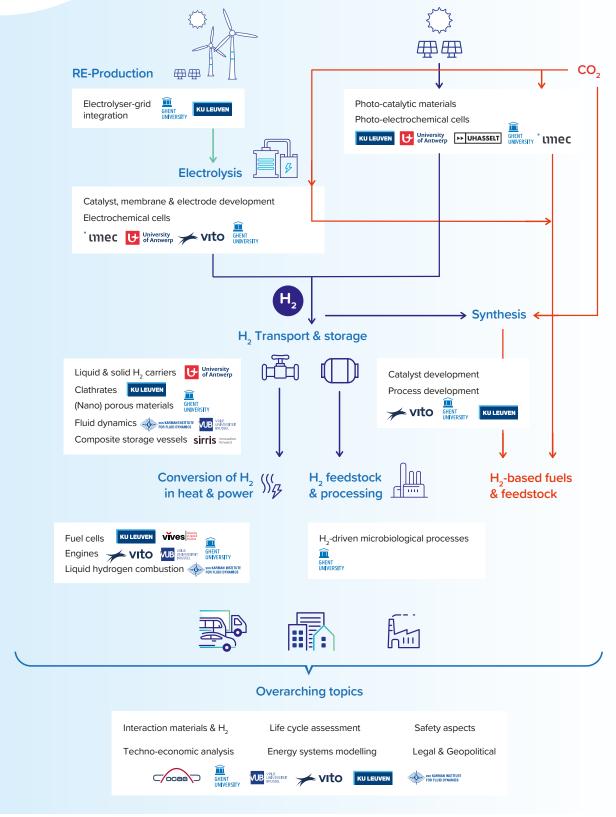
Hydrogen can also play a pivotal role in microbiological processes. The research group CMET at UGent is actively exploring microbial hydrogen metabolism, aiming to produce microbial protein, bioremediate pollutants and enhance nutrient removal for improved potable water quality.

Lastly there is the main R&D of hydrogen, like the work of the Soete Laboratory at UGent. They focus on researching the impact of hydrogen on mechanical properties of steel and roller bearings. Similarly, the MACH & SURF research groups at VUB delve into the interactions between hydrogen and steel, approaching it from a surface-oriented perspective. OCAS boasts a comprehensive expertise in R&D, particularly in understanding the interplay between hydrogen and materials, assessing the impact of hydrogen on material performance and elucidating the behaviour of materials in the presence of hydrogen. Moreover, the SMS research group at UGent has garnered international recognition for its expertise in developing advanced experimental methodologies specifically tailored to studying hydrogen embrittlement.





Academic H₂-related research Flanders





2. Table of Contents

1. Introduction	1
1.1. Content & structure	
2. Table of Contents	7
3. The research	10
3.1. Production, transport & storage	
3.1.1. Imec	11
Energy Department	
3.1.2. KU Leuven	13
Centre for Surface Chemistry and Catalysis (COK-KAT)	13
Electrical Energy Applicati ons (ELECTA)	16
Mecha(tro)nic System Dynamics (LMSD) Composite Materials Group (CMG)	17
3.1.3. Sirris	21
Additive Manufacturing	21
Precision Manufacturing	23
Product Development Hub	25
3.1.4. UAntwerpen	27
Antwerp Engineering, Photoelectrochemistry and Sensing (A-PECS)	27
Applied Electrochemistry and Catalysis (ELCAT)	29
Electron Microscopy for Materials Science (EMAT)	32
Laboratory for the Electrification of Chemical Processes & Hydrogen (ElectrifHy)	35
Laboratory of Adsorption and Catalysis (LADCA)	37
Plasma Lab for Applications in Sustainability & Medicine ANTwerp (PLASMANT)	39
3.1.5. UGent	42
Center for Molecular Modelling (CMM)	42
Center for Ordered Materials, Organometallics & Catalysis (COMOC)	44
Conformal Coating of Nanomaterials (COCOON)	46
Electrical Energy Laboratory (EELAB & Lemcko)	49
Industrial Catalysis and Adsorption Technology (INCAT)	51
Laboratory for Chemical Technology (LCT)	53
Mechanics of Materials and Structures (MMS)	55
Particle and Interfacial Technology Group (PaInT)	57
Pore-scale Processes in Geo-materials (PProGRess)	59



3.1.6. UHasselt	_61
Design and synthesis of inorganic nanomaterials (DESINe)	_61
Electrochemical Engineering (EE)	64
Hybrid Halide Perovskites for Energy Applications (HyMaD)	65
Materials for Energy Applications	68
Organic Opto-Electronics Research (OOE)	_71
3.1.7. VITO	_73
Separation and Conversion Technology (SCT)	_73
3.1.8. VIVES University of Applied Sciences	78
Research group Energy - Hydrogen production	_78
3.1.9. VKI	_80
Research Expertise Group on Liquid & Solid Propulsion (storage & transport)	_80
3.1.10. VUB	_82
Department of Chemical Engineering	_82
Thermodynamics and Fluid Mechanics (FLOW)	_84
3.2. Use of hydrogen	86
3.2.1. KU Leuven	_87
Division of Applied Mechanics and Energy conversion, Mechatronics Group (TME, M-Group)	_87
LowCarb Research Group	89
3.2.2. UGent	_91
Transport Technology (TT)	_91
3.2.3. VIVES University of Applied Sciences	_93
Research Group Energy - Green methanol	_93
Research Group Energy - Hydrogen fuel cell systems	_95
Research Group Energy - Hydrogen ICE	_97
3.2.4. VKI	_99
Research Expertise Group on Environmental Flows & Safety Industrial Flows	_99
Research Expertise Group on High Speed Propulsion & Combustion	101
Research Expertise Group on Liquid & Solid Propulsion (mobility)	104
3.3. Hydrogen general topics	108
3.3.1. KU Leuven	109
Energy Systems Integration and Modelling (ESIM)	109
Interfacial Engineering Research (iR)	111

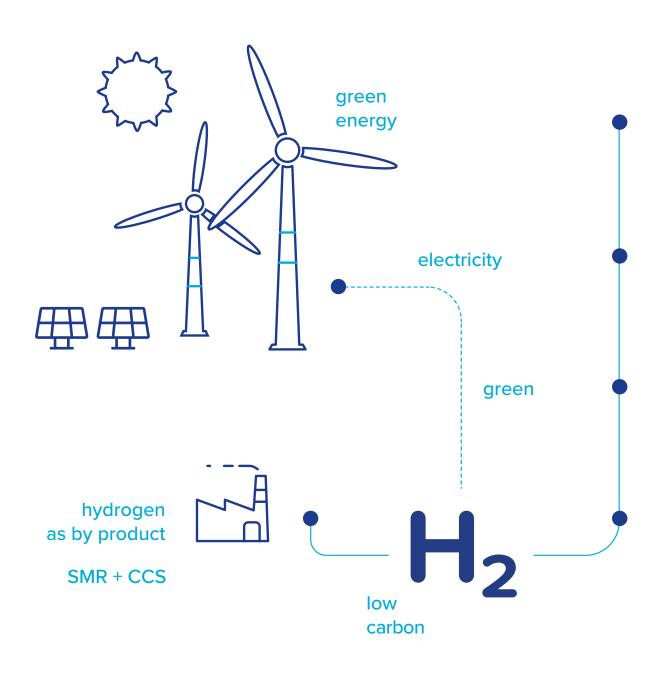


3.3.2. OCAS	113
Department of Applications and solutions	113
Department of Metallurgy	115
Department of surface engineering	118
3.3.3. UGent	120
Center for Microbial Ecology and Technology (CMET)	120
Centre for Sustainable Development (CDO)	122
Centre of environmental & energy law	124
Soete Laboratory	125
Sustainable Materials Science (SMS)	127
Sustainable Systems Engineering (STEN)	130
3.3.4. VITO	132
Techno-economic assessments and LCA analysis	132
3.3.5. VUB	135
Electrochemical and Surface Engineering (SURF)	135
Mobi research centre - EVERGi	137



3. The research

3.1. Production, transport & storage





Materials and components development, process development



3.1.1. Imec

Energy Department

Imec

General expertise of the research group

In the area of energy research Imec is active in the whole value chain from basic material research up to the system level. It spans applications from energy generation (silicon, perovskite and tandem PV cells and modules), energy storage (solid state batteries), energy conversion (power to molecules or electrolysis and fuel cells) and energy systems. For this research, Imec builds on its expertise in (semiconductor) electrochemistry, novel materials (electrodes, catalysts, electrolyte), surface functionalization, design of interfaces, various thin film deposition technologies. Imec also has expertise in characterization of relevant material properties at interfaces and in bulk, of PV-cells and modules, batteries, electrolyzers and fuel cells.

Specific hydrogen - related expertise & research topics

- Development of new solid electrolyte materials and membranes with lower resistance, lower thickness and lower gas cross-over
- Development of new thin electrodes with very large surface area and porosity for ionic conductivity based on controlled and ordered nanostructures to increase current density for thinner MEA
- Development of novel catalysts and related deposition technologies for higher efficiency and durability
- Realization of membrane-electrode assemblies (MEA) as basic component for electrolysers
- Upscaling of all the previous to scales which are industrially relevant
- Study of dynamic behaviour as input for technology-aware modelling
- Integration of PV-elements with electrochemical cells
- Next generation electrolyser using steam or water from the environment (humidity)

Available equipment/tools

- Plating and anodization equipment for sizes up to 200 mm
- Thin-film deposition (sputtering, atomic layer deposition, physical evaporation)
- Printing and coating equipment (small size)
- Sol-gel synthesis and analysis
- · Ionic conductivity and ionic coupling measurements
- · Electrochemical equipment for analysis, synthesis, and characterization
- Single stack electrolyser test cells

Participating in FL/B/EU funded projects with H₂ related research

 PROCURA – ETF – Imec, Vito, KUL, VUB, ULiège, WaterstofNet: PV-EC demonstrator and system modelling

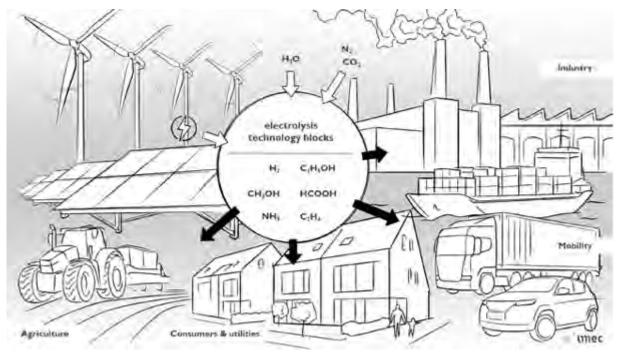


Materials and components development, process development

General



Imec's vision is that the electrolysis technology blocks under development have a wide application in conversion of (green) energy to molecules, including CO₂ Capture and Utilization. The following graphic illustrates that point.



Main relevant publications

- "Combining High Porosity with High Surface Area in Flexible Interconnected Nanowire Meshes
 for Hydrogen Generation and Beyond" Stanislaw Zankowski and Philippe M. Vereecken, ACS Appl.
 Mater. Interfaces, 2018, 10 (51), pp 44634–44644; DOI: 10.1021/acsami.8b15888
- Nanotechnologie: hoe een voetbalveld in een blikje frisdrank onze toekomst kan veranderen | VRT NWS: nieuws (https://www.vrt.be/vrtnws/nl/2019/03/12/nanotechnologie-hoe-een-voetbalveld-in-een-blikje-frisdrank-onz/)
- "Redox Layer Deposition of Thin Films of MnO2 on Nanostructured Substrates from Aqueous Solutions" S.P. Zankowski, L van Hoecke, F Mattelaer, M de Raedt, O. Richard, C. Detavernier, P.M. Vereecken, Chemistry of Materials, 31(13):4805-4816 (2019). IF 9.89.
- "Enhanced Photocatalytic Activity of Nanoroughened GaN by Dry Etching" W. J. Tseng, D. H. van Dorp, R. R. Lieten, B. Mehta, P.M. Vereecken, and G. Borghs, ECS Electrochemistry Letters, 2 (11) H51-H53 (2013).
- "Synthesis of large area carbon nanosheets for energy storage applications", D. Cott, M. Verheijen,
- O. Richard, I. Radu, S. De Gendt, S. Van Elshocht, and P.M. Vereecken, Carbon 58, 59–65 (2013); http://dx.doi.org/10.1016/j.carbon.2013.02.030.

- Technical Philippe Vereecken (philippe.vereecken@imec.be)
- Strategic Jef Poortmans (<u>jef.poortmans@imec.be</u>)
- Business Bart Onsia (<u>bart.onsia@imec.be</u>)



Materials, components & process development

Production & storage of H₂



3.1.2. KU Leuven

Centre for Surface Chemistry and Catalysis (COK-KAT)

KU Leuven, Faculty of Bioscience Engineering, Department of Microbial and Molecular Systems

General expertise of the research group

The research team has a strong focus on porous materials, catalysis and adsorption. The emphasis is on three major themes related to grand societal challenges: water, energy and human health. Energy research is concentrated on renewable fuels (solar hydrogen and ammonia), and hydrogen, CO₂ and green methane storage in clathrate hydrates. Molecular aspects of water upon confinement in nanopores relevant to electrolytic processes and molecular storage are investigated.

Specific hydrogen - related expertise & research topics

- Storage of hydrogen, methane and carbon dioxide in clathrate hydrates
- Green ammonia production and cracking, circular nitrogen economy

Available equipment/tools

- Workstation for advanced testing of photoelectrochemical cells & components, electrolysis lab-scale units
- Analytical equipment including ion chromatography, mass spectrometry
- Solid state NMR spectroscopy and XRD for characterizing hydrogen storage materials

Participating in FL/B/EU funded projects with H₂ related research

- PROCURA (BE ETF)(KUL/Energyville, Waterstofnet, VUB, ULiège): Power-to-X and carbon capture & utilization roadmap for Belgium
- HyPErFarm (EU H2020)(KUL, Aarhus, Fraunhofer): Hydrogen and photovoltaic electrification on farm
- ARCLATH II (FL Moonshot cSBO): hydrogen storage in artificial clathrates
- WATUSO (EU ERC AdG): nanoconfined water: a tunable solvent system





Figure 2: H₂/CH , storage in clathrate hydrates

Main relevant publications

- Beckwée, E.J. et al. (2024). Structure I methane hydrate confined in C8-grafted SBA-15: A highly efficient storage system enabling ultrafast methane loading and unloading. Applied Energy, doi: 10.1016/j.apenergy.2023.122120
- Beckwée, E.J. et al. (2023). Enabling hydrate-based methane storage under mild operating conditions by periodic mesoporous organosilica nanotubes. Heliyon, doi: 10.1016/j.heliyon.2023. e17662
- Thijs, B. et al. (2022). Demonstration of a three compartment solar electrolyser with gas phase cathode producing formic acid from CO₂ and water using Earth abundant metals. Frontiers in Chemical Engineering, doi: 10.3389/fceng.2022.1028811
- Thijs, B. et al. (2022). Matching emerging formic acid synthesis processes with application requirements. Green Chemistry, 24(6), pp. 2287-2295.
- Gupta, A. et al. (2021). Hydrogen Clathrates: Next Generation Hydrogen Storage Materials. Energy Storage Materials. Elsevier B.V., pp. 69–107
- Thijs et al. (2021). Selective electrochemical reduction of CO₂ to formic acid in a gas phase reactor with by-product recirculation. Sustainable Energy Fuels, doi: 10.1039/d1se00218j
- Hollevoet et al. (2020). Energy-Efficient Ammonia Production from Air and Water Using Electrocatalysts with Limited Faradaic Efficiency. ACS Energy Letters, 5(4), 1124–1127.
- Rongé et al. (2019). Bifunctional earth-abundant phosphate/phosphide catalysts prepared via atomic layer deposition for electrocatalytic water splitting. Nanoscale Advances, 1(10), 4166–4172.

- Emeritus professor with formal duties Johan Martens (johan.martens@kuleuven.be)
- Professor Christine Kirschhock (christine.kirschhock@kuleuven.be)



Materials, components & process development

Production & storage of H₂



Spin-offs

- Solhyd (www.Solhyd.eu): «Solar hydrogen for everyone everywhere »
- Contact: Jan Rongé (jan.ronge@solhyd.eu)



Foundation

Solhydair Foundation: Solhydair Foundation's disinterested aim is to increase the positive societal impact of technologies, particularly in the areas of energy supply, water supply, and health. It will manage impact licensed technologies for the purpose of clean cooking and cooling with hydrogen, but also the production, filtration and sustainable management of water, having the main goal of improving the physical well-being of humans.



Electrical Energy Applications (ELECTA)

KU Leuven, Faculty of Engineering, Department of Electrical engineering

The research group carries out applied research related to electrical energy. This comprises: Power electronic applications, storage of electricity, integration of PV, protection of distribution grids under the impact of power electronics and electrical bikes.

Specific hydrogen - related expertise & research topics

• Practical evaluation as hydrogen as a storage for electrical distribution grids

Available equipment/tools

KU LEUVEN

- Power analysers (Yokogawa)
- Power-Quality meters (Fluke)
- Test bench for electrical bikes
- Programmable multi-phase AC current and voltage source (Omicron)
- Programmable DC source and load

Participating in FL/B/EU funded projects with H₂ related research

H₂ for all, TETRA

Contact persons

• Prof. Michael Kleemann (Michael.kleemann@kuleuven.be)



Mecha(tro)nic System Dynamics (LMSD) Composite Materials Group (CMG)

KU Leuven, Faculty of Engineering, Department of Mechanical Engineering

General expertise of the research group

KU LEUVEN

- Experimental identification of material characteristics of fibre-reinforced composites
- Development of numerical modelling strategies for material properties in a multi-scale context, including micro-, meso- and macro-scale
- Development of experimental methodologies for the identification and objective quantification of uncertainty and variability in material properties
- Development of modelling strategies for manufacturing and processing methods of fibre-reinforced composites
- Numerical modelling strategies for structural components at the micro- and macro-scale, both for metals and fibre-reinforced composites
- Development of generic numerical formalisms and methodologies for the propagation of uncertainty and variability in structural components
- Methodologies for the identification and objective quantification of uncertainty and variability in material properties
- Comprehensive methodologies for the propagation of uncertainty and variability in built-up structures, covering processes, materials and structures

Specific hydrogen - related expertise & research topics

Application of generic experimental and simulation procedures to characterize pressure vessels, with a focus on reliability:

- Filament wound pressure vessels based on axisymmetric geometry, including cylindrical components and dome-like end caps: from micro- to macro-scale [1-8 above]
- μ CT-scanning procedures and image analysis for the geometrical identification of material structure at the micro-scale (voids and porosities)
- High-pressure vessels (10²-10³ bar of differential pressure) for applications in storage of hydrogen in gaseous state
- Low-pressure vessels (10-1-100 bar of differential pressure) for applications in storage of hydrogen
 in liquid state, development of efficient design procedures for thin-walled geometries (cylindrical,
 spherical, toroidal, conical primitives) with membrane stress only and high volumetric efficiency
- Topology design and thermo-mechanical analysis of multi-lobe liquid hydrogen fuel storage tanks for application in reusable launchers and blended-wing aircraft
- Topology design and thermo-mechanical analysis of storage tanks for transport of hydrogen as cargo payload in aircraft

Available equipment/tools

KU LEUVEN

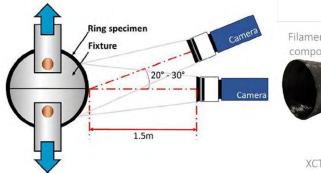
- Composite processing equipment (hot press, autoclave, RTM, infusion)
- Drum winder and filament winding machines
- Mechanical testing of composites, including split-ring test setup
- Damage monitoring tools for mechanical testing (digital image correlation, acoustic emission),
 C-scan
- SEM and optical microscopy
- $\bullet \quad \mu \text{CT-scanning equipment}$ (XCT Core Facilities) and image analysis tools
- DIC equipment and image analysis software
- VoxTex model generation for fibre reinforced composites
- Generic finite element analysis software

International collaborations

- Toyota Motor Europe (BE)
- Mines ParisTech (FR)
- Mines Douai (FR)
- European Space Agency (ESA)
- Hyviate (DE)

Participation in FL/B/EU funded projects with H₂ related research

- SIM ICON project OptiVaS HBC.2019.0070 Optimized pressure vessels through composite Variability Simulation; start 01 Aug 2020 – extended till 31 Jul 2024, coordinator: Toyota Motor Europe; partners: Siemens Industry Software, Plastic Omnium, KU Leuven
- Horizon EU, call CleanH2-2023, ECOHYDRO, Economic manufacturing process of recyclable composite materials for durable hydrogen storage; start 2024 – end 2028, coordinator Institut Mines Telecom, FR; 15 partners from 7 EU countries, including Airbus and Electra Commerical Vehicles Ltd UK
- SIM SBO project RELFICOM HBC.2017.0321 Reliability of fibre-reinforced composites: materials design & variability; start 01 Jan 2018 completion 31 Dec 2021, coordinator: KU Leuven; partners: Toyota Motor Europe, Siemens Industry Software, Plastic Omnium
- FWO doctoral grant strategic basic research, 1SG1523N, Conformable Pressurized Tanks for Hydrogen Storage and Transportation; start 01 Nov 2022 – scheduled till 31 Oct 2026
- VLAIO Baekeland doctoral grant, HBC.2022.0713 Study of the residual stresses in a thermoplastic filament winding process for high-pressure H₂-storage vessels; 2023-2027, in cooperation with Covess





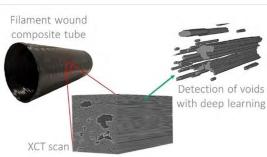


Figure 4: Void characterization in a composite pressure vessel wall via micro-CT





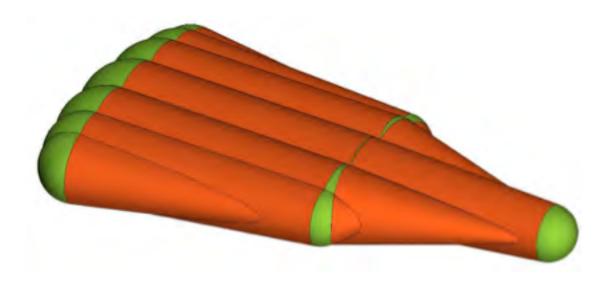


Figure 5: Multi-cell tank topology for maximum volumetric efficiency

Main relevant publications

KU LEUVEN

- Straumit, I., S. V. Lomov and M. Wevers (2015). "Quantification of the internal structure and automatic generation of voxel models of textile composites from X-ray computed tomography data." Composites Part A 69: 150-158. doi:10.1016/j.compositesa.2014.11.016.
- Upadhyay, S., A. G. Smith, D. Vandepitte, S. V. Lomov, Y. Swolfs and M. Mehdikhani (2022). Analysis of voids in filament wound composites using a machine-learning-based segmentation tool. 20th European Conference on Composite Materials (ECCM-20): paper 61918.
- Zhao, Y., P. Druzhinin, J. Ivens, D. Vandepitte and S. V. Lomov (2021). "Split-disk test with 3D digital image correlation strain measurement for filament wound composites." Composite Structures 263: 113686. https://doi.org/10.1016/j.compstruct.2021.113686.
- Zhao, Y., D. Vandepitte and S. V. Lomov (2021). "The effect of delamination on ring specimen failure in the split-disk test with cohesive zone modelling - Comments on the paper: Zhao Y, Druzhinin P, Ivens J, Vandepitte D, Lomov SV. Split-disk test with 3D Digital Image Correlation strain measurement for filament wound composites, Composite Structures, 2021, 263:113686 (doi 10.1016/j. compstruct.2021.113686)." Composite Structures 277: 114517. https://doi.org/10.1016/j.compstruct.2021.114617.
- Niguse Asfew, K., Ivens, J., Moens, D., (2022). "Temperature dependence of thermophysical properties of carbon/polyamide410 composite". Functional Composite Materials, 3, Art.No. 8. doi: 10.1186/s42252-022-00036-6 Open Access
- Ypsilantis, K.I., Faes, M., Ivens, J., Lagaros, N., Moens, D. (2022). "An approach for the concurrent homogenization-based microstructure type and topology optimization problem". Computers & Structures, 272, Art.No. 106859. doi: 10.1016/j.compstruc.2022.106859
- Malfroy, J., Van Bavel, B., Steelant, J., Vandepitte, D. (2023), "Thin-walled tapered conformable pressurized tanks: Concept and principles", submitted to Thin-Walled Structures
- Malfroy, J. (2022) Design and optimization of a tapered multi-bubble tank for hypersonic aircraft, master's thesis dissertation (supervisors D. Vandepitte and J. Steelant)

Materials & components development



- Mechanical engineering Department, LMSD section
 - Dirk Vandepitte (<u>Dirk.vandepitte@kuleuven.be</u>)
 - **David Moens**
 - Johan Steelant
 - Bert Pluymers
- Materials Engineering Department, Composite Materials Group
 - Yentl Swolfs (Yentl.Swolfs@kuleuven.be)
 - Jan Ivens
 - Mahoor Mehdikhani
 - Stepan Lomov
 - Frederik Desplentere



3.1.3. Sirris

Additive Manufacturing

Sirris, Advanced Manufacturing

General expertise of the research group

- Validation of metallic and polymer material for Additive manufacturing in order to use additive
- Manufacturing for increasing the exchange surfaces (specific surface)
- Proof of concepts realisation to test the cells using the potential of AM for iterations

Specific hydrogen - related expertise & research topics

- Dense and porous parts in pure copper (produce by EBM)
- Porous material by using design (lattice) and process setting of L-PBF-LB. (SLM)
- Process validation of porous graded Materials by L-PBF-LB (SLS) process
- Conductive track printing on 3D shapes (3D printing + AJP)

Available equipment/tools

- AM metallic materials validation: 2 PBF-LB (SLM) /1 (PBF-EB) (EBM)/1 DED (cladding)
- AM polymer material validation: 1 MJT/3 VAT PP for loaded material/2 L-PBF-LB (SLS)/2 DLP 3 MEX
- (FDM) covering a wide range of temperatures/ an extrusion head mounted on a Cobot
- AM Feedstock material characterization: Powder lab/ thermal analysis chain adapted to the field of AM
- AM Part quality: Internal stress (DRX) and deformation (Atos 5 Scanner)/mechanical testing

International collaborations

Focus = Belgium as Belgian technology centre



Manufacturig of dense and porous Materials



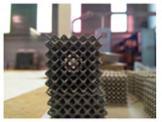






Exemples de structures lattices en polyuréthane thermoplastique (TPU)





Pure Copper for Electrical application









Main relevant publications

- Magnien J, Cosemans P, Nutal N, Kairet T. Current surface issues in additive manufacturing. Plasma Process Polym. 2020;17:e1900154
- YADAV, Pinku, RIGO, Olivier, ARVIEU, Corinne, et al. In situ monitoring systems of the SLM process:
 On the need to develop machine learning models for data processing. Crystals, 2020, vol. 10, no 6, p. 524
- Pauline Delroisse, Matthieu Marteleur, Olivier Rigo, Catherine Doneux, Gregory Pyka, Martine Wevers, Pascal J. Jacques, Aude Simar: "Comparison of the impact resistance of honeycombs and LBM lattice structures "-Workshop on additive manufacturing for space application- ESTEC Noordwijk, Netherlands, 2014.
- Denis Vandormael, Olivier Rigo, Laurent Seronveaux: "Direct deposition of surface acoustic wave by aerosol jet printing technique" - Smart system Integration - VDE verlag publishing, Berlin, 2012

- Guido Heunen (guido.heunen@sirris.be)
- Olivier Rigo (<u>olivier.rigo@sirris.be</u>)



Materials, components & process development

Production 8 storage of Ha



Precision Manufacturing

Sirris, Advanced Manufacturing

General expertise of the research group

Sirris Precision Manufacturing is one of the oldest groups of Sirris and is dedicated towards research and services in the field of advanced manufacturing technologies, and in particular, subtractive manufacturing technologies (e.g. milling, turning, laser ablation) and this in combination with advanced Industry 4.0 practices such as adaptive, data driven machining processes and sensor based manufacturing systems.

Specific hydrogen - related expertise & research topics

- Ultrashort pulsed laser texturing which can potentially:
 - Increase specific surface area of Hydrogen Fuel Cell electrodes (up to 1500-fold) and hence increase efficiency
 - Activate or de-activate parts of the electrode for gas evolving reactions (OER)
 - Produce defects close to the surface to increase wettability and enhance the removal of gas bubbles from the electrodes
 - Create high emissivity (>0,99) and absorption (>99%) surfaces
- Ultrashort pulsed laser machining which can:
 - Cut and structure thin electrode materials in fast and efficient way
 - Engineer coating and selectively remove very thin (200-300 nm) noble metal layers without damage to substrate

Available equipment/tools

- LASEA LS5-1 Femtosecond laser texturing machine
- Keyence vk-x1100 confocal microscope
- COMSOL Thermal modelling & simulation software
- IR Camera & Vacuum tank
- Photo spectrometer

International collaboration

- Sirris Circular Economy, Coatings and renewable materials (T-ICE)
- Sirris Onshore and Offshore Wind Energy Industry (T-OWI)

Participating in FL/B/EU funded projects with H₂ related research

Currently none, but active in ESA GSTP programs to create functional surfaces for space applications and more specifically ultra black surfaces. Recent work by Karsten Lange (Univ. Hannover, Electrode Structuring by Ultrashort Pulsed Lasers: a new tool for the Hydrogen Economy, PhD Thesis, 2019) showed that the same structures are greatly beneficial for Hydrogen applications. This could be potentially a on ground spin-off of space technology developed by Sirris for ESA/Belspo.





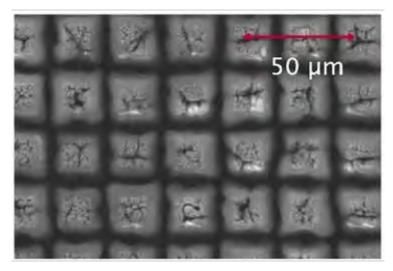


Figure 6: Multiscale structure in Nickel with enormously increase specific surface area, developed for space applications (ESA) but interesting for Hydrogen applications as well.

Main relevant publications

- Ultrafast Laser Selective Phase Removal for surface modification of nanocomposite materials, J. Han,
 O. Malek, J. Vleugels, A. Braem, S. Castagne, Optics Express 29 (16), 24834-24845.
- Ultrashort pulsed laser ablation of zirconia-alumina composites for implant applications, J Han, O Malek, J Vleugels, A Braem, S Castagne, Journal of Materials Processing Technology 299, 117335.
- De Tijd "Belgische Onderzoekers lopen mee naar zwarste zwart" (17/06/2021)

- Senior Engineer Olivier Malek (<u>olivier.malek@sirris.be</u>)
- Program Manager Peter ten Haaf (<u>peter.tenhaaf@sirris.be</u>)



Materials & components development

Storage of H₂



Product Development Hub

Sirris, Composites

General expertise of the research group

Product development in Light, Smart and Micro domains. The Hub combines the expertise of 6 labs (Conception Lab / Fabrication Lab / Micro Lab / Plastics Lab / Hybrids Lab & Smart Lab) to support the companies in the development of innovative products

Specific hydrogen - related expertise & research topics

- Simulation of the structural behaviour of high-pressure composite vessels
- Definition of optimization of the boss and the laminate structure
- Material characterization from specimens produced out of the right process technology

Available equipment/tools

- Simulations through WoundSim/Abaqus chain and Samcef
- Material characterization via universal tensile machine

International collaborations

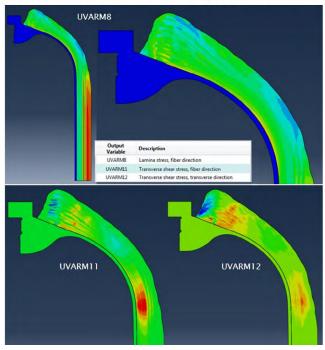
The EY Project THOR described in the next frame

Participating in FL/B/EU funded projects with H₂ related research

- H2020 THOR
 - Partnership: FAURECIA, CETIM & CETIM Grand Est, Air Liquide, RIA, CNRS, NTNU, Sirris
 - The THOR project aims to develop a cost-effective high-pressure "type 4" thermoplastic composite hydrogen storage vessel for transportation applications.
 - Https://thor-fch2.eu/







Main relevant publications

• Only internal reporting within project THOR

Contact persons

SIFFIS innovation forward

• Didier Garray (didier.garray@sirris.be)



3.1.4. UAntwerpen

Antwerp Engineering, Photoelectrochemistry and Sensing (A-PECS)

University of Antwerp, Faculty of Science, Department of Bioscience Engineering

General expertise of the research group

The Antwerp engineering, photoelectrochemistry & sensing (A-PECS) research group has the overall mission to pioneer sustainable solutions for energy, environment & diagnostics. Concerning hydrogen, A-PECS primarily focusses on alternative water production technologies based on photocatalysis, electrolysis and photoelectrocatalysis. We maintain a holistic approach, addressing the problem from nano to macro, starting from the synthesis of new photo(electro)catalysts, all the way to innovative device engineering. In the synthesis of new catalysts, we strive for the exclusive use of non-critical raw materials, thus moving away from platinum group metals. On the level of devices, we study photocatalytic reactors, photo-electrochemical cells, and membraneless (photo)electrolyzers, with the ultimate goal to enable the use of abundant feedstocks (e.g. seawater) or wastewater as the feed.

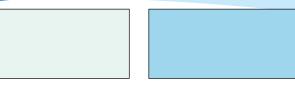
Specific hydrogen - related expertise & research topics

- H₂ production through water splitting by photocatalysis and photo-electrocatalysis
- · Development of innovative membrane-free (photo)electrolyzers
- H₂ recovery from wastewater and contaminated air
- Seawater splitting
- Solar-responsive photo(electro)catalytic materials
- 3D printing of H₂ evolution reactors
- Gas phase analysis of H₂ evolution reactions

Available equipment/tools

- Diverse set of analytics, including GC with pulsed-discharge detector (PDD) for low level H₂
 measurements, thermal conductivity detection (TCD) for high concentrations, etc
- High speed camera for particle/bubble image velocimetry system for non-intrusive fluid flow characterization
- Fully automized gas testing setup with in-line gas detection by FTIR, GC, CLD, Syft-MS,...
- Potentiostat (electrochemical workstation)
- Stereolithographic 3D printer for in-house reactor printing
- Wide array of light sources, ranging from solar simulators, over customized single wavelength LEDs, to a highly tunable CoolLED pE-4000 system







- Simulated moving bed (SMB) with inductively heated thermal swing section for adsorption processes
- Quadrupole mass spectrometer for transient gas analysis
- Refinery gas GC analyser for steady state gas analysis
- Particle image velocimetry system (LED and laser) for non-intrusive fluid flow characterization
- GC with pulsed-discharge detector for low level H₂ measurements
- Fully automized gas testing setup
- Potentiostat
- · Stereolithographic 3D printer for in-house reactor printing

Main relevant publications

- Flow-by membraneless electrolyzer designs: A macroporous flow dividing mesh increases maximum allowable electrode length (2024) R. Borah R., K.R. AG, S.W. Verbruggen. Fuel 377, 132779
- Recent Progress in Developing Non-Noble Metal Based Photocathodes for Solar Green Hydrogen Production. (2024) A.C. Minja, K.R. AG, A. Raes, R. Borah, S.W. Verbruggen. Current Opinion in Chemical Engineering 43, 101000
- Impact of soot deposits on waste gas-to-electricity conversion in a TiO₂/WO₃-based photofuel cell. (2023) K.R. AG, A.C. Minja, R. Ninakanti, M. Van Hal, F. Dingenen, R. Borah, S.W. Verbruggen. Chemical Engineering Journal 470, 144390
- Gas phase photofuel cell consisting of WO3- and TiO2-photoanodes and an air-exposed cathode for simultaneous air purification and electricity generation. (2021) M. Van Hal, R. Campos, S. Lenaerts, K. De Wael, S.W. Verbruggen. Applied Catalysis B: Environmental 292, 120204
- Challenges in the use of hydrogen for maritime applications (2021). L Van Hoecke, L Laffineur, R Campe, P Perreault, S.W. Verbruggen, S. Lenaerts. Energy & Environmental Science 14 (2), 815-843
- Harvesting Hydrogen Gas from Air Pollutants with an Unbiased Gas Phase Photoelectrochemical cell (2017). S.W. Verbruggen, M. Van Hal, T. Bosserez, J. Rongé, B. Hauchecorne, J.A. Martens, S. Lenaerts. ChemSusChem 10, 1413-1418
- Tapping Hydrogen Fuel from the Ocean: a Review on Photocatalytic, Photoelectrochemical and Electrolytic Splitting of Seawater (2021). F. Dingenen, S.W. Verbruggen. Renewable and Sustainable Energy Reviews 142, 110866

Contact persons

Prof. Dr. S.W. Verbruggen (<u>sammy.verbruggen@uantwerpen.be</u>)



Applied Electrochemistry and Catalysis (ELCAT)

University of Antwerp, Faculty of Applied Engineering

General expertise of the research group

Universiteit

Antwerpen

The core research activities within ELCAT are related to the development of state-of-the art electrochemical reactors and its components, with a view towards large-scale industrial development in the field of industrial electrification, in a green and sustainable way to ultimately replace the traditional chemical processes. The scope there is to improve controllability, flexibility and energy efficiency of the reactions through electrocatalyst and reactor design. This research can thus be subdivided in three main topics, which are interrelated: (i) electrocatalysis, (ii) electrosynthesis and (iii) electrochemical reactor engineering. From those research topics, two major aspects of the identity as a group clearly come to the surface: (1) industrial application and (2) sustainable chemistry.

Specific hydrogen - related expertise & research topics

- (Photo-)electrochemical production of hydrogen with a focus on component and reactor development, in-house developed flow-electrolyzers (alkaline and proton-exchange)
- Hydrogen evolution going from catalyst development through GDE preparation and reactor development, with a focus on novel 3D electrodes to improve reactor hydrodynamics (e.g. bubble release, mass transfer, etc.)
- Strategic collaborations already ongoing in the field of alkaline and PEM electrolysis with industry including Agfa and Engie
- Electrochemical production of formic acid and other CO₂-derived chemicals as potential hydrogen carriers, utilizing renewable energy

Available equipment/tools

- A wide range of electrosynthesis set-ups going from batch cells to flow-cells in combination with advanced potentiostats, including boosters required for achieving higher currents
- Electrocatalyst synthesis equipment for wet chemical and electrodeposited catalyst manufacturing: atmosphere-controlled oven, elevated temperature and cryogenic synthesis cells, spray coating, rotavap, hydrostatic pressure vessels, TGA, etc.
- All analytical equipment, including (in-line) GC, HPLC, ICP-MS, DEMS, UV-VIS, etc. to determine the reaction performance and product outcome
- Necessary pumps and sensors (e.g. pressure, flow, pH) to monitor all operating conditions.
- Explosion-safe oven to allow operation at elevated temperatures
- Additionally, ELCAT possesses the required equipment to develop optimized electrolyzers at
 different scales (from 1 cm² to 200 cm²). It can count on its own MP 45, ISEL milling machine, highend 3D metal and polymer printers, an accurate 3D laser micromachining setup, a sputter coater
 and an automated spray coater (up to 1 m² active area)

International collaborations

ELCAT is part of the Center of Excellence on Catalysis at UAntwerp. Additionally, T. Breugelmans is part of the group of experts determining the course of the Capture pipeline with respect to CO₂ conversion.

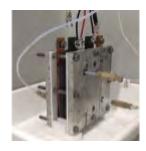
Materials & components development



On an international level, ELCAT has close collaborations with ElectroCat in Slovenia, ICMM-CSIC in Spain, Forschungszentrum Jülich in Germany, TU Delft and TNO in the Netherlands, Fritz Haber Institute in Germany, National Laboratories, etc.

Participating in FL/B/EU funded projects with H₂ related research

- VLAIO O&O with Agfa
 - Topic: ELECZIR: Enhancing Electrolyzer and Zirfon separators for alkaline electrolysis
 - Funding source: VLAIO
 - Main partner: Agfa
- **FWO-WEAVE** proposal
 - Topic: Understanding the role of dopants as a key step towards efficient oxygen evolution catalysts
 - Funding source: FWO-WEAVE
 - Main partners: National Institute of Chemistry, Slovenia
- FWO- PhD Fellowship strategic basic research
 - Topic: Optimisation of Bubble Removal in Alkaline Water Electrolysers at Industrial Current **Densities**
 - Funding source: FWO
 - Main partners: / 0
- **EFFORT**
 - Topic: Development of GDE-MEA for CO₂-electrolysis with low anolyte contribution.
 - Funding source VLAIO-MOT
 - Main partners: KU Leuven, Imec
- Threading-CO₂
 - Topic: Develop CO₂ to CO electrolyzers at pilot and demonstration scale
 - Funding source: Horizon Europe
 - Main partners: Fairbrics, Deutsche institute fur textile- und faserforschung denkendorf, etc.
- SYN-CAT
 - Develop electrocatalysts and photo-electrocatalytic reactor for the conversion of CO₂ to methanol
 - Funding: VLAIO-MOT
 - Main partners: UHasselt, Imec, UGent, VUB
- CLUE
 - Topic: Develop electrocatalytic reactor for the conversion of CO₂ into ethylene at larger scale and directly from flue gases
 - Funding source VLAIO-MOT
 - Main partners: KU Leuven, VITO





Patented zero-gap reactor 2A/cm² current density Trange: 25 – 100°C Prange: up to 2 bar Targeted voltage: < 2.5 V



Materials & components development

Production & storage of H₂



Main relevant publications

- Geboes B., Mintsouli I., Wouters B., Georgieva J., Kakaroglou A., Sotiropoulos S., Valova E., Armyanov S., Hubin A., Breugelmans T., Applied Catalysis B: Environmental, 2014, 150-151, 249.
- Sanchez Gutierrez O., Birdja Y., Bulut M., Vaes J., Breugelmans T., Pant D., Current Opinion in Green and Sustainable Chemistry, 2019, 16, 47-56.
- Daems N., Choukroun D., Merino P., Rettenmaier C., Pacquets L., Bergmann A., Santoro G., Vazquez L., Martinez L. Roldan Cuenya B., Martin Gago J.A., Breugelmans T., ACS Applied Materials & Interfaces, 2022, 14, 2691.
- D. Choukroun, N. Daems, T. Kenis, T. Van Everbroeck, J. Hereijgers, T. Altantzis, S. Bals, P. Cool, T. Breugelmans, The Journal of Physical Chemistry C, 2020, 124, 1369.
- De Mot B., Hereijgers J., Duarte M., Breugelmans T., Chemical Engineering Journal, 2020, 378, 122224-122232.
- De Mot B., Ramdin M., Hereijgers J., Vlugt T., Breugelmans T., ChemElectroChem, 2020, 7, 3839.
- Duarte M., De Mot B., Hereijgers J., Breugelmans T., ChemElectroChem, 2019, 6, 5596.
- Van Daele K., De Mot B., Pupo M., Daems N., Deepak P., Kortlever R., Breugelmans T., ACS Energy Letters, 2021, 6, 4317

- Spokesperson Professor Tom Breugelmans (tom.breugelmans@uantwerpen.be)
- Technological manager Nick Daems (<u>nick.daems@uantwerpen.be</u>)
- Research manager Kevin Van Daele (<u>kevin.vandaele@uantwerpen.be</u>)





Electron Microscopy for Materials Science (EMAT)

Universiteit Antwerpen, Faculty of Sciences, Department of Physics

General expertise of the research group

Electron Microscopy for Materials Science (EMAT) is the core research group in the NANOlight Centre of Excellence. EMAT is an electron microscopy center for materials research specialized in:

- Structure of nanomaterials and interfaces through electron diffraction (ED), high resolution transmission electron microscopy (TEM) and scanning TEM (STEM) imaging
- Electron energy loss spectroscopy (EELS), energy filtered TEM (EFTEM) and energy-dipersive X-ray (EDX) analysis
- Three-dimensional imaging through electron tomography and FIB/SEM slice-and-view
- In-situ TEM analysis while heating/biasing in a gas/humid/liquid environment

Specific hydrogen- related expertise & research topics

- Investigation of the structure of radiation sensitive nanomaterials and interfaces through electron
 diffraction and high-resolution TEM imaging, electron energy loss spectroscopy (EELS), energy
 filtered TEM, three-dimensional imaging through electron tomography and imaging interfaces in
 hybrid compounds
- Catalyst nanoparticle shape/size/distribution analysis with nanometer or atomic resolution
- Stability studies of materials with respect to material morphology, composition and crystal structure, under relevant working conditions while heating/biasing in a gas/humid/liquid environment

Available equipment/tools

- 6 Transmission Electron Microscopes (Thermo Fisher Titan, Tecnai, Jeol)
- 3 Scanning Electron Microscopes (FEI QUANTA FEG 250, FEI Helios Nanolab 650, JEOL)
- Specimen preparation (focused ion beam, etc)
- Image simulation and processing (commercial scientific software packages and in-house developed packages available)
- X-ray powder diffractometers

International collaborations

EMAT has a wide network of collaborators developing nanomaterials used in electrophotocatalysis applications. For example: Utrecht University – Netherlands, IIT – Italy, IMDEA Energy – Spain, CIC bioMAGUNE, Spain.



Materials & components development

Production and/or storage of H₂



Participating in FL/B/EU funded projects with H₂ related research

- NANOlight Centre of Excellence, "Nanoparticles in the spotlight: light-driven nanoscience from the lab to society", some subtopics are related to photoelectrocatalytic hydrogen production. Main partners: Universiteit Antwerpen groups EMAT, CMT, AXIS, A-PECS, EnvEcon
- TEMPEL, "Temperature assisted water electrolysis". Main partners: VLAIO Moonshot, VITO, IMEC, KU Leuven, Ghent University, Universiteit Antwerpen
- ARCLATH, "Artificial clathrates for safe storage, transport and delivery of hydrogen". Main partners: VLAIO Moonshot, KU Leuven, Ghent University, VUB, Universiteit Antwerpen
- DELIGHT, "Designing of multifunctional nanomaterials for light-driven innovation technologies",
 Horizon Europe MSCA Staff Exchange, some topics are related to photocatalysis and hydrogen
 production. Main partners: Universiteit Antwerpen, Italian institute of technology, CNRS, Utrecht
 University, Institute of Polymer Research Dresden
- Correlating Surface Evolution with Electrocatalytic Efficacy in Perovskite Electrocatalysts, FWO project. Partner: University of Louisville, USA

Main relevant publications

- "Tuneable mesoporous silica material for hydrogen storage application via nano-confined clathrate hydrate construction". Ciocarlan R-G, Farrando-Perez J, Arenas Esteban D, Houlleberghs M, Daemen LL, Cheng Y, Ramirez-Cuesta AJ, Breynaert E, Martens J, Bals S, Silvestre-Albero J, Cool P, Nature communications 15, 8697 (2024). http://doi.org/10.1038/S41467-024-52893-3
- "An atomically dispersed Mn-photocatalyst for generating hydrogen peroxide from seawater via the Water Oxidation Reaction (WOR)". Ren P, Zhang T, Jain N, Ching HYV, Jaworski A, Barcaro G, Monti S, Silvestre-Albero J, Celorrio V, Chouhan L, Rokicinska A, Debroye E, Kustrowski P, Van Doorslaer S, Van Aert S, Bals S, Das S, Journal of the American Chemical Society 145, 16584 (2023). http://doi.org/10.1021/JACS.3C03785
- "Enabling hydrate-based methane storage under mild operating conditions by periodic mesoporous organosilica nanotubes". Beckwee EJ, Watson G, Houlleberghs M, Arenas Esteban D, Bals S, Van Der Voort P, Breynaert E, Martens J, Baron GV, Denayer JFM, Heliyon 9, e17662 (2023). http://doi.org/10.1016/J.HELIYON.2023.E17662
- "Hierarchical zeolites containing embedded Cd0.2Zn0.8S as a photocatalyst for hydrogen production from seawater". Yuan Y, Wu F-J, Xiao S-T, Wang Y-T, Yin Z-W, Van Tendeloo G, Chang G-G, Tian G, Hu Z-Y, Wu S-M, Yang X-Y, Chemical communications 59, 7275 (2023). http://doi.org/10.1039/ D3CC01409F
- "Restructuring of titanium oxide overlayers over nickel nanoparticles during catalysis". Monai M,
 Jenkinson K, Melcherts AEM, Louwen JN, Irmak EA, Van Aert S, Altantzis T, Vogt C, van der Stam W,
 Duchon T, Smid B, Groeneveld E, Berben P, Bals S, Weckhuysen BM, Science 380, 644 (2023). http://doi.org/10.1126/SCIENCE.ADF6984
- "A high-entropy oxide as high-activity electrocatalyst for water oxidation". Kante MV, Weber ML, Ni S, van den Bosch ICG, van der Minne E, Heymann L, Falling LJ, Gauquelin N, Tsvetanova M, Cunha DM, Koster G, Gunkel F, Nemsak S, Hahn H, Estrada LV, Baeumer C, ACS nano 17, 5329 (2023). http://doi.org/10.1021/ACSNANO.2C08096
- "Selective anodes for seawater splitting via functionalization of manganese oxides by a lasma-assisted process". Bigiani L, Barreca D, Gasparotto A, Andreu T, Verbeeck J, Sada C, Modin E, Lebedev OI, Morante JR, Maccato C, Applied Catalysis B-Environmental 284, 119684 (2021). http://doi.org/10.1016/J.APCATB.2020.119684



Materials & components development



"Nanostructured materials for solid-state hydrogen storage: a review of the achievement of COST Action MP1103". Callini E, Aguey-Zinsou KF, Ahuja R, Ares JR, Bals S, Biliškov N, Chakraborty S, Charalambopoulou G, Chaudhary AL, Cuevas F, Dam B, de Jongh P, Dornheim M, Filinchuk Y, Grbović Novaković J, Hirscher M, Jensen TR, Jensen PB, Novaković N, Lai Q, Leardini F, Gattia DM, Pasquini L, Steriotis T, Turner S, Vegge T, Züttel A, Montone A, International journal of hydrogen energyT2 - E-MRS Fall Meeting / Symposium C on Hydrogen Storage in Solids -, Materials, Systems and Aplication Trends, SEP 15-18, 2015, Warsaw, POLAND 41, 14404 (2016). http://doi.org/10.1016/j. ijhydene.2016.04.025

- Sara Bals (<u>sara.bals@uantwerpen.be</u>)
- Joke Hadermann (joke.hadermann@uantwerpen.be)
- Jo Verbeeck (jo.verbeck@uantwerpen.be)

Electrification of processes (joule & induction heating)

Production & storage of H₂



Laboratory for the Electrification of Chemical Processes & Hydrogen(ElectrifHy)

University of Antwerp & Faculty of Science, Department of Chemistry/Blue App

General expertise of the research group

At ElectrifHy, we work on the development of electrified chemical reactors, adsorbers, etc. (Power-to-Heat via resistive and induction heating, and the use of electric fields), as well as on (electrified) hydrogen storage and production. Our scope includes the design, simulation (including CFD code development for multiphase turbulent reacting slows), prototyping, experimental characterization and scale-up of intensified reactors. We have a lot of experience in fluidization, counting on various reactors (from 3 to 10 cm ID), including a pre-pilot electrothermal fluidized bed reactors available for tests. Located in the Blue App building, we can also count on world class laboratories, including a 3 story high pilot hall.

Specific hydrogen- related expertise & research topics

- Design of electrically-assisted chemical carriers (e.g., ammonia) cracking reactors
- Design of dehydrogenation units for liquid organic hydrogen carriers (LOHC)
- Test rig for LOHC (up to 250 lpm)
- Design of dense Pd-Ag supported membranes for H₂ removal from reactors
- Pre-pilot electrothermal fluidized bed designed for the pyrolysis of methane into H₂
- Design, simulation, and experimental validation of e-reactors
- Coke-resistant catalysts for biogas (CH4 and CO₂) to syngas applications

Available equipment/tools

- 10 cm ID electrothermal fluidized bed coupled to an online RGA GC
- Up to 250 lpm LOHC test rig
- Various inductively- and resistively-heated reactors fully instrumented
- Various inductively- and resistively-heated fluidized bed reactors (up to 100 bar), fully instrumented, including highly sensitive pressure transducers for indirect reactor diagnostic
- Various Sieverts (volumetric) apparatus for the characterization of adsorbents, using highly sensitive pressure transducers, coupled to -50-200 °C cryostats
- Simulated moving bed (SMB) with inductively-heated thermal swing section for adsorption processes
- Quadrupole mass spectrometer for transient gas analysis
- Refinery gas GC analyzer for steady state gas analysis
- · Particle image velocimetry system (LED and laser) for non-intrusive fluid flow characterization

International collaborations

- Hydrogenious LOHC Technologies, Germany
- Various spin-offs in the direct air capture, energy generation and CCS sector



Electrification of processes (joule & induction heating)

Production & storage of H₂



Participating in FL/B/EU funded projects with H₂ related research

- 'CAMELEON': Electrified catalytic non-oxidative methane coupling for separated hydrogen and ethylene production (2024-2028); VLAIO Moonshot cSBO project (2017-2024). Collaboration with LCT (UGent), and STEN (Ugent)
- Cracking of green ammonia to hydrogen using innovative catalyst and adsorbent assisted plasma technology (HYPACT) (2022-2025); FOD Economie. Federal Government of Belgium; Collaboration with COK-KAT (KULeuven), and PLASMANT (UAntwerp)
- Electrical Cracking of Ammonia for Hydrogen Production (AMELEC) (2024-2025); UAntwerp's industrial valorization funds (IOF SBO) Research Grant. Supported by the Port of Antwerp-Bruges
- "Design of innovative reactors for the release of hydrogen from chemical carriers such as liquid organic hydrogen carriers" (2023-2024); UAntwerp's industrial valorization funds (IOF SBO) Research Grant. Supported by the Port of Antwerp-Bruges
- 'Arclath' 1 and 2 projects on the storage of hydrogen in hydrate clathrates. VLAIO Moonshot cSBO projects (2017-2024); Collaboration with COK-KAT (KULeuven), Comoc (Ugent), Center for Molecular Modeling (Ugent), STEPChem (VUB), and LADCA (UAntwerp)
- "Design of innovative reactors for the release of hydrogen from chemical carriers such as liquid organic hydrogen carriers" (2023-2024); UAntwerp's industrial valorization funds (IOF SBO) Research Grant. Supported by the Port of Antwerp-Bruges
- "Electrified chemical reactor for fast release of hydrogen (H₂) from liquid organic hydrogen carriers (LOHCs) for generator set (genset); H₂ genset testing on a ship (Port of Future)" (2019-2020).
 UAntwerp's industrial valorization funds (IOF SBO) Research Grant. Supported by the Port of Antwerp-Bruges
- BOF DOCPRO4 PhD Fellowship, "CFD-Assisted Design of an Innovative Multiphase Chemical Reactor for Hydrogen Release"

Main relevant publications

- Challenges in the use of hydrogen for maritime applications (2021). L Van Hoecke, L Laffineur, R
 Campe, P Perreault, et al. Energy & Environmental Science 14 (2), 815-843
- Combined Methane Pyrolysis and Solid Carbon Gasification for Electrified CO₂-Free Hydrogen and Syngas Production (2023). P Perreault, CR Boruntea, et al. Energies 16 (21), 7316
- Intensified swirling reactor for the dehydrogenation of LOHC (2023). L Van Hoecke, NB Kummamuru, et al. International Journal of Hydrogen Energy
- Critical challenges towards the commercial rollouts of a LOHC-based H₂ economy (2023). P
 Perreault, L Van Hoecke, et al. Current Opinion in Green and Sustainable Chemistry, 100836
- Hydrogen clathrates: Next generation hydrogen storage materials (2021). A Gupta, GV Baron,
 P Perreault, et al. Energy Storage Materials 41, 69-107

Contact persons

Prof Dr Ir Patrice Perreault (<u>Patrice.perreault@uantwerpen.be</u>)

Production & storage of H₂



Laboratory of Adsorption and Catalysis (LADCA)

University of Antwerp, Faculty of Science, Department of Chemistry

General expertise of the research group

- The Laboratory of Adsorption and Catalysis (LADCA) is a pioneer in the synthesis and applications of
 porous materials and metal-oxides in the field of adsorption and catalysis. The research activities in
 the laboratory of Adsorption and Catalysis are focussed on:
 - The development of new micro- and mesoporous inorganic materials
 - Optimalization of synthesis pathways for inorganic materials with a controlled porosity and surface properties
 - Catalytic activation of porous materials
 - Optimalization of porous materials for efficient gas- and liquid separations
 - Characterization of porous materials
 - Catalytic applications (redox and photocatalysis)

Specific hydrogen - related expertise & research topics

- Design of heterogeneous catalysts for in-situ hydrogen production for sustainable reduction reactions in water (BOF-GOA project in collaboration with the Organic Chemistry group (prof. B. Maes)
- Development of porous materials with tuned properties as matrix for hydrogen clathrate formation (Vlaio Moonshot project on Artificial clathrates for safe storage, transport and delivery of hydrogen (ARCLATH))
- Photocatalytic and photo-electrocatalytic reduction of CO₂ with hydrogen into added value chemicals (Vlaio Moonshot D2M and Vlaio Moonshot SYN-CAT projects)

Available equipment/tools

- Micro-Raman, in-situ Raman
- FT-IR, in-situ FT-IR
- UV-VIS
- TGA/DTG, TGA-MS
- N2-sorption, chemisorption
- TOC
- TPR, TPO
- Photocatalytic set-ups and lamps
- Reactors (photocatalytic, plasma and automotive)
- GC detection

International collaborations

- UNIPD, Padova, Italy
- NCSRD Athens, Greece
- National Institute of Chemistry, Ljubljana, Slovenia
- University of Alicante, Alicante, Spain
- Technical University Gheorghe Asachi, Iasi, Romania
- ENMIX (European Nanoporous Materials Institute of Excellence aisbl)
- DZA (Dutch zeolite association)



Production, storage, transport & use of H₂ and H₂-based carriers



Main relevant publications

- Suligoj A. Arcon I., Mazaj M., Drazic G., Arcon D., Cool P., Stangar U.L., Tusar N.N., Surface modified titanium dioxide using transition metals: nickels as winning transition metal for solar light photocatalysis, J. Mat. Chem. A, 6 (21), 9882-9892, 2018
- Xin Q., Papavasiliou A., Boukos N., Glisenti A., Li JPH, Yang Y., Philippopoulos C.J., Poulakis E., Katsaros F.K., Meynen V., Cool P., Preparation of CuO/SBA-15 catalyst by the modified ammonia driven deposition precipitation method with a high thermal stability and an efficient automotive CO and hydrocarbons conversion, Applied Catalysis B- Environmental, 223, 103-115, 2018
- N. Blommaerts, N. Hoeven, D. Arenas Esteban, R. Campos, M. Mertens, R. Borah, A. Glisenti, K. De Wael, S. Bals, S. Lenaerts, S.W. Verbruggen, P. Cool, Tuning the turnover frequency and selectivity of photocatalytic CO₂ reduction to CO and methane using platinum and palladium nanoparticles on Ti-Beta zeolites, Chemical Engineering Journal 410, 128234, 2021
- R.-G Ciocarlan, N. Hoeven, E. Irtem, V. Van Acker, M. Mertens, E.M. Seftel, T. Breugelmans, P. Cool, <u>Ferrite@TiO2-nan</u>ocomposites as Z-scheme photocatalysts for CO₂ conversion: Insight into the correlation of the Co-Zn metal composition and the catalytic activity, Journal of CO₂ Utilization, 36, 177-186, 2020
- Y. Uytdenhouwen, V. Meynen, P. Cool, A. Bogaerts, The potential use of core-shell structured spheres in a packed-bed DBD plasma reactor for CO₂ conversion, Catalysts, 10, 5, 2020, DOI: 10.3390/catal10050530
- A. Gupta, G. V. Baron, P. Perreault, S. Lenaerts, R.-G. Ciocarlan, P. Cool, P. G.M. Milea, S. Rogge, V. Van Speybroeck, G. Watson, P. Van Der Voort, M. Houlleberghs, E. Breynaert, J. Martens, J. F.M. Denayer, Hydrogen clathrates: next generation hydrogen storage materials, Energy Storage Materials 41, 69-107, 2021.
- N. B. Kummamuru, G. Watson, R.-G. Ciocarlan, S.W. Verbruggen, P. Cool, P. Van Der Voort, P. Perreault, Accelerated methane storage in clathrate hydrates using mesoporous (Organo-) silica materials, Fuel 354, 129403, 2023.
- E.J. Beckwée, M. Houlleberghs, R-G Ciocarlan, C.V. Chandran, S. Radhakrishnan, L. Hanssens, P. Cool, J. Martens, E. Breynaert, G.V. Baron, J.F.M. Denayer, Structure I methane hydrate confined in C8-grafted SBA-15: A highly efficient storage system enabling ultrafast methane loading and unloading, Applied Energy 353, 122120, 2024.

Contact persons

Prof. Pegie Cool (pegie.cool@uantwerpen.be)

Production, storage, transport & use of H₂ and H₂-based carriers



Plasma Lab for Applications in Sustainability & Medicine ANTwerp (PLASMANT)

University of Antwerp, Faculty of Science, Department of Chemistry

General expertise of the research group

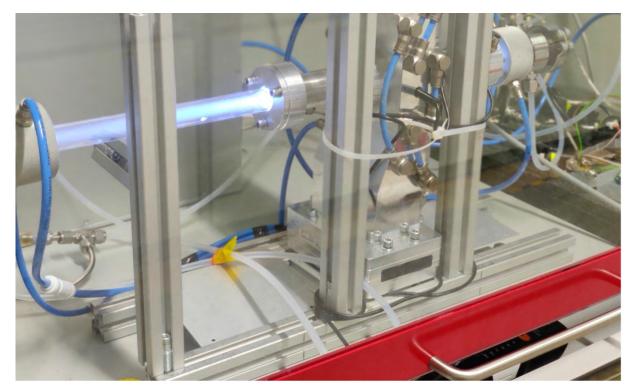
Plasma research by means of computer modelling and experiments, for two main applications, i.e.:

- Green chemistry, including CO₂, CH4 and N2 conversion into value-added chemicals and fuels, or into fertilizers, but also NH3 cracking for green H₂ production
- Plasma medicine, focusing mainly on cancer treatment, but also virus inactivation

The aim is to obtain better insights in the underlying mechanisms, in order to improve the applications. Indeed, plasma technology is very promising for green chemistry, as energy-efficient alternative to the existing classical conversion methods, because the splitting of inert molecules (such as CO_2 , CH_4 and N_2) is initiated by energetic electrons present in the plasma.

Specific hydrogen - related expertise & research topics

- Plasma-based CH₄ conversion into H₂ (and value-added carbon) and into higher hydrocarbons (e.g., ethylene, acetylene) and oxygenates
- Plasma-based dry reforming of methane, including plasma catalysis, for the production of syngas and other value-added chemicals and fuels
- Plasma-based H₂ synthesis from other hydrocarbons (e.g., methanol, ethanol, and even plastic waste pyrolysis products), as well as from NH₃
- We perform research for all these applications, by a combination of plasma chemistry and plasma reactor modelling, and experiments



Production of H₂



Available equipment/tools

- Various (gliding) arc plasma reactors, atmospheric pressure glow discharges, microwave plasmas and dielectric barrier discharge plasmas
- Analysis equipment (GC, MS, non-dispersive IR/UR, optical sensors) for gas conversion
- Various types of models: quasi-1D chemical reaction kinetics models, 2D/3D fluid dynamics simulations, Monte Carlo, particle-in-cell Monte Carlo, hybrid models, molecular dynamics, density functional theory simulations

International collaborations

- ERC Synergy Grant "SCOPE", together with G. Centi, V. Hessel and E. Rebrov: See website ERC Synergy SCOPE
- DIFFER (Dutch Institute for Fundamental Energy Research)
- Eindhoven University of Technology
- Maastricht University
- University of Liverpool
- · University of Messina
- University of Warwick
- University of Adelaide
- University of Manchester
- University of Notre Dame
- Dalian University of Technology
- CSIRO-Australia

Participating in FL/B/EU funded projects with H₂ related research

- HyPACT: Cracking of green ammonia to hydrogen using innovative catalyst and adsorbent assisted
 plasma technology, ETF project, with Waterstofnet, KU Leuven (J. Martens), and UAntwerpen (P.
 Perreault)
- OPTANIC: Energy-efficient plasma conversion of greenhouse gases to methanol, the fuel of the future, BlueApp POC project, with our spinoff Optanic
- PLASyntH2: Plasma-based green hydrogen synthesis from hydrocarbons, FWO-FNRS Excellence of Science project, with UGent (N. De Geyter, R. Morent), UMONS (R. Snyders) and ULB (F. Reniers)
- P2O: Power to olefins: Electrified steam cracking and plasma booster, Catalisti-Moonshot SBO project, with UGent (K. Van Geem, G. Stefanidis, R. Morent) and VKI
- SCOPE: Surface-COnfined fast-modulated Plasma for process and Energy intensification in small
 molecules conversion, ERC Synergy Grant, with Univ. Messina (G. Centi), Warwick Univ. (E. Rebrov)
 and Univ. Adelaide (V. Hessel)
- ALCHEMHY: Horizon Europe RIA project with several international partners, where we focus on: Plasma-catalytic hydrogenation of CO₂ to CH3OH



Production of H₂



Main relevant publications

- Plasma-assisted NH3 cracking in warm plasma reactors for green H₂ production, I. Fedirchyk, I.
 Tsonev, R. Quiroz Marnef and A. Bogaerts, Chem. Eng. J. 499, 155946 (2024)
- Plasma technology a novel solution for CO₂ conversion R. Snoeckx and A. Bogaerts, Chem. Soc. Rev. 46, 5805-5863 (2017). Selected for the cover of the journal (IF 40.182).
- Plasma technology: An emerging technology for energy storage. A. Bogaerts and E. Neyts, ACS
 Energy Lett. 3, 1013-1027 (2018). Invited feature article, and selected to be featured in ACS Editors'
 Choice + Free Open Access (IF 16.331)
- Plasma-based CH₄ conversion into higher hydrocarbons and H₂: Modelling to reveal the reaction mechanisms of different plasma sources. S. Heijkers, M. Aghaei, A. Bogaerts, J. Phys. Chem. C, 124, 7016-7030 (2020). Featured in "ACS Editors' Choice", and given open access due to its potential for broad public interest.
- Plasma-catalytic ammonia reforming of methane over Cu-based catalysts for the production of HCN and H₂ at reduced temperature. Y. Yi, X. Wang, A. Jafarzadeh, L. Wang, P. Liu, B. He, J. Yan, R. Zhang, H. Zhang, X. Liu, H. Guo, E.C. Neyts and A. Bogaerts, ACS Catal., 11, 1765-1773 (2021).
- Plasma-catalytic ammonia decomposition using a packed-bed dielectric barrier discharge reactor. J. A. Andersen, J. M. Christensen, M. Østberg, A. Bogaerts and A. D. Jensen, Int. J. Hydrog. Energy, 47, 32081-32091 (2022).
- Methane coupling in nanosecond pulsed plasmas: correlation between temperature and pressure and effects on product selectivity. E. Morais, E. Delikonstantis, M. Scapinello, G. Smith, G. D. Stefanidis and A. Bogaerts, Chem. Eng. J. 462, 142227 (2023). (15 pages)
- Modelling the dynamics of hydrogen synthesis from methane in nanosecond-pulsed plasmas. E.
 Morais and A. Bogaerts, Plasma Process. Polymers, 2300149 (2023). (10 pages)
- NH3 decomposition for H₂ production by thermal and plasma catalysis using bimetallic catalysts. S.
 Meng, S. Li, S. Sun, A Bogaerts, Y. Liu and Y. Yi, Chem. Eng. Sci, 283, 119449 (2024).

Contact persons

Annemie Bogaerts (annemie.bogaerts@uantwerpen.be)





3.1.5. UGent

Center for Molecular Modelling (CMM)

Ghent University, Faculty of Engineering and Architecture/Sciences, Department of Physics and Astronomy

General expertise of the research group

The Center for Molecular Modelling focuses on frontier research in six major areas - chemical kinetics in nanoporous materials, computational material research on the nanoscale, spectroscopy, many-particle physics, model development & bio- and organic chemistry. Our multidisciplinary research team is currently composed of about 40 researchers from the Faculties of Sciences (WE05) and Engineering and Architecture (EA17, EA08) of Ghent University.

Specific hydrogen - related expertise & research topics

Design of Materials for H₂ storage and conversion of chemicals

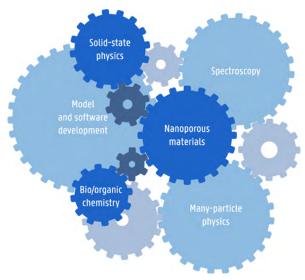
Available equipment/tools

- Expertise in a very broad range of molecular modelling engines (Gaussian, ADF, MOLPRO, CHARMM,
- CPMD, CP2K, Orca, VASP,...)
- Developer of own software codes available via https://molmod.ugent.be/software, Member of the developer teams of large-scale software engines such as LAMMPS, CP2K,...
- Largest user of HPC infrastructure at the Flemish level and pilot user in newly installed HPC clusters



Fransport of H_2





Main relevant publications

- See website: biblio.ugent.be
- Vandeputte A, Sabbe M, Reyniers M-F, Van Speybroeck V, Waroquier M, Marin G. Theoretical study
 of the thermodynamics and kinetics of hydrogen abstractions from hydrocarbons. JOURNAL OF
 PHYSICAL CHEMISTRY A. AMER CHEMICAL SOC; 2007;111(46):11771–86.
- Martínez-Espín JS, De Wispelaere K, Janssens TVW, Svelle S, Lillerud KP, Beato P, et al. Hydrogen transfer versus methylation: on the genesis of aromatics formation in the Methanol-To-Hydrocarbons reaction over H-ZSM-5. ACS CATALYSIS. 2017;7(9):5773–80.
- Van Houteghem M, Verstraelen T, Ghysels A, Vanduyfhuys L, Waroquier M, Van Speybroeck V. Analysis of the basis set superposition error in molecular dynamics of hydrogen-bonded liquids: application to methanol. JOURNAL OF CHEMICAL PHYSICS. 2012;137(10).

Contact persons

Prof. Veronique Van Speybroeck (<u>Veronique.VanSpeybroeck@ugent.be</u>)



Center for Ordered Materials, Organometallics & Catalysis (COMOC)

Ghent University, Faculty of Science, Department of Chemistry

General expertise of the research group

The synthesis of new porous materials and their application in heterogeneous catalysis, adsorption and biomedical systems.

The Center for Ordered Materials, Organometallics and Catalysis (COMOC) is internationally very renowned for the development of novel porous materials, as adsorbents, heterogeneous catalysts, photocatalysts, electrodes for photocatalysis, electrodes for electrocatalysis, materials for sensing and luminescence.

The group typically consists of 1 director (Prof. Pascal Van Der Voort), 5 postdocs, 10-15 PhD students, 5-10 undergraduates and visiting PhD students (interns). They are fully equipped for the characterization and testing of the materials.

Specific hydrogen - related expertise & research topics

- Development and synthesis of novel crystalline highly porous materials
- Development and synthesis of highly porous crystalline polymers
- Storage/Separation of gases in highly porous media (MOFs, COFs)
- Hydrogenation reactions
- Photocatalytic total water splitting
- Z-scheme tandem cells for photocatalysis (heterojunctions)
- Electrocatalysis
- Development of COF

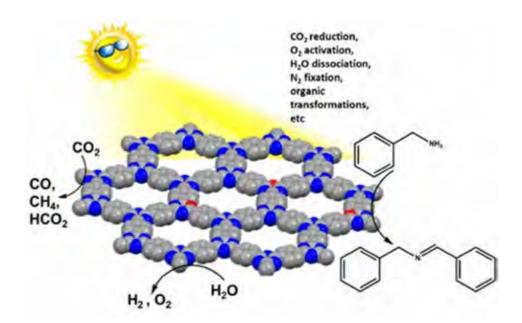
Available equipment/tools

• GC, HPLC, state of the art sorption equipment (high pressure, low pressure, chemisorption, TPD, TPR, TPD), CHNS elemental analysis, FTIR, FT-Raman, dispersive Raman, UV-VIS, electrocatalytic setups, photocatalytic setups, powder XRD, single crystal XRD, ...

International collaborations

COMOC collaborates with the leading international groups on porous materials, heterogeneous catalysis, photo-and electrocatalysis, including prof. Markus Antonietti (MPI-Potsdam), prof. Bettina Lotch (MPI-Stuttgart), prof. Christian Serre (Versailles), prof. Arne Thomas (TU Berlin), prof. Mietek Jaroniec (Kent State Univ, USA), and many others.





Participating in FL/B/EU funded projects with H₂ related research

- See website: research.ugent.be
- Group website: www.ugent.comoc.be
- Twitter: @COMOC_research
- COMOC is active in the Flanders Moonshot Projects on Hydrogen Generation and Hydrogen Storage (MOT-4) with one running project and one project currently being reviewed.

Main relevant publications

- See website: biblio.ugent.be
- Group website: www.comoc.ugent.be
- RESEARCH-ID: http://www.researcherid.com/rid/D-3800-2012
- ORCID: http://orcid.org/0000-0002-1248-479X
- GOOGLE SCHOLAR: https://scholar.google.be/citations?user=DdI5E8QAAAAJ&hl=en
- PUBLONS: https://publons.com/researcher/1309466/pascal-van-der-voort/

Contact persons

Prof. dr. Pascal Van Der Voort (<u>Pascal.VanDerVoort@ugent.be</u>)



Process development



Conformal Coating of Nanomaterials (COCOON)

Ghent University, Faculty of Sciences, Department of Solid State Science

General expertise of the research group

The research group COCOON is part of the Department of Solid State Sciences and is led by Christophe Detavernier and Jolien Dendooven. Our research is directed at developing and understanding thin film materials within a context of applications relevant to society. We develop thin films and nanomaterials and systematically study their properties governed by their composition, structure, and surface and interface nature. We are particularly interested in (1) physical phenomena that occur at surfaces and interfaces during thin film growth or electrochemical energy conversion reactions, (2) solid state reactions that occur at the nanoscale, and (3) ion transport in solid state nanoscale systems. Understanding these fundamental aspects provides the necessary foundation for optimizing deposition processes and developing materials with an improved functionality for the targeted applications. Important research topics include:

- Atomic layer deposition for ultrathin coatings, surface engineering and conformal coating of nanostructured materials
- In-situ characterization of thin films during deposition/annealing treatments
- Combinatorial thin film research for fast screening of composition-dependent properties of binary, ternary or even quaternary mixtures

Specific hydrogen - related expertise & research topics

The COCOON group has a strong track record in investigating thin film materials for applications in microelectronics and battery technology. Since several years, the group is expanding its expertise in thin film technology to applications in electrocatalysis:

- Atomic layer deposition (ALD) of electrocatalysts for hydrogen and oxygen evolution reactions: metal nanoparticles, oxides, phosphates and sulphides with controllable composition and dimensions
- ALD for tailoring electrochemical interfaces, e.g. passivation layers for photoelectrodes, stabilizing layers to prevent metal nanoparticle catalyst degradation, thin films of mixed ionic electronic conductors
- Combinatorial magnetron sputtering of alloy thin film libraries for catalyst composition screening

Process development

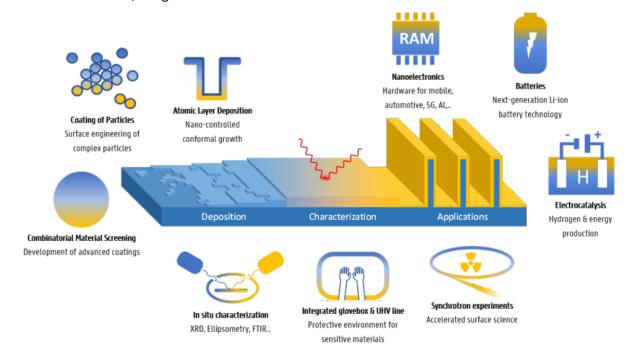


Available equipment/tools

- Thermal and plasma-enhanced ALD systems with several integrated in-situ characterization techniques to monitor surface reactions and film deposition during ALD processes
- Dedicated setups for the sputter deposition of combinatorial thin film libraries; wafers can be coated
 with a film that has a uniform thickness and a linear gradient in composition, resulting in a "printed"
 compositional library of binary, ternary or even quaternary mixtures; in this way, one can easily
 investigate the properties of >100 different compositions in parallel
- Several home-built systems for in situ XRD during annealing under controlled ambient (oxidizing, inert, reducing) offering opportunities to efficiently study the evolution of phase, grain size and phenomena such as crystallization and phase transformations during annealing
- An integrated glovebox infrastructure for thin film deposition onto air-sensitive materials, and for surface and electrochemical characterization, all without exposure to air. All gloveboxes are Ar-filled.
 Several commercial and home-built potentiostat/galvanostat devices are available
- UHV cluster tool consisting of an ALD tool, a scanning probe microscope, an instrument for XPS and a vacuum transfer line, which allows for transferring samples between glovebox, deposition and analytical chambers without air exposure

Participating in FL/B/EU funded projects with H₂ related research

- SYN-CAT (SBO, VLAIO-MOT, UA, UHasselt, Imec, UGent, VUB): Synergetic design of catalytic materials for integrated photo- and electrochemical CO₂ conversion processes
- TEMPEL (SBO, VLAIO-MOT, VITO, Imec, UGent, KU Leuven, UA): Temperature assisted water electrolysis
- ALTERPEM (SBO, VLAIO-MOT, KUL, Imec, UGent): Alternative for PEM technology with nonfluorinated, integrated membranes and PGM-free nanoarchitecture









Main relevant publications

IIIIIII

GHENT UNIVERSITY

- Blomme, R.; Ramesh, R.; Henderick, L.; Minjauw, M.; Vereecken, P.; Adriaens, M.; ... Dendooven, J.
 Atomic layer deposition for tuning the surface chemical composition of nickel iron phosphates for oxygen evolution reaction in alkaline electrolyzers, IOP Nanotechnology 35 (23), 235401 (2024)
- Mathew, F.; Van den Hoek, J.; Poonkottil, N.; Zhao, B.; Rampelberg, G.; Choukroun, D.; Hereijgers, J.; Hens, Z.; Poelman, D.; Breugelmans, T.; Detavernier, C.; Dendooven, J. Crystalline Tin Disulfide by Low-Temperature Plasma-Enhanced Atomic Layer Deposition as an Electrode Material for Li-Ion Batteries and CO₂ Electroreduction, ACS Applied Energy Materials 6 (24), 12526-12538 (2023)
- Henderick, L.; Dhara, A.; Werbrouck, A.; Dendooven, J.; Detavernier, C. Atomic layer deposition of metal phosphates, Applied Physics Reviews 9, 011310 (2022)
- Trompoukis, C.; Feng, J.-Y.; Bosserez, T.; Rongé, J.; Dendooven, J.; Detavernier, C.; Baets, R.; Martens, J. A. ALD Pt nanoparticles and thin-film coatings enhancing the stability and performance of silicon photocathodes for solar water splitting, Sustainable Energy Fuels 5, 3115-3123 (2021)
- Rongé, J.; Dobbelaere, T.; Henderick, L.; Minjauw, M. M.; Sree, S. P.; Dendooven, J.; Martens, J. A.;
 Detavernier, C. Bifunctional earth-abundant phosphate/phosphide catalysts prepared via atomic layer deposition for electrocatalytic water splitting, Nanoscale Advances 1, 4166 4172 (2019)
- Dendooven, J.; Ramachandran, R. K.; Solano, E.; Kurttepeli, M.; Geerts, L.; Heremans, G.; Minjauw, M. M.; Dobbelaere, T.; Devloo-Casier, K.; Martens, J. A.; Vantomme, A.; Bals, S.; Portale, G.; Coati, A.; Detavernier, C. Independent tuning of size and coverage of supported Pt nanoparticles using atomic layer deposition, Nature Communications 8, 1074 (2017)
- Mattelaer, F.; Bosserez, T.; Rongé, J.; Martens, J. A.; Dendooven, J.; Detavernier, C. Manganese oxide films with controlled oxidation state for water splitting devices through a combination of atomic layer deposition and post-deposition annealing, RSC Advances 6, 98337-98343 (2016)
- Rongé, J.; Deng, D.; Sree, S. P.; Bosserez, T.; Verbruggen, S. W.; Singh, N. K.; Dendooven, J.; Roeffaers, M. B. J.; Taulelle, F.; De Volder, M.; Detavernier, C.; Martens, J. A., Air-based photoelectrochemical cell capturing water molecules from ambient air for hydrogen production, RSC Advances 4 (55), 29286-29290 (2014)

- Prof. Dr. Christophe Detavernier (Christophe.Detavernier@UGent.be)
- Prof. Dr. Jolien Dendooven (<u>Jolien.Dendooven@UGent.be</u>)



System modelling



Electrical Energy Laboratory (EELAB & Lemcko)

Ghent University, Faculty of Engineering and Architecture, Department of ElectroMechanical, Systems and Metal Engineering

General expertise of the research group

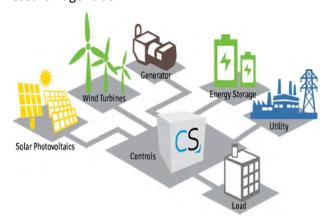
- Low frequency electromagnetic fields and magnetic materials
- Power Systems
- Power Electronics
- Drive systems and control for electrical machines
- Energy and cluster management

Specific hydrogen - related expertise & research topics

- Electrolyser electrical grid integration aspects, flexibility
- Power-to-X
- Power generation grid support (X-to-power)

Participating in FL/B/EU funded projects with H₂ related research

- BEST (Energy Transition Fund, PhD with UCLouvain)
- InduFlexControl (Catalisti cSBO)
- CO2PERATE (Catalisti SBO)
- GREENPORTS (Flux50 ICON)
- See website: research.ugent.be









Main relevant publications

IIIIII

GHENT UNIVERSITY

- See website: biblio.ugent.be
- Dadkhah A, Bozalakov D, De Kooning J, Vandevelde L. On the optimal planning of a hydrogen refuelling station participating in the electricity and balancing markets. INTERNATIONAL JOURNAL OF HYDROGEN ENERGY. 2021;46(2):1488–500.
- Ebneali Samani A, D'Amicis A, De Kooning J, Bozalakov D, Silva P, Vandevelde L. Grid balancing with a large-scale electrolyser providing primary reserve. IET RENEWABLE POWER GENERATION. 2020;14(16):3070–8.
- Baetens J, De Kooning J, Van Eetvelde G, Vandevelde L. A two-stage stochastic optimisation methodology for the operation of a chlor-alkali electrolyser under variable DAM and FCR market prices. ENERGIES. 2020;13(21).

- Prof. Lieven Vandevelde (lieven.vandevelde@ugent.be)
- Prof. Greet Van Eetvelde (greet.vaneetvelde@ugent.be)
- Prof. Jan Desmet (<u>janj.desmet@ugent.be</u>)

Process development



Industrial Catalysis and Adsorption Technology (INCAT)

Ghent University, Faculty of Engineering and Architecture, Department of Materials, Textiles and Chemical Engineering

General expertise of the research group

The Industrial Catalysis and Adsorption Technology research group (INCAT) focuses mainly on the development of catalysts and adsorbents with a strong focus on renewable resources and environmental management. This involves the catalytic conversion of biomass-derived streams, their upgrading and separation into useful chemicals, with a strong application-oriented goal. This goal is pursued by the many running research projects in collaboration with consortium and industrial partners, including smaller and middle-sized companies in the broader chemical industry.

- Heterogeneous catalysis
- Membrane technologies
- Separation technologies
- Separation and membrane technologies not elsewhere classified
- (Waste)water treatment processes

Specific hydrogen - related expertise & research topics

Catalyzed sodium borohydride hydrolysis (NaBH4 as storage for hydrogen)

Available equipment/tools

- Reactors
- Catalyst synthesis
- Characterization
- See: https://incat.ugent.be/infrastructure.html

International collaborations

- H2Fuel: www.H₂-fuel.nl
- Bilateral projects with H2CiF, H2Fuel
- See website: research.ugent.be







Main relevant publications

- See website: biblio.ugent.be
- B. Van Vaerenbergh, J. Lauwaert, P. Vermeir, J. Thybaut, and J. De Clercq, "Towards highperformance heterogeneous palladium nanoparticle catalysts for sustainable liquid-phase reactions," REACTION CHEMISTRY & ENGINEERING, vol. 5, no. 9, pp. 1556–1618, 2020.

Contact persons

 $\widehat{\underline{\underline{}}}$

GHENT UNIVERSITY

Prof. Jeriffa De Clercq (Jeriffa.DeClercq@ugent.be)



Process development



Laboratory for Chemical Technology (LCT)

Ghent University, Faculty of Engineering and Architecture, Department of Materials, Textiles and Chemical Engineering

General expertise of the research group

The Laboratory for Chemical Technology (LCT) integrates chemical science and engineering in its research on catalysis, polymerization, kinetics, reactor design and process design. LCT is part of the Department of Materials, Textiles and Chemical Engineering within the Faculty of Engineering and Architecture at Ghent University in Belgium and member of the Centre for Sustainable Chemistry (CSC) of Ghent University. LCT aims at research excellence and bottom-up innovation in the framework of technological, industrial, and societal challenges.

Specific hydrogen - related expertise & research topics

- · Production of e-fuels
- · Economics of e-fuels
- Chemical looping
- Catalytic processes

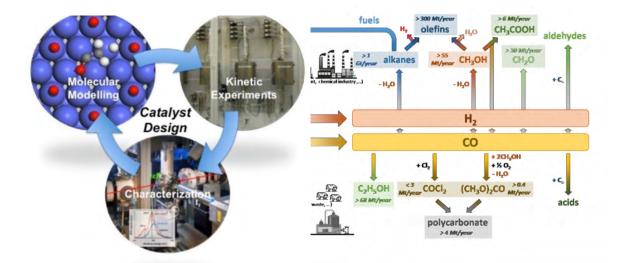
Available equipment/tools

- Lab scale reactors for investigating thermal, catalytic, chemical looping and adsorptive reaction processes
- Chemical looping pilot plant with a production capacity in the order of kg/day
- Catalyst synthesis
- Materials characterization (redox/acid-base properties, porosity, ...)
- Software for:
 - Mechanistic investigations
 - Fluid Dynamics calculations
 - Process design
 - (Micro)kinetic modelling

Participating in FL/B/EU funded projects with H₂ related research

- MuSE (Energy Transition Fund, 2022-2025, 1 PhD)
- CATCO2RE (SBO, 2018-2021, 3 PhD)
- CO2PERATE (cSBO, 2018-2022, 1 PhD)
- C2O (MOT3 sSBO, 2021-2022, 2 PhD)
- Be-HyStore (Energy Transition Fund, 2023-2026, 1 PhD)
- See website: research.ugent.be





Main relevant publications

- See website: biblio.ugent.be
- V. Singh, L. C. Buelens, H. Poelman, M. Saeys, G. B. Marin, V. V. Galvita, Intensifying blue hydrogen production by in situ CO₂ utilisation, Journal of CO₂ Utilization, 2022, 61, 102014.
- De Vrieze J, Urbina Blanco CA, Thybaut J, Saeys M. Autocatalytic role of molecular hydrogen in copper-catalyzed transfer hydrogenation of ketones. ACS CATALYSIS. 2019;9(9):8073–82.
- Van Geem K, Galvita V, Marin G. Making chemicals with electricity. SCIENCE. American Association for the Advancement of Science (AAAS); 2019. p. 734–5.

- Prof. Kevin Van Geem (Kevin.VanGeem@ugent.be)
- Prof. Mark Saeys (Mark.Saeys@ugent.be)
- Prof. Vladimir Galvita (<u>Vladimir.Galvita@ugent.be</u>)
- Prof. Joris Thybaut (<u>Joris.Thybaut@ugent.be</u>)



Storage & transport of H



Mechanics of Materials and Structures (MMS)

Ghent University, Faculty of Engineering and Architecture, Department of Materials, Textiles and Chemical Engineering

General expertise of the research group

The research group Mechanics of Materials and Structures (MMS) is part of the Department of Materials, Textiles and Chemical Engineering (MaTCh). This group has more than 40 years of experience in the design, simulation, testing and inspection of fiber-reinforced composites. In the last decade, also expertise in additive manufactured materials has been developed.

The group has a long-term tradition in numerical simulation and design of composites, in static, impact, fatigue and creep loading conditions. A wide range of experimental test facilities is available for mechanical characterization of materials, and also for Non-destructive Testing (NDT) of materials and components.

Specific hydrogen - related expertise & research topics

- Simulation and design of filament wound composite pressure vessels for hydrogen storage.
 Investigated topics relate to the vessel design, the effect of fatigue damage during filling/depleting cycles, the instability of the liner (buckling, cracking), the interaction with the metallic inserts, etc.
- Analytical theories for stress calculation of filament wound composite hydrogen tanks and pipes, to improve on the currently used netting theory for tank design
- Non-destructive Testing (NDT) techniques are developed for inspection of these thick-walled composites. Ultrasound, thermography and shearography techniques are investigated to detect manufacturing defects or in-service damage in the tank, and locate and size the defects. Acoustic Emission is explored for Structural Health Monitoring of hydrogen tanks in service
- Micro-mechanical tests to characterize the fibre/matrix interface in composites. Those tests could also be used for ageing tests in the presence of hydrogen
- Design and simulation of fuel cell stacks in terms of stiffness, strength and durability (impact/crash, bolting/gaskets)
- Topology optimization codes for material choice in thermo-mechanical loading scenarios
- Simulation of performance and damage development in flexible transport pipes (typically for offshore applications)



Storage & transport of H



Available equipment/tools

- Wide range of lab equipment for static/dynamic/fatigue testing of composite materials and components
- Variety of Non-destructive Testing (NDT) techniques for inspection of parts and components
- Finite Element software for mechanical design and simulation (relevant for hydrogen storage tanks, fuel cell engineering, flexible pipelines)
- In-house Topology Optimization codes for multi-material design in thermo-mechanical loading conditions
- Micro-mechanical testing facilities for ageing of fibre/matrix interfaces

Main relevant publications

- Hondekyn, M., Ali, N. and Van Paepegem, W. (2024). Closed-form analytical model for the cylinder region of thick-walled composite pressure vessels for hydrogen storage. International Journal of Hydrogen Energy 87 (2024) 457–468
 - Open access: https://doi.org/10.1016/j.ijhydene.2024.08.447
- Finazzi, D., Seychal, G., Raquez, J.-M., Robert, G., De Clerck, K., Daelemans, L. and Van Paepegem, W. (2024). Study of the temperature-humidity equivalence and the time-temperature superposition principle in the finite-strain response of polyamide-6 and short glass fibre-reinforced polyamide-6. Accepted for Polymer Testing.

Contact persons

Prof. dr. ir. Wim Van Paepegem (<u>Wim.VanPaepegem@ugent.be</u>)



Particle and Interfacial Technology Group (PaInT)

Ghent University, Faculty of Bioscience Engineering, Department of Green Chemistry and Technology

General expertise of the research group

The Particle and Interfacial Technology Group (PaInT) is a research group within the Faculty of Bioscience Engineering at Ghent University, which focuses on separation processes for physical-chemical water treatment. The name PainT stems from the fact that the group focusses it's research on interfacial phenomena and selective separations. The key know-how of the group lies in:

- Industrial water treatment (high-quality applications, cooling & ultrapure water)
- Membrane-based processes (focus on transport phenomena), including reverse and forward osmosis, nano/micro/ultra-filtration, membrane distillation, and electrolysis/electrodialysis
- Increasing selectivity and fouling resistance of interfaces
- Resource recovery

Specific hydrogen - related expertise & research topics

- Physical and chemical water treatment for ultrapure water for H₂ production in electrolysis
- Decentralised & alternative energy-powered desalination for ultrapure water
- Link between thermolysis of organic matter, formation of organics acids and H₂-assisted corrosion phenomena in steam-water cycles (in collaboration with Prof. Kim Verbeken)

Available equipment/tools

- Lab- & pilot-scale (ultrapure) water treatment technology
- Mobile IMPROVED pilot-plant infrastructure for on-site water treatment, coupled with process (e.g., steam boiler) simulation and online corrosion measurements
- Lab-scale stacks for conventional electrodialysis and bipolar membrane and mono-selective membrane applications, including automated potentiostats
- Lab-scale stacks for electrolysis applications
- Medium and large-size Pilot scale units for electrodialysis applications

International collaborations

- · Large academic network throughout Europe, United States, Australia & South-East Africa
- Numerous industrial research collaborations with large multinationals (DOW, Yara, Sabic, DSM, Kurita,...)

Production of H₂



Participating in FL/B/EU funded projects with H₂ related research

- AquaSPICE (H2020; started 12/2020)
- Improved (Interreg; finished 2020)
- RUSTICA (H2020; started 1/2021)
- BIOSTABLE (SBO; started 10/2020)
- REvivED (H2020, finished 2021)
- Condensate Polishing (ISPT, started 2019)
- MUSE (Molecules At Sea, FPS economy in the ETF category)
- Numerous local grants
- See website: research.ugent.be



Figure 7: Electrodialysis reversal (EDR) pilot plant, capacity: 1.75 m3/d product water.

Main relevant publications

• See website: biblio.ugent.be

- Prof. Emile Cornelissen (Emile.Cornelissen@ugent.be)
- Prof. Arne Verliefde (<u>Arne.Verliefde@ugent.be</u>)
- Dr. Leo Gutierrez (<u>Leonardo.GutierrezGarces@ugent.be</u>)

Process development & system modelling



Pore-scale Processes in Geo-materials (PProGRess)

Ghent University, Faculty of Sciences, Department of Geology

General expertise of the research group

The research group PProGRess is part of Ghent University's department of Geology and Center for X-ray tomography (UGCT). PProGRess studies the various physical and chemical processes that occur inside porous rocks and sediments. The group specializes in non-destructive 3D and 4D imaging of pore structures and processes in them, from the nano- to macro-scale, mainly using X-ray micro-computed tomography.

Specific hydrogen - related expertise & research topics

- Storage of hydrogen and CO₂ in subsurface rock formations (the latter in the context of Carbon Capture and Storage, e.g. for blue hydrogen). Microscopic (pore-scale) studies of:
 - Multiphase flow in porous rocks (gas and brine natively present)
 - Salt precipitation in porous rocks due brine evaporation in hydrogen/CO₂
 - Rock alteration processes due to hydrogen-mineral or CO₂-mineral interactions
 - Relation between geo-mechanics and fluid transport in the subsurface
- Imaging of fluid menisci in porous materials (e.g. hydrogen-water in fuel cells)

Available equipment/tools

- · Micro-computed tomography: time-resolved and high-resolution 3D imaging of the internal structure of a sample
- X-ray transparent fluid flow cells (up to 120 bars/100°C)
- High-pressure high-precision piston pumps

International collaborations

On pore-scale fluid transport and interactions in rocks:

- Université de Pau et Pays de l'Adour (UPPA)
- Universiteit Hasselt
- Heriot-Watt University
- TU Eindhoven
- Imperial College London, Shell

Participating in FL/B/EU funded projects with H₂ related research

- FWO junior research project: "Energy storage in the geological subsurface: impact of salt precipitation in porous media". Collaboration with H. Derluyn (CNRS/UPPA)
- FWO research project: "VisioFlow: Advanced macro-model generation based on micro-scale visualization experiments of two-phase flow through porous sedimentary rocks". Collaboration with S. Pop (UHasselt)
- H2020 INFRAIA-grant EXCITE: "Electron and X-ray microscopy Community for structural and chemical Imaging Techniques for Earth materials"

IIIIIII

GHENT

UNIVERSITY



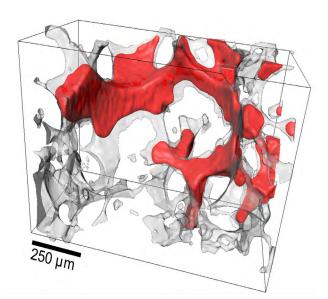


Figure 8: High-resolution 3D image of fluid menisci in the pores of a rock sample, made by X-ray imaging.

Main relevant publications

- Withers, P. J., Bouman, C., Carmignato, S., Cnudde, V., Grimaldi, D., Hagen, C. K., ... Stock, S. R. (2021). X-ray computed tomography. NATURE REVIEWS METHODS PRIMERS, 1(1)
- Mascini A, Cnudde V, Bultreys T. Event-based contact angle measurements inside porous media using time-resolved micro-computed tomography. JOURNAL OF COLLOID AND INTERFACE SCIENCE. 2020;572:354–63
- Bultreys T, Lin Q, Gao Y, Raeini AQ, AlRatrout A, Bijeljic B, et al. Validation of model predictions of pore-scale fluid distributions during two-phase flow. PHYSICAL REVIEW E. 2018;97(5)
- Bultreys T, De Boever W, Cnudde V. Imaging and image-based fluid transport modelling at the pore scale in geological materials: a practical introduction to the current state-of-the-art. EARTH-SCIENCE REVIEWS. 2016;155:93–128
- Bultreys T, Boone M, Boone M, De Schryver T, Masschaele B, Van Hoorebeke L, Cnudde, V. Fast laboratory-based micro-computed tomography for pore-scale research: illustrative experiments and perspectives on the future. ADVANCES IN WATER RESOURCES. 2016;95:341–51

- Prof. Veerle Cnudde (Veerle.Cnudde@ugent.be)
- Prof. Tom Bultreys (<u>Tom.Bultreys@ugent.be</u>)





3.1.6. UHasselt

Design and synthesis of inorganic nanomaterials (DESINe)

Hasselt University, Faculty of Science, Institue for Materials Research (IMO-IMOMEC)

General expertise of the research group

The DESINe group specializes in environmentally friendly methods for synthesizing nanostructured inorganic materials for sustainable energy applications. Recent efforts target oxide, metal, polyanionic, and sulfide-based materials for energy storage in batteries, including lithium-ion, sodium-ion, and lithium-sulfur batteries. The applications extend to thermochromic coating windows, photo/electrocatalytic CO₂ reduction, and hydrogen production, contributing to enhanced energy efficiency and diverse power supply applications.

Specific hydrogen -related expertise & research topics

- Regarding H₂ generation, the DESINe group is currently focusing on materials for:
 - Photocatalytic hydrogen generation: stabilizing ZnOAl as a photocatalyst, understanding the interplay between synthesis, formation of defects, and catalytic function
 - Photoelectrochemical hydrogen generation: design and synthesis of thin films and powder-based materials with catalytic activity in the photoelectrochemical water splitting
 - (PEM) electrolysis: design and synthesis of catalysts for hydrogen and oxygen evolution reactions in PEM electrolysis cells
- DESINe's research activities in this scope concentrate on:
 - The design and synthesis of light harvesting and electrocatalytic materials with optimal composition and morphology
 - Establishing innovative synthesis methods while assessing atom and energy efficiency,
 enabling precise control over material properties such as light absorption, crystal phase, size,
 morphology, porosity, and surface characteristics
 - Analysing structure-morphology-function relationships comprehensively using spectroscopic and microscopic tools
 - Assessing the fundamental functional properties of materials, both as solar absorbers and electrocatalysts in standalone components

Available equipment/tools

- State-of-the-art chemical synthesis and analytical laboratories (commissioned in 2020) including Nanolabs up to risk level 3 (high risk)
- Solution synthesis equipment (solvothermal reactors with sampling possibilities, Schlenk lines, etc)
- Spraydryer for particle production
- High-temperature furnaces and RTP
- High-speed centrifuge (max. 20.000g)
- Coating equipment (tape-casting, Spin-coater, dip-coater and spray-coater)
- Gloveboxes (N2 and Ar)
- Potentiostats and (photo-)electrochemical cells
- Custom built setup for evaluating the light-assisted catalytic reactions, equipped with a Xe-arc light source and MicroGC Gas chromatography
- N2 sorption BET





- XRD
- SEM and TEM
- FTIR and Raman, UV-Vis spectroscopy
- Mass spectrometry

International collaborations

- Nederlandse Organisatie voor toegepast-natuurwetenschappelijk onderzoek (TNO) Eindhoven, The Netherlands dr. Pascal Buskens
- Korea Advanced Institute of Science & Technology (KAIST) Daejeon, South-Korea Prof. dr. Byungha Shin

Participating in FL/B/EU funded projects with H₂-related research

- Interreg FOTON: High-tech systems and materials for a sunlight-driven sustainable chemical industry
- Green Hydrogen Lab: Relance Vlaamse Veerkracht project
- Grand challenges BOF project UHasselt, Clean H₂, partnering Dirk Vanderzande, An Hardy, Koen Vandewal, Momo Safari, and Robert Malina of UHasselt
- Bilateral BOF PhD scholarship UHasselt UNamur on photocatalytic water splitting with AZO, partners: M.K. Van Bael, An Hardy, and Peter Adriaensens (UHasselt), Carmela Aprile and Luca Fusaro (UNamur). Also, in collaboration with Sammy Verbruggen, Pegie Cool and Silvia Lenaerts at **UAntwerp**
- BE-HYFE: BE-HyFE Belgian Hydrogen Fundamental Expertise; ETF project
- T-REX: On the transition to more Renewable Energy in power-to-X applications: ETF project
- SYN-CAT: Synergetic design of catalytic materials for integrated photo- and electrochemical CO₂ conversion processes; Funding: VLAIO-MOT
- LUMEN: Zonlicht als brandstof voor duurzame chemische processen; Interreg VI-NI project
- SPOTLIGHT: SPOTLIGHT solar fuels: a disruptive photonic technology to create carbon neutral fuels: Horizon 2020 project

Main relevant publications

- Facile Aqueous Solution-Gel Route toward Thin Film CuBi2O4 Photocathodes for Solar Hydrogen Production; Bjorn Joos, Ken Elen, Jonathan van den Ham, Nicole Meulendijks, Pascal Buskens, Andreas Paulus, Koen Wouters, Jean Manca, Jan D'Haen, Sudhanshu Shukla, Bart Vermang, Marlies Van Bael, An Hardy; Advanced Sustainable Systems, 2300083
- Photocatalytic Performance of Undoped and Al-Doped ZnO Nanoparticles in the Degradation of Rhodamine B under UV-Visible Light: The Role of Defects and Morphology; Alessandra Piras, Chiara Olla, Gunter Reekmans, An-Sofie Kelchtermans, Dries De Sloovere, Ken Elen, Carlo Maria Carbonaro, Luca Fusaro, Peter Adriaensens, An Hardy, Carmela Aprile, Marlies K Van Bael; International Journal of Molecular Sciences 23 (24), 15459
- Sunlight-Powered Reverse Water Gas Shift Reaction Catalysed by Plasmonic Au/TiO₂ Nanocatalysts: Effects of Au Particle Size on the Activity and Selectivity; Jordi Volders, Ken Elen, Arno Raes, Rajeshreddy Ninakanti, An-Sofie Kelchtermans, Francesc Sastre, An Hardy, Pegie Cool, Sammy W Verbruggen, Pascal Buskens, Marlies K Van Bael; Nanomaterials 12 (23), 4153
- Comparing the Performance of Supported Ru Nanocatalysts Prepared by Chemical Reduction of RuCl3 and Thermal Decomposition of Ru3 (CO) 12 in the Sunlight-Powered Sabatier Reaction; Daria Burova, Jelle Rohlfs, Francesc Sastre, Pau Martinez Molina, Nicole Meulendijks, Marcel A Verheijen, An-Sofie Kelchtermans, Ken Elen, An Hardy, Marlies K Van Bael, Pascal Buskens; Catalysts 12 (3), 284



Production of H₂



- Precursor Design Strategies for the Low-Temperature Synthesis of Functional Oxides: It's All in the Chemistry; W Marchal, D De Sloovere, M Daenen, MK Van Bael, A Hardy; Chemistry

 –A European Journal 26 (42), 9070-9083
- Remarkable lowering in the synthesis temperature of LiMn2O4 via citrate solution-gel synthesis facilitated by ethanol, Maino, G; Carleer, R.; Marchal, W.; Bonneux, G.; Hardy, A.; Van Bael, M.K. Dalton Transactions, 2017 46 (43) 14934-14946
- Ultrasonic spray deposition of metal oxide films on high aspect ratio microstructures for 3D all-solidstate Li-ion batteries; E. Jonathan van den Ham, Sven Gielis, Marlies Van Bael, An Hardy; ACS Energy Letters, 2016 1, p.1184-1188
- Factors influencing the conductivity of aqueous sol(ution)-gel processed Al-doped ZnO films; H.
 Damm, P. Adriaensens, C. De Dobbelaere, B. Capon, K. Elen, J. Drijkoningen, B. Conings, J. Manca, J. D'Haen, C. Detavernier, P.C.M.M. Magusin, J. Hadermann, A. Hardy, M.K. Van Bael, Chemistry of Materials 26(20) (2014) 5839-5851

- Lieve De Doncker (<u>lieve.dedoncker@uhasselt.be</u>)
- An Hardy (an.hardy@uhasselt.be)
- Marlies K. Van Bael (marlies.vanbael@uhasselt.be)



Production, storage and transport of H₂



Electrochemical Engineering (EE)

Hasselt University, Faculty of Engineering Technology & Electrochemical Engineering, Institue for Materials Research (IMO-IMOMEC)

General expertise of the research group

- · Electrochemical engineering
 - Porous electrode design & characterization
 - Kinetics & charge transport
 - Electrochemical characterization
 - Mathematical modelling
 - Aging and post-mortem analysis

Specific hydrogen - related expertise & research topics

- PEM water electrolyzer
 - MEA preparation and optimization
 - Polarization and aging tests
 - Electrochemical characterization and physics-based modelling

Available equipment/tools

- MEA preparation: Mixing, Coating, hot press
- Mercury porosimeter
- 500W PEM water electrolyzer automatic test station
- Electrochemical characterization: Potentio- and Galvano-static + EIS

Participating in FL/B/EU funded projects with H₂ related research

CleanH2 (BOF)

Main relevant publications

- 'A techno-economic evaluation of solar-powered green hydrogen production for sustainable energy consumption in Belgium', N Srettiwat, M Safari, H Olcay, R Malina, *International Journal of Hydrogen Energy (2023)* 48 (100), 39731-39746
- 'Bridging the microstructural evolutions from slurry to porous electrode of a lithium-ion battery', H Hamed, Z Alamooti, A Agrawal, J D'Haen, A Hardy, M Safari, *Energy Chemistry* (2023) 84, 329-334.
- 'Non-Uniform Distribution of Current in Plane of Large-Area Lithium Electrodes', S Yari, MK Van Bael, A Hardy, M Safari, *Batteries & Supercaps (2022)* 5 (10), e202200217.

- Prof. Momo Safari (momo.safari@uhasselt.be)
- Dr. Lieve De Doncker (lieve.dedoncker@uhasselt)



Production, storage and transport of H₂



Hybrid Halide Perovskites for Energy Applications (HyMaD)

Hasselt University, Faculty of Science, Institue for Materials Research (IMO-IMOMEC)

General expertise of the research group

About half of our research activity is related to thin film photovoltaic, including CIGS, organic, inorganic, hybrid perovskites PV. The expertise of our 3 divisions (Chemistry, Physics and Engineering Technology) is brought together and use towards fundamental research, applied research and device engineering of (semi-)conductor materials. It covers synthesis, structural characterization, material processing and device physics. The institute has developed many original contributions to the chemistry and physics of conjugated small molecules and polymers including development of novel synthesis routes and has built up an internationally recognized strong reputation in the domain. Since 2016, the synthesis activities include ammonium functionalized chromophores for integration in 2D layered Hybrid Organic Inorganic Perovskites (HOIP) Dirk VANDERZANDE (UHasselt), Laurence LUTSEN (Imec-imomec).

Specific hydrogen - related expertise & research topics

- Development of high-efficiency and stable hybrid perovskite (3D and 2D layered) and organic semiconductor molecules for application in PEC and PV+EC
- Structural characterization
- Thin film morphology

Available equipment/tools

- Fully equipped organic and hybrid materials synthesise and spectroscopic characterisations including Schlenk lines to work under inert conditions
- Liquid NMR
- Solid state NMR to evaluate both amorphous and crystalline phases and molecular miscibility of blends at the nm scale
- State-of-the-art glovebox systems to produce perovskite materials under inert conditions
- Solvent purification system connected to the glovebox
- MALDI-TOF
- Vacuum sublimation system for small organic molecules
- FTIR, Raman, UV-Vis spectroscopy
- SEM and TEM



Production, storage and transport of H₂



International collaborations

- TUDelft, Prof. Dr. Ferdinand Grozema, Time-resolved Microwave Conductivity
- Arizona State University, Prof. Dr. Brent Nannenga, Cryo Electron Microscopy
- CSEM, Dr. Brett Kamino and Dr. Björn Niesen, large area perovskite solar cells
- Solaronix, Dr. David Martineau, large area perovskite solar cells
- University of Toronto, Dr. Amin Morteza Najarian (Sargent group), Electro Optical Modulation
- Rijksuniversiteit Groningen, Prof. Dr. Maria Antonietta Loi, photophysics and solar cells
- Victoria University of Wellington, Dr. Kai Chen, femtosecond luminescence
- TUEindhoven, Prof. Dr. René Janssen, in-situ absorption spectroscopy during spin-coating

Participating in FL/B/EU funded projects with H₂ related research

- CLEANH2, Fundamental Research in Solar-driven Hydrogen Generation using Earth-abundant Catalysts and Durable Hybrid Perovskites as Light Absorbers. Funding agency: BOF project. UHasselt research groups, 5 principal Investigators. 2021-2025
- PROCEED, Hybrid Perovskites as Material Platform for Conversion, Emission and Detection of Light.
 Funding agency: FWO, SBO project. UHasselt, UGent, KU Leuven, UAntwerpen and Imec as the coordinator of the project. 2020-2024
- FWO senior research project. A fundamental study of energy and charge transfer processes in low dimensional organic-inorganic hybrid perovskites. Funding agency: FWO. PI: Dirk Vanderzande. FWO 019-16
- FWO PhD fellowship Martijn Mertens. 2D perovskite-induced self-organization of conjugated chromophores for efficient and stable optoelectronic applications. 01/01/2018-31/12/2021
- FWO PhD fellowship Arthur Maufort. Self-assembly of organic donor-acceptor complexes within a perovskite structure: a fundamental study of the relationship between optoelectronic and structure properties.01/11/2020-31/10/2024





Production, storage and transport of H₂



Main relevant publications

- 2D layered perovskite containing functionalised benzothieno-benzothiophene molecules: formation, degradation, optical properties and photoconductivity. Van Gompel, Wouter T. M.; Herckens, Roald; Denis, Paul-Henry; Mertens, Martijn; Gelvez-Rueda, Maria C.; Van Hecke, Kristof; Ruttens, Bart; D'Haen, Jan; Grozema, Ferdinand C.; Lutsen, Laurence; Vanderzande, Dirk. Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2020, 8(21), 7181-7188.
- Inducing charge separation in solid-state two-dimensional hybrid perovskites through the
 incorporation of organic charge-transfer complexes. Gelvez-Rueda, Maria C.; Van Gompel, Wouter T.
 M.; Herckens, Roald; Lutsen, Laurence; Vanderzande, Dirk; Grozema, Ferdinand C. Journal of Physical
 Chemistry Letters, 2020, 11(3), 824-830.
- Lead-Halide Perovskites Meet Donor-Acceptor Charge-Transfer Complexes. Marchal, Nadege; Van Gompel, Wouter; Gelvez-Rueda, Maria C.; Vandewal, Koen; Van Hecke, Kristof; Boyen, Hans-Gerd; Conings, Bert; Herckens, Roald; Maheshwari, Sudeep; Lutsen, Laurence; Quarti, Claudio; Grozema, Ferdinand C.; Vanderzande, Dirk; Beljonne, David. Chemistry of Materials, 2019, 31(17), 6880-6888.
- Low-Dimensional Hybrid Perovskites Containing an Organic Cation with an Extended Conjugated System: Tuning the Excitonic Absorption Features. Van Gompel, Wouter T. M.; Herckens, Roald; Van Hecke, Kristof; Ruttens, Bart; D'Haen, Jan; Lutsen, Laurence; Vanderzande, Dirk. ChemNanoMat, 2019, 5(3), 323-327.
- Towards 2D layered hybrid perovskites with enhanced functionality: introducing charge-transfer complexes via self-assembly. Van Gompel, Wouter T. M.; Herckens, Roald; Van Hecke, Kristof; Ruttens, Bart; D'Haen, Jan; Lutsen, Laurence; Vanderzande, Dirk. Chemical Communications, 2019, 55(17), 2481-2484.
- Layered hybrid organic-inorganic perovskite materials. Lutsen, Laurence; Vanderzande, Dirk. Imec VZW, Belg.; Universiteit Hasselt. Jan 31, 2019. Patent WO 2019020612A1.
- Multi-layered hybrid perovskites templated with carbazole derivatives: optical properties, enhanced moisture stability and solar cell characteristics. Herckens, Roald; Van Gompel, Wouter T. M.; Song, Wenya; Gelvez-Rueda, Maria C.; Maufort, Arthur; Ruttens, Bart; D'Haen, Jan; Grozema, Ferdinand C.; Aernouts, Tom; Lutsen, Laurence; Vanderzande, Dirk. Journal of Materials Chemistry A: Materials for Energy and Sustainability, 2018, 6(45), 22899-22908.
- Degradation of the Formamidinium Cation and the Quantification of the Formamidinium Methylammonium Ratio in Lead Iodide Hybrid Perovskites by Nuclear Magnetic Resonance Spectroscopy. Van Gompel, Wouter T. M.; Herckens, Roald; Reekmans, Gunter; Ruttens, Bart; DHaen, Jan; Adriaensens, Peter; Lutsen, Laurence; Vanderzande, Dirk. Journal of Physical Chemistry C, 2018, 122(8), 4117-4124.

- Dirk Vanderzande (dirk.vanderzande@uhasselt.be)
- Laurence Lutsen (<u>Laurence.lutsen@uhasselt.be</u> / <u>laurence.lutsen@imec.be</u>)

Production of H₂



Materials for Energy Applications

Hasselt University, Faculty of Engineering Technology, Institue for Materials Research (IMO-IMOMEC)

General expertise of the research group

Our research team focuses on developing chalcogenide and new materials for Photovoltaic (PV) and PV-integrated solar fuel devices. Additionally, Photoelectrochemical and photocatalytic pathways are being explored as a testbed to study fundamental interactions at semiconductor electrolyte interface. Our research team consists of around 16 members including 5 senior researchers, 8 PhD students and various thesis/internship students with strong expertise in materials development, advanced optoelectronic characterization and catalyst engineering.

Specific hydrogen - related expertise & research topics

- Development of high-efficiency PV tandem devices which can be integrated to water electrolytic cells for PV-EC applications
- Engineering various chalcogenide and emerging promising materials as photo absorbers and cocatalysts for photoelectrochemical water splitting
- Development of photoelectrochemical (PEC) and photocatalytic (PC) cells for direct solar to hydrogen generation
- Designing flow cells and electrode materials for efficient and low-overpotential electrocatalytic hydrogen generation systems
- Advanced opto-electrical, structural, and configuration characterization of potential materials and devices applicable to PV and photo-electrochemical studies

Available equipment/tools

- In-line connected photoelectrochemical reactor with GC detection system
- Physical vapor deposition tool including large scale (35 x 35 cm2) deposition
- Tabletop Tescan SEM equipped with EDX for elemental analysis
- Electrical D.C. Hall measurement Setup
- Steady state and transient Photoluminescence spectrometer
- X-ray diffractometer (XRD)
- LCR electronics for capacitance measurements (temperature and illumination dependent)
- Secondary Ion Mass Spectrometer (SIMS)
- State-of-the-art facility for hybrid PV cells development under controlled environment
- Solar simulators
- Electrochemical workstation for photoelectrochemical PV-electrolyzer testing



International collaborations

IMO-IMOMEC

▶► UHASSELT

- International Iberian Nanotechnology Laboratory, Portugal
- Technical University of Denmark
- University of California, Berkeley
- University of New South Wales, Australia
- Nanyang Technological University Singapore, Singapore
- Foundation for Research and Technology Hellas, Greece
- Karlstad University, Sweden

Participating in FL/B/EU funded projects with H₂ related research

- Development of high-efficiency tandem PV, e.g. for PV-EC
 - PHOENIX (Photo-electro Integrated Next-Generation energy technologies | PHOENIX | Project | Fact sheet | HORIZON | CORDIS | European Commission) Coupling efficient PV-EC and PEC systems for converting CO₂ to propanol and PET to valuable products
 - SolVa (Solar To Value | SolVa | Project | Fact sheet | HORIZON | CORDIS | European Commission) Couple electrocatalysts and highly performing photoabsorbers for designing novel photoelectrodes and PEC cells for reducing CO2 to formic acid
 - PERCISTAND (https://cordis.europa.eu/project/id/850937) Development of all thin-film perovskite on cis tandem photovoltaics
 - LASERGRAPH (https://www.era-learn.eu/network-information/networks/fetflag-02-2018/ flag-era-joint-transnational-call-jtc-2019/in-situ-laser-fabrication-of-graphene-electrodesandinterlayers-for-next-generation-cigs-perovskite-solar-cells) In-situ laser fabrication of graphene electrodes and interlayers for next generation CIGS/ Perovskite solar cells
 - LAFLEX2T (https://projecten.topsectorenergie.nl/projecten/flexible-large-area-2tmonolithictandem-psc-cigs-33526) Flexible Large area 2T monolithic Tandem PSC-CIGS
 - ARLEA (https://www.uhasselt.be/nl/projecten/detail/23616-project-r-13035) Advanced Recombination Junction Layer Engineering and Application for Scalable and Stable Monolithic Perovskite Tandem Solar Cells with Two Different Bottom Cells. (Si-CIGS)
 - SITA (https://www.sitasolarcells.eu/Imec) Stable Inorganic TAndem solar cell with superior device efficiency and increased durability
- Development of chalcopyrite materials for photo-electrochemical applications
 - SYNCAT (https://moonshotflanders.be/mot3-syn-cat/) Synergetic design of catalytic materials for integrated photo-and electrochemical CO₂ conversion
 - T-REX (https://www.uhasselt.be/en/projects/detail/21780-project-r-12321) Conversion of CO₂ into renewable materials via electrified routes
 - Procura Belgium (https://procurabelgium.be/en) Power to X, carbon capture & utilization roadmap for Belgium
 - CHALCON (https://cordis.europa.eu/project/id/101067667) Chalcogenide-Silicon tandem PEC for CO₂ reduction
- Development of kesterite materials for photo-electrochemical applications
 - KESPER (https://www.uhasselt.be/en/projects/detail/24269-project-r-13406) Kesteritebased Photoelectrodes for Water and Nitrogen Reduction
 - Hydrogen Booster, EMR Interreg project (https://www.emrh2booster.eu/) Energy transition towards the development of carbon-free energy solutions by SMEs







Main relevant publications

- Santos, D., Shukla, S., Vermang, B., (2023) Prospects of copper—bismuth chalcogenide absorbers for photovoltaics and photoelectrocatalysis, J. Mater Chem A, 11, 22087-22104. https://doi.org/10.1039/D3TA03564F
- Scaffidi, R., Birant, G., Brammertz, G., de Wild, J., Flandre, D., Vermang, B. (2023) Ge-alloyed kesterite thin-film solar cells: previous investigations and current status a comprehensive review. J. Mater. Chem. A, 11, 13174-13194. https://doi.org/10.1039/D3TA01218B
- Silvano, J., Hamtaei, S., Verding, P., Vermang, B., Deferme, W., (2023) Investigating the Fabrication of Perovskite Solar Cells by Ultrasonic Spray Coating: A Design of Experiments Approach. ACS Appl. Energy Mater., 6, 14, 7363–7376. https://doi.org/10.1021/acsaem.3c00491
- Joos, B., Elen, K., Ham, J., Meulendijks, N., Buskens, P., Paulus, A., Wouters, K., Manca, J., D'Haen, J., Shukla, S., Vermang, B., Van Bael, M., Hardy, A. (2023) Facile Aqueous Solution-Gel Route toward Thin Film CuBi2O4 Photocathodes for Solar Hydrogen Production. Adv. Sustainable Syst. 7, 8, 2300083. https://doi.org/10.1002/adsu.202300083
- De Wild, J., Scaffidi, R., Brammertz, G., Birant, G. and Vermang, B., (2023) Dielectric Front Passivation for Cu(In,Ga)Se2 Solar Cells: Status and Prospect. Adv. Energy Sustainability Res. 2200132. https://doi.org/10.1002/aesr.202200132
- Ramesh, S., Tuomiranta, A., Hajjiah, A., M. Meuris, B. Vermang, J. Poortmans. (2022) Physics-based electrical modelling of CIGS thin-film photovoltaic modules for system-level energy yield simulations. npj Flex Electron 6, 87. https://doi.org/10.1038/s41528-022-00220-5
- Birant, G., de Wild, J., Meuris, M., Poortmans, J. and Vermang, B. (2022) "To Spin or Not to Spin?"—
 Is Spin-Coating the Ideal Technique for Pre-Deposition of Sodium Fluoride for CIGS Rear Surface
 Passivated Ultrathin Solar Cells?. Phys. Status Solidi A, 219: 2100830. https://doi.org/10.1002/
 pssa.202100830
- Ratz, T., Nguyen, N. D., Brammertz, G., Vermang, B., Jean-Yves Raty, J.-Y., (2022) Relevance of Ge incorporation to control the physical behaviour of point defects in kesterite, J. Mater. Chem. A, 10, 4355-4365. https://doi.org/10.1039/d1ta09620f

Contact persons

Prof. Bart Vermang (bart.vermang@uhasselt.be)



Materials & components development

Production, storage and transport of H₂



Organic Opto-Electronics Research (OOE)

Hasselt University, Faculty of Sciences&Materials Physics, Institue for Materials Research (IMO-IMOMEC)

General expertise of the research group

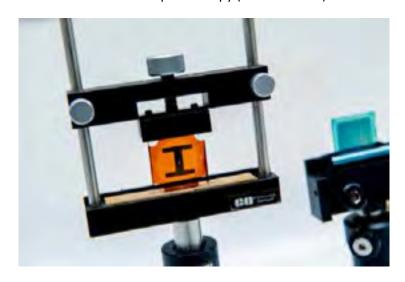
The organic opto-electronics research group has the aim to solve fundamental questions in organic, hybrid and molecular electronics with relevance in opto-electronic devices such as OLEDs, sensors, solar cells and photovoltaic systems. The group is led by Prof. Dr. Ir. Koen Vandewal, who is well known for his seminal work on the characterization and description of charge-transfer states at organic interfaces. The groups expertise lies in the fabrication and characterization of thin film devices based on organic and hybrid perovskite materials, as well as advanced device characterization and device physics.

Specific hydrogen - related expertise & research topics

- Integration of organic and perovskite PV-elements with electrochemical cells
- Engineering of photovoltaic interfaces

Available equipment/tools

- Glovebox with spincoater and thermal evaporator for sample and device preparation
- AM1.5g solar simulator
- Steady-state spectroscopy: UV/Vis/NIR transmission/reflection/absorption and photocurrent
- Spectroscopy (350 nm 2500 nm), emission (photoluminescence/electroluminescence/thermal) spectroscopy (350 nm – 20 um)
- Photothermal deflection and photoluminescence excitation spectroscopy with wavelength tuneable laser excitation (450 650 nm & 900 1300 nm)
- Time gated iCCD for time resolved spectroscopy (400 800 nm). 2 ns minimum gating time





Materials & components development

Production, storage and transport of H₂



International collaborations

- TU Dresden (device physics and engineering)
- Stanford University (Synchrotron x-ray analysis)

Participating in FL/B/EU funded projects with H₂ related research

- CLEANH2 Fundamental Research in Solar-driven Hydrogen Generation using Earth-abundant
- Catalysts and Durable Hybrid Perovskites as Light Absorbers, BOF
- ConTROL Charge-transfer states for high performance organic electronics, ERC Consolidator Grant
- Joint FWO project with HyMAT Self-assembly of organic donor-acceptor complexes within the confinement of a perovskite lattice: a fundamental study of the relation between structure and opto-electronic properties (R-11232)

Main relevant publications

- Emissive and charge-generating donor—acceptor interfaces for organic optoelectronics with low voltage losses. S. Ullbrich, J. Benduhn, X. Jia, V. C. Nikolis, K. Tvingstedt, F. Piersimoni, S. Roland, Y. Liu, J. Wu, A. Fischer, D. Neher, S. Reineke, D. Spoltore, K. Vandewal. Nature materials, 2019, 18.5: 459-464
- Lead-Halide Perovskites Meet Donor–Acceptor Charge-Transfer Complexes. N. Marchal, W. Van Gompel, M. C. Gélvez-Rueda, K. Vandewal, K. Van Hecke, H-G. Boyen, B. Conings, R. Herckens, S. Maheshwari, L. Lutsen, C. Quarti, F. C. Grozema, D. Vanderzande, D. Beljonne. Chemistry of Materials, 2019, 31(17), 6880-6888
- High voltage vacuum-deposited CH3NH3PbI3—CH3NH3 PbI3 tandem solar cells. J. Ávila, C.
 Momblona, P. Boix, M. Sessolo, M. Anaya, G. Lozano, K. Vandewal, H. Míguez, H. J. Bolink. Energy & Environmental Science, 2018, 11(11), 3292-3297
- Intrinsic non-radiative voltage losses in fullerene-based organic solar cells. J. Benduhn, K. Tvingstedt, F. Piersimoni, S. Ullbrich, Y. Fan, M. Tropiano, K. A. McGarry, O. Zeika, M. K Riede, C. J. Douglas, S. Barlow, S. R. Marder, D. Neher, D. Spoltore, K. Vandewal. Nature Energy, 2017, 2(6), 17053
- Reducing voltage losses in cascade organic solar cells while maintaining high external quantum efficiencies. V. C. Nikolis, J. Benduhn, F. Holzmueller, F. Piersimoni, M. Lau, O. Zeika, D. Neher, C. Koerner, D. Spoltore, K. Vandewal. Advanced Energy Materials, 2017, 7(21), 1700855

Contact persons

Koen Vandewal (koen.vandewal@uhasselt.be)



Materials & components development, process development & economic aspects



3.1.7. VITO

Separation and Conversion Technology (SCT)

VITO, Sustainable chemistry

General expertise of the research group

VITO is a leading European independent research/consultancy centre in the areas of cleantech and sustainable development, elaborating solutions for the grand societal challenges of tomorrow: climate change, food security, a sustainable energy supply, the ageing population and scarcity of resources. The business unit of Separation and Conversion Technology is composed of >100 researchers, managers, support staff and students and has organized its strategic research program around the theme 'Sustainable Chemistry' with special focus on (1) process intensification through the integration of separation processes with chemical, microbial, enzymatic or bio-electrochemical conversion processes, and (2) the use of alternative feedstocks, such as CO2.

Specific hydrogen - related expertise & research topics

- Integration of reaction technology (bio, electrochemical) and separation technologies
- Expertise in alkaline and PEM fuel cell development and testing
- Development of low cost and efficient electrodes and membranes
- The gas diffusion electrodes to be used as air cathodes in MFCs are considered as the state-of-theart and are currently being optimized for CO₂ conversion processes
- Activities in the electrosynthesis field with projects on conversion of CO₂ to ethanol, methanol, formic acid and conversion of acids to alcohols and production of ionic liquids
- Techno-economic and life cycle assessment of the hydrogen value chain
- Energy system modelling, long-term system scenario modelling (2030-2050)

Available equipment/tools

- 3 laboratory test stands
 - Single cell/small stack
 - Operational ranges
 - 15 bar, 90°C
 - 35 bar, 90°C
 - 15 bar, 70°C
 - Labview
 - Sensoring Pressure, Temp, Q_flows
 - Gas quality (HTO, Gas Chromatography...)
 - Electrochemical characterization (I-V,EIS)
- Demo setup
 - Up to 3 kW
 - Design range: 50 bar, 90°C
 - PLC based
 - Sensoring P,T,Q,HTO...
 - GC/EIS



Materials & components development, process development & economic aspects

Production and general use of H₂



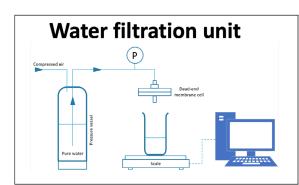
- Durability test benches
 - Parallel 2x2 cm testing of 5 samples
 - 10 bar, 80°C- 120°C



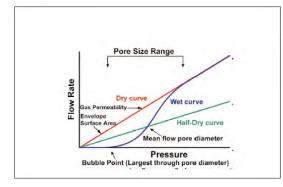




- Ex-situ tools for membrane characterization
 - Water permeability (via Water filtration unit)
 - IEC measurement (via titration)
 - Capillary Flow Porometry (CFP) (via Porolux) to determine:
 - First Bubble Point (FBP)
 - Smallest pore size (SP)
 - Mean Flow Pore diameter (MFP)
 - Gas permeability (GP)
 - Scanning electron microscopy (SEM)
 - Hg porosimetry measurements
 - Thermogravimetric analysis
 - Tensile strength measurements











Materials & components development, process development & economic aspects

Production and general use of H₂



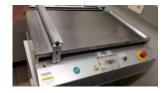






ELCOMETER 4340 Automatic Film Applicator

- Dimensions: 20/30cm
- Heated coating bed



BRAVE 4340 SP Automatic Film Applicator

Dimensions: 50/60cm



Roll-to-Roll Film Applicator

Dimensions: 15cm width

• Speed: 1 to 800 cm/min



Pressurized polymer solution delivery system





MIXERS / DISOLVERS
0.1 -> 8 kg



20-ton hydraulic press



Materials & components development, process development & economic aspects

Production and general use of H₂



Participating in FL/B/EU funded projects with H₂ related research

- Bac-To-Fuel, Bacterial conversion of CO₂ and renewable H₂ into biofuels, H2020 Project ID: 825999
- BIORECO2VER, Biological routes for CO₂ conversion into chemical building blocks, H2020 Project ID: 760431
- LOTER.CO2M, CRM-free low temperature electrochemical reduction of CO₂ to methanol, H2020 Project ID 761093-2
- PERFORM, PowerPlatform: Establishment of platform infrastructure for highly selective electrochemical conversions, H2020 Project ID: 820723
- CATCO2RE, Conversion of solar energy and CO₂ to chemicals and fuels, FWO, VITO/UGent/KUL/VUB
- CO2PERATE, The catalytic conversion of CO₂ to formic acid, Cluster SBO, VITO/UGent/KUL/UA/BEPP
- PROCURA, Power to X and carbon capture and utilization roadmap for Belgium, ETF, VITO/Imec/ Waterstofnet/KUL/VUB/University of Liège
- BREGILAB, Investigation of the practical realisation of further expansion of renewable electricity sources in Belgium, ETF, VITO/KUL/UHasselt/Imec/KMI
- E2C Interreg Project: Electrons to high value Chemical products
- ELYINTEGRATION Horizon 2020 project "Grid integrated multi megawatt high pressure alkaline electrolysers for energy applications", FCH Initiative
- REselyser FP7 Project "Hydrogen from RES: pressurised alkaline electrolyser with high efficiency",
 FCH Initiative





Materials & components development, process development & economic aspects



Main relevant publications

- Sánchez, O.G.*, Birdja, Y.Y.*, Bulut, M., Vaes, J., Breugelmans, T. and Pant, D, Recent advances in industrial CO₂ electroreduction. Current Opinion in Green and Sustainable Chemistry. 2019, 16, 47-
- König, M., Vaes, J., Klemm, E. and Pant, D., Solvents and Supporting Electrolytes in the Electrocatalytic Reduction of CO₂. iScience, 2019, 19, p.135
- Doyen, W., Alvarez Gallego, Y., Stoops, L., Molenbergh, B., Reissner, R., Schiller, G., Guelzow, E., Vaes, J. and Bowen, J.R., 2014. The e-bypass separator: the solution to the inherent problem of alkaline water electrolysis under challenging working conditions. 2014 Membrane Symposium, 08. Sept. 2014, Aachen, Deutschland
- König, M, Bulut, M., Vaes, J., Klemm, E., Pant, D. 2019. Electrochemical CO₂ conversion. EU patent EP19213008
- Prato, R.A., Van Vught, V., Eggermont, S., Pozo, G., Marin, P., Fransaer, J. and Dominguez-Benetton, X., 2019. Gas Diffusion Electrodes on the Electrosynthesis of Controllable Iron Oxide Nanoparticles. Scientific reports, 9(1), pp.1-11
- Van Dael, M., Kreps, S., Virag, A., Kessels, K., Remans K., Thomas, D., and De Wilde, F., 2018, Technoeconomic assessment of a microbial power-to-gas plant – case study in Belgium, Applied Energy, 2015, pp.416-425

- Metin Bulut (<u>metin.bulut@vito.be</u>)
- Jan Vaes (jan.vaes@vito.be)





3.1.8. VIVES University of Applied Sciences

Research group Energy - Hydrogen production

VIVES University of Applied Sciences

General expertise of the research group

The research group hydrogen can rely on a fully equipped laboratory of the hydrogen energy chain. From production, up to the use of hydrogen in different applications. The group has gained expertise in practical use and implementation of various aspects, including green hydrogen production, hydrogen storage, regulatory aspects and safety considerations related to hydrogen, utilization of hydrogen as a fuel for internal combustion engines, hydrogen fuel cell systems, fuel cell vehicles, and the production and utilization of green methanol.

Specific hydrogen - related expertise & research topics

- Expertise in production of green hydrogen with solar and wind energy and PEM electrolyser (10 kW)
- Control management and data acquisition and visualisation of a PEM electrolyzer
- System modelling and optimalization
- Training and education

Available equipment/tools

- Solar panels
- PEM electrolyser 10 kW with water treatment
- Compressor 300 bar
- Hydrogen storage
- · Hydrogen supply infrastructure

International collaborations

- TU Delft
- Solent University Southampton
- UPHF Université Polytechnique Hauts-de-France
- NICE Noordelijk Innovatielab Circulaire Economie
- BDI Bretagne Développement Innovation

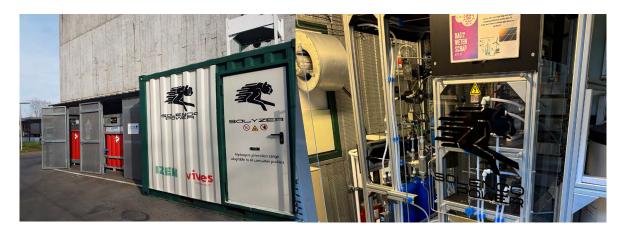






Participating in FL/B/EU funded projects with H₂ related research

- Project: H₂ ElektrolyzE topic: PEM electrolyser demonstrator for production of green hydrogen
 funding source: VLAIO PWO (projectmatig wetenschappelijk onderzoek) industrial partners:
 Cinergy, AA Technics, e-BO enterprises, Bekaert, Van Marcke Technics
- Project: Hyde, sustainable and "green" energy applications for military use topic: modelling and building of a demonstrator – funding source: BELSPO DEFRA – project partners: KU Leuven, Solenco and Royal Military Academy



Main relevant publications

- J. Mus et al., "Design and Characterisation of an Alkaline Electrolyser," 2022 11th International Conference on Renewable Energy Research and Application (ICRERA), 2022, pp. 253-259, doi: 10.1109/ICRERA55966.2022.9922902
- De Wilde, B., Schotte, S. (contr.) (2022). Hogeschool VIVES opent nieuw waterstofcentrum VRT NWS
- Mus, J., Mylle, S., Schotte, S., Fevery, S., Latré, S., Buysschaert, F. (2022). CFD Modelling and

- Sam Schotte (<u>sam.schotte@vives.be</u>)
- Steven De Tollenaere (<u>steven.detollenaere@vives.be</u>)

Storage & transport of H₂



3.1.9. VKI

Research Expertise Group on Liquid & Solid Propulsion (storage & transport)

von Karman Institute for Fluid Dynamics, Department of Aerospace

General expertise of the research group

Experimental testing and numerical simulation of the fluid dynamic behaviour for 2-phase flows and multiphase flows, with application for liquid hydrogen and other cryogenic (e-)fuels. Extensive expertise is available from research on the propellant management system for space launchers. This expertise which has been developed for space applications, is now being transferred to terrestrial applications, both for terrestrial mobility (in ships, aircraft, heavy duty trucks...) and for energy applications (long term H_2 storage and long distance H_2 transport).

Specific hydrogen - related expertise & research topics

- In general: numerical simulations of liquid hydrogen behaviour and performing experimental tests to validate the modelling
- Densified Cryogenic eFuels ("Slush"): hydrogen, methane, LNG (also applicable to CO₂)

Available equipment/tools

- Numerical simulation platforms for CFD (Computational Fluid Dynamics), e.g. EcosimPro, OpenFOAM®
- Experimental test facilities:
 - PREDICT and BECASSINE Facility: for testing for densified cryogenic (e-)fuels
 - Particle Image Velocimetry

International and industrial collaborations:

- Ariane Group (FR, DE)
- CiRA (UK)
- DLR (DE)
- Numeca (BE)
- Open Engineering (BE)
- Waseda University Tokyo (JPN)



Figure 9: PREDICT Facility, for experimental characterization of densified cryogenic fuels



Storage & transport of H



Participating in FL/B/EU funded projects with H₂ related research

- [SPACE] PREDICT DREAMS is the continuation of PREDICT (experimental characterization of a slurry flow or densified cryogenic flow in hydraulic similitude with future cryogenic propellant at the triple point) in the framework of a PhD thesis. In this activity, both numerical simulation and experimental investigations are carried out. A CFD solver based on a Euler-Euler approach coupled with the Granular Kinetic Energy theory is in development, satisfactory results were obtained once validated against the PREDICT experimental data. The final ambitious goal targets experiments characterizing a slush flow and possibly evaluate the solver performances. Funding: FRIA/FNRS and ESA NPI
- [ENERGY] Be-HyFE (Belgian Hydrogen Fundamental Expertise): this project aims at developing a Belgian PhD network with PhD level research on hydrogen, about many different topics across the hydrogen value chain. The VKI PhD will focus on advanced characterization of thermodynamic properties of densified cryogenic hydrogen (or e-fuels more in general): composition (crystals shape and size), aging dynamics (stratification, melting), rheology and behaviour in pipelines and their components. This densified cryogenic slush is a promising solution to increase the volumetric density for storage and increase the resistance against boil-offs and heat losses during long distance transportation. Funding: Energy Transition Fund, by the Belgian Federal Public Services "Economy"

Main relevant publications

• Two-Phase Flows Investigations in Liquid Propulsion Systems: "TRL Booster" research at the von Karman Institute, by Jean-Baptiste Gouriet, Cryogenic Heat & Mass Transfer symposium, TU Twente (Enschede), november 2019

- Research manager Jean-Baptiste Gouriet (<u>jeanbaptiste.gouriet@vki.ac</u>.be)
- Business development manager Peter Simkens (<u>peter.simkens@vki.ac</u>.be)





VRIJE

UNIVERSITEIT BRUSSEL

Department of Chemical Engineering

Vrije Universiteit Brussel, Faculty of Engineering Sciences

General expertise of the research group

The Department of Chemical Engineering at VUB has extended expertise in separation processes, in particular separation and purification of gas and liquid mixtures by adsorption and chromatography. Advanced experimental techniques (lab on a chip, high- throughput experimentation, ...) are combined with state-of-the-art computer modelling methods, including molecular modelling and computational fluid dynamics, to obtain insight in the fundamental adsorption, diffusion and mass and heat transfer effects. The department has 3 core research topics adsorptive separation processes, HPLC technology and analysis and microfluidics and microreactors

Specific hydrogen - related expertise & research topics

- Adsorption, gas separation, purification and storage
- Hydrogen storage in porous solids
- Hydrogen clathrate formation
- Study of kinetics, uptake and thermodynamics of hydrogen storage
- Experimental assessment and modelling of storage
- CFD modelling for flow field design of electrolysers and fuel cells
- Know-how on gas sampling, in-line/on-line / off-line gas analysis

Available equipment/tools

- Ultra-precise (in-house built) gravimetric experimental setup to study H₂-storage in porous solids: kinetics of storage, uptake capacity, thermodynamics in a broad range of conditions (77K, -30 to 70°C, up to 15 MPa, density measurement, many types of gases)
- Volumetric setup to study gas storage in porous solids
- Breakthrough setup to study purification of hydrogen streams (removal of trace impurities)
- Gas analysis equipment (GC, GC-MS, MS)
- Software tools to simulate H₂-storage processes

International collaborations

- ITQ Valencia (Prof. F. Rey): micro- and mesoporous solids
- Université de Montpellier (Prof. G. Maurin): molecular modelling of adsorption

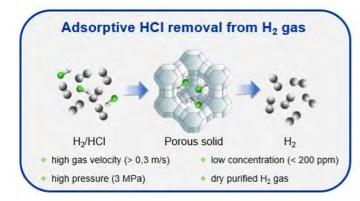
Process development System modelling

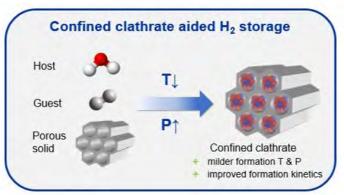
Storage of H₂



Participating in FL/B/EU funded projects with H₂ related research

• ARCLATH, H₂ storage in artificial clathrates, VLAIO, Project coordinator: KU Leuven, Prof. J. Martens, main partners: KU Leuven, UGent, UAntwerpen, VUB





Main relevant publications

- Gupta, A., Baron, G. V., Perreault, P., Lenaerts, S., Ciocarlan, R.-G., Cool, P., ..., Denayer, J. F. M. (2021). Hydrogen Clathrates: Next Generation Hydrogen Storage Materials. Energy Storage Materials, 41, 69–107. https://doi.org/10.1016/j.ensm.2021.05.044
- Sharma, R., Cousin-saint-remi, J., Tiriana, S., Delplancke, M., Pletincx, S., Baert, K., ... Denayer, J.
- F. M. (2022). Metal-organic framework ZIF-8 for exceptional HCl removal from Hydrogen gas by reaction. International Journal of Hydrogen Energy, 47(47), 20556–20560. https://doi.org/10.1016/j. ijhydene.2022.04.244
- Sharma, R., Segato, T., Delplancke, M.-P., Terryn, H., Baron, G. V., Denayer, J. F. M., & Cousin-Saint-Remi, J. (2020). Hydrogen chloride removal from hydrogen gas by adsorption on hydrated ion-exchanged zeolites. Chemical Engineering Journal, 381(August 2019), 122512. https://doi.org/10.1016/j.cej.2019.122512
- De Schepper, P., Danilov, V. A., & Denayer, J. F. M. (2016). Cathode flow field design for nitric oxide/ hydrogen fuel cell in cogeneration of hydroxylamine and electricity. International Journal of Energy Research, 40(10), 1355–1366. https://doi.org/10.1002/er.3519

- Prof. Joeri Denayer (joeri.denayer@vub.be)
- Business developer dr. ir. Marleen Claeys (<u>marleen.claeys@vub.be</u>)

Process development System modelling

Storage of H₂ & use of H₂ or H₂-based carriers



Thermodynamics and Fluid Mechanics (FLOW)

Vrije Universiteit Brussel, Faculty of Engineering, Department of Applied Mechanics

General expertise of the research group

At FLOW, we focus on ensuring access to sustainable energy for all, which is one of the sustainable development goals of the United Nations. We tackle this challenging mission through 3 research topics circular energy, low emissions, and flexible energy systems. We have expertise in thermodynamics, fluid mechanics, combustion, CFD simulations, system modelling and data driven modelling. In the field of Hydrogen, our current focus in on the combustion of hydrogen and related e-fuels for heat and power production and other industrial applications, including safety issues related to hydrogen storage and use.

Specific hydrogen - related expertise & research topics

- Combustion of H₂ and H₂-based carriers
- · CFD simulations
- Kinetic mechanisms
- Thermodynamic process modelling and integration
- Power plants
- Flue gas treatment
- Storage
- H₂ leakages

Available equipment/tools

• Micro-gas turbine Turbec T100 (100 kWe)

Participating in FL/B/EU funded projects with H₂ related research

- BEST: Belgian Energy System. Role of e-fuels in the Belgian energy system, 2020-2024, ETF: Energy Transition Funds. Partners: UCL, ULB, UMons, UGent
- BE-HyFE: Belgian Hydrogen Fundamental Expertise, 2021-2025, ETF: Energy Transition Funds. Partners: UGent, UCLouvain, ULB, UAntwerpen, UMons, KU Leuven, ULiège, UHasselt, Imec,VKI,VITO, WaterstofNet, TWEED
- H₂-HeatNet: A planification tool for the integration of hydrogen-based energy systems into urban district heating networks, 2022-2024, Innoviris: Joint R&D project; Partners: ULB, Sibelga.
- H₂-GridTwin: A digital twin of a hydrogen-to-grid living lab, 2023-2025, ETF: Energy Transition Funds. Partners: ULB, Sibelga



Process development System modelling

Storage of H_2 & use of H_3 or H_3 -based carriers



Main relevant publications

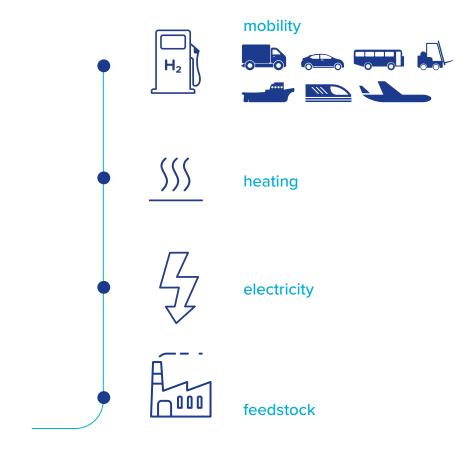
- Is Blue Hydrogen a Better Alternative Than Post-Combustion Carbon Capture for Combined Cycle Gas Turbines? A Thermodynamic Point of View, MJ Mendoza Morales, A Verhaeghe, L Bricteux, J Blondeau, W De Paepe, Turbo Expo: Power for Land, Sea, and Air 86946, V002T03A012, 2023
- Large Eddy Simulation investigation of pressure and wall heat loss effects on rich ammoniahydrogen-air combustion in a gas turbine burner. K Bioche, J Blondeau, L Bricteux. International Journal of Hydrogen Energy 47 (85), 36342-36353, 2022
- Towards Zero-Carbon Emission Cogeneration Through Hydrogen Fueling: Assessment of the Impact of CH4/H₂ Blends on the Thermodynamic Performance of a Gas Turbine CHP Unit. MJ Mendoza Morales, J Blondeau, W De Paepe. International Conference on Applied Energy, 2022
- Large Eddy Simulation of rich ammonia/hydrogen/air combustion in a gas turbine burner, K Bioche,
 L Bricteux, A Bertolino, A Parente, J Blondeau, International Journal of Hydrogen Energy 46 (79),
 39548-39562, 2021

Contact persons

Julien Blondeau (<u>Julien.blondeau@vub.be</u>)



3.2. Use of hydrogen





Process development & system modelling

Use of H₂ or H₃-based carriers



3.2.1. KU Leuven

Division of Applied Mechanics and Energy conversion, Mechatronics Group (TME, M-Group)

KU Leuven, Faculty of Engineering Technology, Department of Mechanical Engineering

General expertise of the research group

The M-Group research team has a unique composition, including three departments - Mechanical Engineering, Electrical Engineering, and Computer Science. The primary focus of the M-Group is to investigate the reliability and dependability of highly automated interconnected mechatronic systems, where the TME@M-Group has a particular emphasis on unmanned aerial systems and hybrid hydrogen-based propulsion systems. The team consists of experts in various areas, including sensor networks and algorithms (Prof. H. Hallez), software dependability (Prof. J. Boydens), hardware and system safety (Prof. D. Pissoort), Artificial Intelligence and machine learning (Prof. M. Verbeke), H₂ based systems for drone applications (Prof. F. Buysschaert), and dependable lightweight structures for aeronautics (Prof. G. Serhat).

Specific hydrogen - related expertise & research topics

Dependable hybrid drone propulsion with fuel cells

Participating in FL/B/EU funded projects with H₂ related research

- HYDE: Hydrogen technology for Defence applications, DEFRA Belspo. Partners: KU Leuven, VIVES Zuid, VIVES Noord, Solenco Power
- H₂-4-All: Fuel cell technologies for industry, VLAIO TETRA. Partners: VIVES-Zuid, KU Leuven, VIVES-Noord

Available equipment/tools

- Electronic loads
- FRA
- Fuel cells
- Modified Climate chambers, including mechanical stress (tension, pressure and shearing) and UV radiation
- Halt (Highly Accelerated lifetime testing)
- EMC test equipment (via FMEC, M-Group)



System modelling & components development

Use of H₂ or H₂-based carriers



Main relevant publications

- Mus, J., Madhav, D., Vanierschot, M., Vandeginste, V., Buysschaert, F., 2024. A review of the impact of ambient conditions and degradation in hybrid fuel cell powered unmanned aerial vehicles.
 Journal of Power Sources 624, 235571. URL: https://www.sciencedirect.com/science/article/pii/S0378775324015234, doi:https://doi.org/10.1016/j.jpowsour.2024.235571
- Mus, J., Vanhoutte, B., Schotte, S., Fevery, S., Latré, S., Kleemann, M., Buysschaert, F. (2022).
 Design and Characterisation of an Alkaline Electrolyser. In: 2022 11th International Conference on Renewable Energy Research and Application (ICRERA), (253-259). Presented at the International Conference on Renewable Energy Research and Application (ICRERA), Istanbul, Turkey, 18 Sep 2022-21 Sep 2022. ISBN: 978-1-6654-7140-4. doi: 10.1109/ICRERA55966.2022.9922902
- Mus, J., Mylle, S., Schotte, S., Fevery, S., Latré, S., Buysschaert, F. (2022). CFD Modelling and Simulation of PEMFCs in STAR-CCM+. In: 2022 11th International Conference on Renewable Energy Research and Application (ICRERA), (260-267). Presented at the International Conference on Renewable Energy Research and Application (ICRERA), Istanbul, Turkey, 18 Sep 2022-21 Oct 2022. ISBN: 978-1-6654-7140-4. doi: 10.1109/ICRERA55966.2022.9922908
- Buysschaert, F., Mus, J. (2022). Waterstof en drones. Presented at the Drone West 22, Ostend, Belgium. (professionally oriented)
- Buysschaert, F., Van Luchem, P. (2022). Hydrogen Tech Day Workshop: Regulations. Presented at the Hydrogen Tech Day, Kortrijk, Belgium. (professionally oriented)
- Mus, J., Buysschaert, F. (2022). Modelling & Characterization of Electrochemical Energy Systems.
 Presented at the Chemical Research in Flanders Chemistry Conference for Young Scientists (CRF-ChemCYS), Blankenberge, Belgium.
- Schotte, S., De Tollenaere, S., Buysschaert, F., Mus, J., Uytterhaegen, B., van luchem, P. (2020). H₂-4-All presentation Fuel cell system. Presentation H₂-4-All basics Fuel cells system.
- Buysschaert, F., Mus, J., De Tollenaere, S., Schotte, S., Van Luchem, P. (2021). Webinar: Hoe starten met toepassingen op waterstofgas?

- Frank Buysschaert (<u>frank.buysschaert@kuleuven.be</u>)
- Dries Vanoost (<u>dries.vanoost@kuleuven.be</u>)



Process development & system modelling

Use of H₂ or H₂-based carriers



LowCarb Research Group

KU Leuven, Faculty of Engineering Technology, Department of Mechanical Engineering

General expertise of the research group

The LowCarb Research Group specializes in the decarbonization of transportation and power generation through the use of electrification and low- and zero-carbon alternative fuels. The group utilizes a variety of experimental and numerical methodologies to characterize the combustion of alternative fuels, and to evaluate the energy efficiency of novel powertrains and propulsion systems. There is significant experience within the group concerning hydrogen engine systems in particular and more general expertise in the direct injection of gaseous fuels.

Specific hydrogen - related expertise & research topics

- Use of hydrogen for heat and power
- Advanced direct injection strategies for hydrogen in reciprocating engines
- · Abnormal combustion limit of hydrogen, hydrogen/natural gas blends
- · Flexible oxy-fuel combustors with hydrogen-enrichment
- Combustion of zero carbon fuel blends (ammonia/hydrogen), in-situ cracking of ammonia for hydrogen-enhanced ammonia combustion
- Storage of intermittent, renewable energy using 'green' hydrogen injected into the natural gas network



Modified engine cylinder head with instrumentation for direct measurement of surface temperature and wall heat flux (small cylinder near the centre of the image) as well as a prototype direct injector for hydrogen (large cylindrical object in the top right of the image)



Process development & system modelling

Use of H₂ or



Available equipment/tools

- 300 kW ABB DC dynamometer
- Engine test bed with suite of instrumentation (i.e. in-cylinder pressure transducers, etc.
- CO₂ analyser with 0-100% volume range for oxy-fuel combustion testing
- High-speed tomographic particle image velocimetry (PIV) system
- Phase doppler anemometry (PDA) instrument for measurements of velocity and particle size
- Flexible 20 kW burner apparatus (premixed-swirl or diffusion flame modes)
- High-speed image-intensifier, Nikkor UV lens and visualization hardware
- Array of mass flow controllers to mix gases for air/partial oxy-fuel/full oxy-fuel combustion
- Electron impact ionization mass spectrometer for H₂ detection
- In-house LabVIEW-based combustion analysis software and commercial GT-Power software for combustion and powertrain simulation
- Vehicle powertrain and drive cycle simulation software via Argonne National Labs Autonomie

International collaborations

- University of Melbourne Thermodynamics Laboratory
- Engine Combustion Network (ECN)

Participating in FL/B/EU funded projects with H₂ related research

- BeHyFE (Belgian Hydrogen Fundamental Expertise) targeting projects for PhD students involving all
 aspects of the hydrogen value chain (hydrogen production, storage/logistics and end-use), FOD ETF,
 knowledge institutions and universities throughout Belgium (12 total partners)
- ICO2CH (Integrated CO₂ Capture and Hydrogen Production) novel reactor producing green hydrogen connected to oxy-fuel reciprocating engine valorising CO₂/O2 byproducts, VLAIO Moonshot, VITO/Imec/VUB/KU Leuven
- Highly efficient and robust zero-carbon emission engines using directly-injected, spark-ignited hydrogen – conducting innovative engine experiments with directly-injected hydrogen, the capability to inject multiple times per cycle and direct measurements of wall heat flux, KU Leuven Internal Funds C3 project, KUL/VIVES Kortrijk/Eneria

Main relevant publications

- Joel Mortimer, Farzad Poursadegh, Michael Brear, Stephen Yoannidis, Joshua Lacey, Yi Yang, Extending the knock limits of hydrogen DI ICE using water injection, Fuel, 2022.
- M.R. Yosri, J.Z. Ho, M. Meulemans, M. Talei, R.L. Gordon, M.J. Brear, D. Cosby, J.S. Lacey, Large-eddy simulation of methane direct injection using the full injector geometry, Fuel, Volume 290, 2021.
- Zhewen Lu, Junqiu Jiang, Yi Yang, Joshua Lacey, Michael J. Brear, Hydrogen oxidation near the second explosion limit in a flow reactor, Proceedings of the Combustion Institute, 2020.
- Mortimer, J, Yoannidis, S, Poursadegh, F, Lu, Z, Brear, M, Yang, Y, Etherington, D, Heijkoop, M, & Lacey, J. "An Experimental and Numerical Study of a Hydrogen Fueled, Directly Injected, Heavy Duty Engine at Knock-Limited Conditions." Proceedings of the ASME 2020 Internal Combustion Engine Division Fall Technical Conference. ASME 2020 Internal Combustion Engine Division Fall Technical Conference. Virtual, Online. November 4–6, 2020. V001T01A002. ASME.

Contact persons

• Assistant Professor Joshua Lacey (josh.lacey@kuleuven.be)





3.2.2. UGent

Transport Technology (TT)

Ghent University, Faculty of Engineering and Architecture, Department of Electromechanical, Systems and Metal Engineering

General expertise of the research group

The research group Transport Technology at Ghent University is specialized in internal combustion engines operating on renewable fuels. The group's research is going from the heart of the engine: the in-cylinder processes (spray formation, combustion, heat transfer and emission formation), to the engine as part of a sustainable energy system (power-to-x, vehicle propulsion, ...). The group's vision is to enable the transition to sustainable transportation through finding the best engine and fuel for each application. Its mission is therefore to provide appropriate R&D tools to the research community and industry, training to students and researchers, and guidelines to policy makers.

Specific hydrogen - related expertise & research topics

- Internal combustion engines (ICEs) on e-fuels, with the main expertise being on hydrogen and methanol
- Power, efficiency, emissions
- · Simulations of ICE on e-fuels

Available equipment/tools

- 5 engine test benches, with dynamometer capability to 300 kW
- Combustion vessel with high-speed camera
- Gaseous emissions measurement (CO, CO₂, NOx, O2)

Participating in FL/B/EU funded projects with H₂ related research

- FASTWATER (EU, 2020-2024, 1 PhD)
- BEST (National, 2020-2024, 1 PhD)
- PhD Baekeland (Flemish, 2020-2024, 1 PhD)
- CHyPS (Intercluster cSBO, 2022-2024, 1 PhD)
- MMU (VIL COOCK, 2021-2024, 1 PhD)
- See website: research.ugent.be





System modelling



Main relevant publications

- See website: biblio.ugent.be
- Verhelst S., Sierens R., A quasi-dimensional model for the power cycle of a hydrogen fuelled ICE. International Journal of Hydrogen Energy, Vol. 32, pp. 3545-3554, October 2007
- Verhelst S., Wallner T., Hydrogen-Fueled Internal Combustion Engines. Progress in Energy and Combustion Science, Vol. 35, pp. 490-527, December 2009
- Verhelst S., Wallner T., Eichlseder H., Naganuma K., Gerbig F., Boyer B., Tanno S., Electricity Powering Combustion: Hydrogen Engines, Proceedings of the IEEE Vol. 100, pp. 427-439, February 2012
- Vancoillie J., Demuynck J., Sileghem L., Van De Ginste M., Verhelst S., Comparison of the renewable transportation fuels, hydrogen and methanol formed from hydrogen, with gasoline - Engine efficiency study, International Journal of Hydrogen Energy Vol. 37, pp. 9914-9924
- Verhelst S., Recent progress in the use of hydrogen as a fuel for internal combustion engines, International Journal of Hydrogen Energy, invited paper, Vol. 39, pp. 1071-1085, January 2014
- Verhelst S., Demuynck J., Sierens R., Scarcelli R., Matthias N., Wallner T., Hydrogen-fueled internal combustion engines, in 'Renewable Hydrogen Technologies. Production, Purification, Storage, Applications and Safety', Chapter 16, pp381-400, edited by L.M. Gandía, G. Arzamendi, P.M. Diéguez, Elsevier, ISBN 978-0444563521
- Verhelst S., Wallner T., Hydrogen-fueled internal combustion engines, in 'Handbook of Hydrogen Energy', pp. 821-901, edited by S.A. Sherif, Y. Goswami, E. Stefanakos, A. Steinfeld; CRC/Taylor and Francis, ISBN 978-1420054477

Contact persons

Prof. Sebastian Verhelst (Sebastian. Verhelst@ugent.be)





3.2.3. VIVES University of Applied Sciences

Research Group Energy - Green methanol

VIVES University of Applied Sciences

General expertise of the research group

The research group hydrogen can rely on a fully equipped laboratory of the hydrogen energy chain. From production, up to the use of hydrogen in different applications. The group has gained expertise in practical use and implementation of various aspects, including green hydrogen production, hydrogen storage, regulatory aspects and safety considerations related to hydrogen, utilization of hydrogen as a fuel for internal combustion engines, hydrogen fuel cell systems, fuel cell vehicles, and the production and utilization of green methanol.

Specific hydrogen - related expertise & research topics

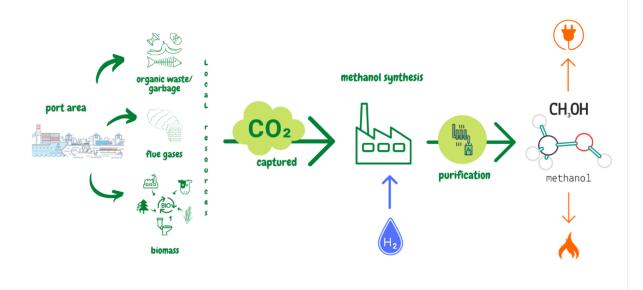
- Expertise in green methanol production from CO₂ and H₂
- Expertise in green methanol utilization
- Methanol combustion systems (dual-fuel, mono-fuel)
- Methanol combustion characteristics, performance, etc

Available equipment/tools

- Set-up methanol production from CO₂ and H₂
- Genset Atlas Copco (250 kVA) on dual fuel technology (diesel methanol)
- One-cylinder combuston engine on methanol
- Testbench with single cylinder experimental setup for PFI and DFI
- Resistive load bench 20 kW & 300 kW
- Engine test bench water brake

International collaborations

Assistant professor Atul Bansode and prof. Urakawa (TuDelft)

















Participating in FL/B/EU funded projects with H₂ related research

- Project: REDII ports: Renewable energy development an intelligent implementation in PORTS
 - Topic: resource study and building of a CCU demonstrator for green methanol production and use in an internal combustion engine
 - Funding source: European Interreg north sea region
 - Project partners: Port of Skagen, Ports Niedersachsen, Korsor Havn, NICE, BDI, Port of Brest, Port of Brussels

- Sam Schotte (<u>sam.schotte@vives.be</u>)
- Steven De Tollenaere (<u>steven.detollenaere@vives.be</u>)





Research Group Energy - Hydrogen fuel cell systems

VIVES University of Applied Sciences

General expertise of the research group

The research group hydrogen can rely on a fully equipped laboratory of the hydrogen energy chain. From production, up to the use of hydrogen in different applications. The group has gained expertise in practical use and implementation of various aspects, including green hydrogen production, hydrogen storage, regulatory aspects and safety considerations related to hydrogen, utilization of hydrogen as a fuel for internal combustion engines, hydrogen fuel cell systems, fuel cell vehicles, and the production and utilization of green methanol.

Specific hydrogen - related expertise & research topics

- Expertise in hydrogen PEM Fuel cell systems (small size), system design, control, and data acquisition
- Expertise in fuel cell vehicle technology, reverse engineering, system layout, and working principles
- Fuel cell system modelling, control, and implementation
- Fuel cell system testing

Available equipment/tools

- Slow filling station for FCEV
- Fuel cell system 8 kW
- Fuel cell system 6.8 kW
- Toyota Mirai
- 4W vehicle Test bench
- 2W vehicle Test bench
- Engine test bench water brake
- ZERT 002 H₂ KART 12.5 kW FC
- Didactical IX35 FCEV setup

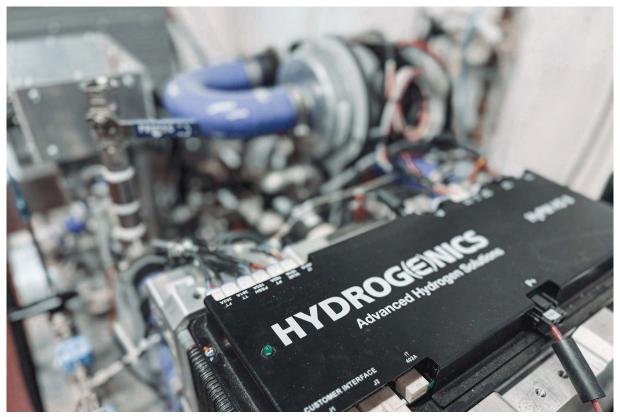
Participating in FL/B/EU funded projects with H₂ related research

- Project: H₂-4-All
 - Topic: H₂-4-All is developing a testbed for fuel cell systems and consolidating regulations for hydrogen use in businesses
 - Funding source: Flemisch Tetra-project from VLAIO project partners: KU Leuven, Solenco Power, Agoria, EUKA, Eliet, Eoly, Addax motors, Atlas Copco, WaterstofNet, Bekaert, E-Bo enterprises, Geoxyz, Kaseco, Lieven Deneckere, Mol Cy, Vandaele machinery, Stad Kortrijk, Schneider Electric, Van Marcke, Robuust









Main relevant publications

- Conference on Renewable Energy Research and Application (ICRERA), 2022, pp. 253-259, doi:10.1109/ICRERA55966.2022.9922902.
- Buysschaert, F., Mus, J., De Tollenaere, S., Schotte, S., Van Luchem, P. (contr.) (2021). Webinar: Hoe starten met toepassingen op waterstofgas?
- Mus, J., Mylle, S., Schotte, S., Fevery, S., Latré, S., Buysschaert, F. (2022). CFD Modelling and Simulation of PEMFCs in STAR-CCM+. In: 2022 11th International Conference on Renewable Energy Research and Application (ICRERA), (260-267). Presented at the International Conference on Renewable Energy Research and Application (ICRERA), Istanbul, Turkey
- All energy Australia, Melbourne 25/10/2023 Green hydrogen in Flanders

- Sam Schotte (<u>sam.schotte@vives.be</u>)
- Steven De Tollenaere (<u>steven.detollenaere@vives.be</u>)





Research Group Energy - Hydrogen ICE

VIVES University of Applied Sciences

General expertise of the research group

The research group hydrogen can rely on a fully equipped laboratory of the hydrogen energy chain. From production, up to the use of hydrogen in different applications. The group has gained expertise in practical use and implementation of various aspects, including green hydrogen production, hydrogen storage, regulatory aspects and safety considerations related to hydrogen, utilization of hydrogen as a fuel for internal combustion engines, hydrogen fuel cell systems, fuel cell vehicles, and the production and utilization of green methanol.

Specific hydrogen - related expertise & research topics

- Expertise in H₂-ICE technology (hydrogen internal combustion engine)
- In-house proficiency in dual fuel technology, particularly diesel-hydrogen systems, demonstrated with a 250 kVA generator set
- Specialization in converting petrol engines into 100% hydrogen combustion engines
- Specialized knowledge in low-level control management for dual fuel systems
- Proficient in control management, data acquisition, and visualization techniques

Available equipment/tools

- Genset Atlas Copco dual fuel diesel hydrogen methanol 250 kVA
- Genset Caterpillar Direct injection 33kVA
- Testbench with single cylinder experimental setup for PFI and DFI
- Resistive load bench 20 kW & 300 kW
- Engine test bench water brake

International collaborations

- TU Delft
- Solent University Southampton
- UPHF Université Polytechnique Hauts-de-France
- NICE Noordelijk Innovatielab Circulaire Economie
- BDI Bretagne Développement Innovation





Participating in FL/B/EU funded projects with H₂ related research

- Project: ISHY (implementation of ship hybridisation)
 - Topic: retrofit of an existing diesel genset 250 kVA to dual fuel mode (hydrogen and pilot diesel)
 - Funding source: Europe Interreg 2 Seas
 - Industrial partners: Port of Ostend, Parkwind, GeoXYZ, TU Delft, Solent University, Hybrid marine
- Project: Direct injection of hydrogen for ICE
 - Topic: building a demonstrator for testing of direct injection of hydrogen and strategies
 - Funding source: Industrial research Fund (IOF) Category 3 (C3)
 - Project partners: In cooperation with KU Leuven







Main relevant publications

- Conference on Renewable Energy Research and Application (ICRERA), 2022, pp. 253-259, doi:10.1109/ICRERA55966.2022.9922902.
- De Wilde, B., Schotte, S. (contr.) (2022). Hogeschool VIVES opent nieuw waterstofcentrum VRT NWS.
- Buysschaert, F., Mus, J., De Tollenaere, S., Schotte, S., Van Luchem, P. (contr.) (2021). Webinar: Hoe starten met toepassingen op waterstofgas?
- Mus, J., Mylle, S., Schotte, S., Fevery, S., Latré, S., Buysschaert, F. (2022). CFD Modelling and Simulation of PEMFCs in STAR-CCM+. In: 2022 11th International Conference on Renewable Energy Research and Application (ICRERA), (260-267). Presented at the International Conference on Renewable Energy Research and Application (ICRERA), Istanbul, Turkey
- All Energy Australia, Melbourne 25/10/2023 Green hydrogen in Flanders

- Sam Schotte (<u>sam.schotte@vives.be</u>)
- Steven De Tollenaere (<u>steven.detollenaere@vives.be</u>)

Use of H₂ for Mobility



3.2.4. VKI

Research Expertise Group on Environmental Flows & Safety Industrial Flows

von Karman Institute for Fluid Dynamics, Department of Environmental & Applied Fluid Dynamics

General expertise of the research group

Numerical simulation, Computational Fluid Dynamics (CFD) and experimental testing for industrial and environmental hydrogen flows and for safety analysis for hydrogen applications.

Specific hydrogen- related expertise & research topics

- Safety:
 - Detonation risk
 - Risk mitigation of explosions
 - Leakage
- Industrial application:
 - Cooling of steel with hydrogen

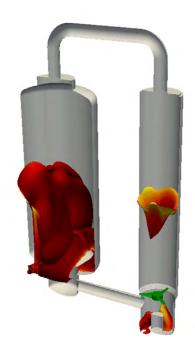
Available equipment/tools

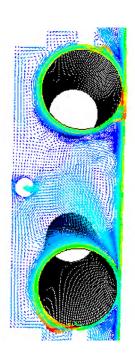
- Software platforms for CFD
 - OpenFOAM®
 - WRF
 - High Performance Computing (HPC) cluster
- · Testing facilities
 - Water Spray Facility: The Water-Spray facility is designed for the general study of liquid sprays that are generated by pneumatic and pressure nozzles. It is equipped with a pump capable of delivering spray flow rates up to 1 dm3/s at a pressure of 8 bar, with metering of both flow rate and feed pressure, into a 3x4 m2 collecting pool. The facility is also equipped with a set of gas burners and vertical flat plates, which are instrumented with thermocouples and radiometers, to simulate thermal shielding by a water curtain.



International and Industrial collaborations

- Arcelor Mittal
- Total
- Solvay
- GDF Suez





Left: CFD Simulation of inflammation / combustion of H_2 . Right: Use of H_2 for cooling application in steel manufacturing

- Research manager EA department Philippe Planquart (philippe.planquart@vki.ac.be)
- Professor Delphine Laboureur (<u>delphine.laboureur@vki.ac.be</u>)
- Business development manager Peter Simkens (peter.simkens@vki.ac.be)

Use of H₂



Research Expertise Group on High Speed Propulsion & Combustion

von Karman Institute for Fluid Dynamics, Department Turbomachinery & Propulsion

General expertise of the research group

Utilisation of (liquid) hydrogen as propellant in airplanes or spacecraft, in combustion engines or thrusters:

- Combustion of hydrogen in turbines, for jet engines and for energy production
- (Pulsed) Detonation of hydrogen for aerospace propulsion

Specific hydrogen- related expertise & research topics

- Combustion models for thermodynamic modelling of hydrogen powered engines for hypersonic flight
- Numerical modelling, experimental validation
- Emission calculation
- · Jet-noise modelling and testing

Available equipment/tools

- Facilities:
 - JAFAAR (Jet Aeroacoustic Facility for Aeronautical & Aerospace Research): the aeronautical applications concern mainly airframe noise with a focus on high-lift devices. The aerospace applications include launcher rocket noise, and supersonic boundary layer studies. The facility permits jet noise studies up to Mach 2, in single or a coaxial jet configurations with an outlet diameter of the order of 0.05 m. The flow is quietened by means of a silencer, and the jet discharges in an anechoic room with dimensions (4 x 3 x 4) m3 and with a cut-off frequency of 200 Hz. The facility can also accommodate a free-jet test section with side-plates for airframe noise research.
 - H3 (Mach 6 Hypersonic Wind Tunnel): the hypersonic tunnel H3 is a blow-down facility with an axisymmetric nozzle giving a uniform Mach 6 free jet 12 cm in diameter. Air is supplied at 7-35 bar stagnation pressure and a maximum 550 K stagnation temperature. Reynolds number may be varied from 3 x 106 to 30 x 106/m.
- Software & CFD platforms:
 - Ecosimpro
 - Fluent
 - Chemkin
 - WRF
 - OpenFOAM®







International & Industrial Collaborations

- BOEING (USA)
- BOOM (USA)
- CiRA (UK)
- CNRS (FR)
- DLR (DE)
- Politechnico di Torino (IT)
- LUND University (SE)
- QinetiQ (BE / UK)
- TU Delft (NL)

Participating in FL/B/EU funded projects with H₂ related research

- STRATOFLY investigates the feasibility analysis of high-speed passenger stratospheric flight with respect to key technological, societal and economical aspects. The goal of STRATOFLY is to refine the design of a hypersonic vehicle able to fly at about 10,000 Km/h (Mach 8) above 30 km of altitude. The project will focus on the integration of innovative propulsion systems, unconventional structural configurations and systems for the thermal and energy management of the vehicle. Taking into account sustainability, the project will investigate strategies to reduce gas and noise emissions, while at the same time ensuring the required safety levels for passengers. The project aims at drastically increasing the efficiency of the thermodynamic cycle (>15%) by exploiting fuels cryogenically stored in the tanks. This efficiency gain will be quantified in terms of reduction of fuel consumption, emissions (75% to 100% reduction in CO₂ emissions per passenger kilometer, 90% reduction in NOx emissions) and noise. Funding: EC H2020. Partners: Politechnico di Torino, TUHH, UDC, CiRA, DLR
- MORE & LESS aims at MORE sustainable fuels, environmental protection and citizens protection, and LESS pollutant emissions, noise emissions and impact on air quality, ozone layer and climate: it aims at low-boom and environmentally sustainable supersonic aviation. The objective is to thermodynamically design and optimize 3 propulsion system components (inlet, turbomachinery and nozzle) for Mach 2 aircraft and for a Stratofly concept for Mach 5. MORE & LESS runs URANS simulations of hydrogen and bio-fuel combustion, for propulsion and pollutant emission determination. MORE & LESS performs aerodynamic testing, aeroacoustic jet noise modeling and experimental testing, and sonic boom propagation. Funding: Cleansky 2. Partners: Polito, BOOM, CIRA, CNRS, DLR, ECATS, FICG, INCAS, ISL, LUND University, BOEING, TU Delft, TUHH
- PDT aims at numerically and experimentally proving/disproving pulse-detonation thrustering as a viable option for spacecraft propulsion. After doing a thorough requirement review, 1D simulations on a number of viable solutions, and 3D CFD simulations, 2 PDT candidates are selected. With a trade-off analysis, the final PDT design is consolidated for testing. H₂-O2 detonation experiments are performed under vacuum conditions, providing a vast amount of data to validate the numerical tools. Funding: ESA; partners: COMOTI, UPM, QinetiQ

Use of H₂





Main relevant publications

- Saracoglu B.H., Cutrone L., Marini M., Assessment of combustion models for thermodynamic modeling of the engines for hypersonic propulsion, International Conference on Flight vehicles, Aerothermodynamics and Re-entry Missions and Engineering (FAR) 30 September 3 October 2019
- Ispir A.C., Gonçalves P.M., Saracoglu B.H., Analysis of a combined cycle propulsion system for STRATOFLY hypersonic vehicle over an extended trajectory, MATEC Web of Conferences 304
- Goncalves P.M., Ispir A.C., Saracoglu B.H., Development and optimization of a hypersonic civil aircraft propulsion plant with regenerator system, AIAA Propulsion and Energy 2019 Forum
- Ali C. Ispir, Pedro M. Goncalves & Bayindir H Saracoglu, Thermodynamic efficiency analysis and investigation of exergetic effectiveness of STRATOFLY aircraft propulsion plant, by., AIAA 2020-1108, January 2020

- Research manager Bayindir Saracoglu (<u>bayindir.saracoglu@vki.ac.be</u>)
- Business development manager Peter Simkens (<u>peter.simkens@vki.ac.be</u>)



Use of H₂ for Mobility



Research Expertise Group on Liquid & Solid Propulsion (mobility)

von Karman Institute for Fluid Dynamics, Department Aerospace

General expertise of the research group

Design and optimisation of critical components for a LH2 propulsion system, such as LH2 fuel tanks, valves, heat exchangers...

Experimental testing and numerical simulation of the fluid dynamics behaviour for two-phase flows, with application for liquid hydrogen (LH2). Extensive expertise is available from research on the propellant management system for space launchers. This expertise which has been developed for space applications, is now being transferred to terrestrial mobility applications in ships, aircraft, heavy duty trucks...

Specific hydrogen- related expertise & research topics

- In general: numerical simulations of fluid dynamics behaviour of liquid hydrogen (LH2) and performing experimental tests to validate the modelling
- Fluid Dynamics Phenomena of Liquid Hydrogen in a propellant management system (in pumps, piping, valves...):
 - Cavitation
 - Boil-offs and heat transfer
 - Fluid hammering
- Sloshing of cryogenic fuels in a fuel tank (on board of a ship, a plane, a truck or in a space launcher...)

Available equipment/tools

- Numerical simulation platforms for CFD (Computational Fluid Dynamics), e.g. EcosimPro, OpenFOAM®
- Experimental test facilities:
 - Cryoline Facility: a large multipurpose facility, which allows the characterization of cryogenic valves and the study of cryogenic water hammer and chill-down phenomena. The CryoLine facility can be placed horizontally, vertically and at intermediate angles to study the effect of gravity direction on cryogenic two-phase flows. Characterization of the facility allows measurement of temperature, pressure, flow rate and visualization of the flow (single phase or two-phase) during transient and at steady state.
 - The "CryME" (Cryogenic Microgravity Experiments) facility is a fully customized cryostat, for the characterization of cryogenic sloshing, boiling and thermal stratifi cation on earth and in microgravity conditions at temperature down to 70 K. The presence of large windows allows the use of non-intrusive optical techniques such as particle image velocimetry or high-speed visualization.
 - CHIEF Facility and upgraded CHIEF Facility: for testing cryo-valves

Use of H₂ for Mobility



- PREDICT and BECASSINE Facility: for testing for densified cryogenic (e-)fuels.
- Sloshing table
- Particle Image Velocimetry

International and industrial collaborations

- Airbus
- Ariane Group (FR, DE)
- CiRA (UK)
- DLR (DE)
- Numeca (BE)
- Open Engineering (BE)
- Pipistrel Vertical Solutions (SLO)
- Polytecnico di Torino (IT)
- Safran Aero Boosters (BE, FR)
- Waseda University Tokyo (JPN)







Experimental testing of sloshing of liquid hydrogen in a fuel tank, in the "Cryostat" test facility, with visualisation with Particle Image Velocimetry (PIV)

Participating in FL/B/EU funded projects with H₂ related research

- [SPACE] CRYOSLOSH and its continuation SLOSH II deal with the problem of sloshing in cryogenic propellants, stored in a reservoir. The main scope is to improve the state-of-the-art knowledge of the numerical simulation of liquid hydrogen, by refining actual models and performing coordinated experiments for their validation. SLOSH II focuses on introducing non-isothermal conditions on the hydrodynamic problem and provides model(s) for the contact-angle boundary condition. Funding: ESA GSTP; partners: Numeca).
- [SPACE] The SPARGE I & II projects concern the isothermal characterization of sloshing in microgravity conditions, when surface tension forces are dominant. Parabolic flights represent a good tool to achieve microgravity conditions which are compatible with the ones obtained in real conditions (satellite or space vehicle propeller tanks). Funding: ESA – Continuously Open Research Announcement.



Use of H₂ for Mobility



- [SPACE] CRYOBUBBLE is related to the experimental study and modelling of the transient chill down phenomena occurring when a cryogenic liquid is introduced into a system at ambient conditions. Such situation is happening at the initial start of a cryogenic system prior to operation. Heat exchanges between the cryogenic fluid and the system lead to vaporization and boiling phenomena as well as a cool down of the whole system. In this project, the cool-down created by a LN2 flow into a pipe at ambient temperature is studied both experimentally and numerically.
- [SPACE] CRYOVANNE II focuses on the multiphysics study of the behavior of a cavitating valve in cryogenic conditions. The development of new valves for space applications is going more and more towards electromechanically operated valves to reduce the mass demands. It requires improving the prediction of the expected thermo-mechanical loads on the valves, in particular during its transient operations. Due to the complexity of the multi-phase phenomena and the lack of literature describing benchmark experiments, the physical models implemented in the numerical codes cannot be validated properly. Therefore, the scope of this project was to investigate the physics involved during transient phenomena, such as flashing and water hammer, due to the fast closure or opening of valves designed for cryogenic fluids. Funding: ESA GSPT. Partners: Safran Aero Boosters, Open Engineering, ET Energy Technology.
- [MARITIME / SHIPPING] CHyPS (Clean Hydrogen Propulsion for Ships) focuses on development of high fidelity 3D simulation models, needed for the engineering of clean propulsion for ships, with fuels such as H₂, e-methane or methanol. The projects aims at developing models for the storage of cryogenic fuels in a tank, looking at phenomena such as sloshing and boil-off, and models for the combustion of these fuels in an Internal Combustion Engine (ICE) for ships. Flemish regional funding via VLAIO and the Blue Cluster.
- [AVIATION] HYPSTER (HYdrogen Propulsion System: Thermique Et Régulation): aims at designing, manufacturing and demonstrating 2 key components in the fuel delivery system for future hydrogen powered aircraft, namely the cryogenic valves and the heat exchanger. The project team, lead by Safran Aero Booster, will provide these components to Airbus, for integration in the ZEROe A380 flying testbed. In this project team, VKI is in charge of the design of the heat exchanger and of the testing in subcritical and supercritical regimes. The heat exchanger is used to bring the cryogenic LH2 to the right gaseous conditions. VKI also does the 1D modeling of the fuel delivery system. Walloon regional funding via the Skywin cluster.
- [AVIATION] fLHYing tank: this project, lead by Pipistrel Vertical Solutions from Slovenia, aims at
 developing a liquid hydrogen (LH2) load bearing fuel tank, which can fit in the tail cone of smaller
 aircraft. It will be demonstrated in flight with a Pipistrel NUUVA large cargo UAV. VKI will develop
 the digital twin for the thermo-fluid dynamics of the LH2 tank, will design the instrumentation for
 the performance characterisation and will perform the experimental validation. Funding by the
 European Clean Aviation R&D programme.



Component Development System Modeling

Use of H₂ for Mobility







Flying testbeds on which components for hydrogen powered aviation, designed by VKI, will be demonstrated: the Airbus ZEROe A380 flying testbed and the Pipistrel NUUVA large cargo UAV.

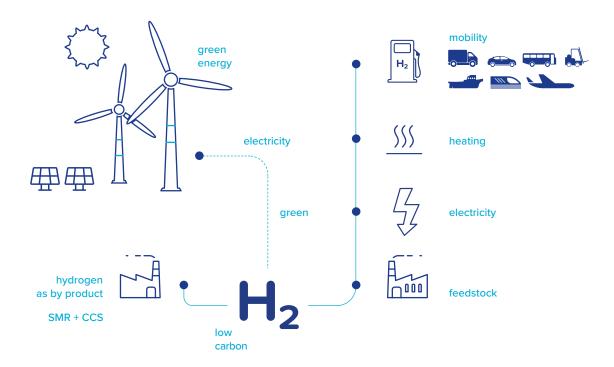
Main relevant publications

 Two-Phase Flows Investigations in Liquid Propulsion Systems: "TRL Booster" research at the von Karman Institute, by Jean-Baptiste Gouriet, Cryogenic Heat & Mass Transfer symposium, TU Twente (Enschede), november 2019

- Research manager Jean-Baptiste Gouriet (<u>jeanbaptiste.gouriet@vki.ac.be</u>)
- Business development manager Peter Simkens (<u>peter.simkens@vki.ac.be</u>)



3.3. Hydrogen general topics







3.3.1. KU Leuven

Energy Systems Integration and Modelling (ESIM)

KU Leuven, Faculty of Engineering Science, Department of Mechanical Engineering

General expertise of the research group

Research focus and expertise is on quantitative tools, supporting an efficient operation of, and transition towards, a low-carbon energy system (mathematical modelling of energy systems). A major strength of the group is its interdisciplinary focus (techno-economic models considering multiple energy vectors, link to energy markets and policies). Modelling focus is on unit commitment models, generation expansion planning models, equilibrium models and agent-based models. Applications relate to flexibility through energy systems integration, market design, renewables support mechanisms and emission trading.

Specific hydrogen - related expertise & research topics

- Integrated energy systems modelling
 - Including natural gas networks
 - Long term (seasonal) storage modelling
 - Interactions between electricity, heat, gas H₂ and CO₂
- Policy impact assessment
 - Interaction with, e.g., emission trading systems (EU ETS)

Available equipment/tools

- Optimization models for the operation of energy systems (e.g., using Mixed Integer Linear Programming MILP)
- Optimization models for energy planning and scenario analyses
- Equilibrium models describing the interactions of various (market) actors in the liberalized electric power sector (e.g., consumers, generators, system operators)
- Agent-based models to describe the electricity system as a complex adaptive system. This modelling
 approach captures the complex interactions among the physical infrastructure, the actors'
 behaviour, and the institutions that govern those behaviours in an energy system
- All of the above can be combined with various policy instruments

International collaborations

Hydrogen workgroup in EERA Joint Program on Energy Systems Integration

Participating in FL/B/EU funded projects with H₂ related research

- 2024-2028 AMIGDALA Alliance for Modelling Industries towards the Green Deal's objectives And circuLArity – Horizon Europe
- 2020-2025 PROCURA Power to X and Carbon Capture & Utilization Roadmap for Belgium Energy Transition Fund Belgium







Main relevant publications

KU LEUVEN

- Verbist, F., Meus, J., Moncada, J.A., Valkering, P., Delarue, E. (2024). Implications of the EU ETS on the level-playing field between carbon capture storage & utilisation. International Journal Of Greenhouse Gas Control, 136. doi:10.1016/j.ijggc.2024.104165
- Namazifard, N., Vingerhoets, P., Delarue, E. (2024). Long-term cost optimization of a national lowcarbon hydrogen infrastructure for industrial decarbonization. International Journal Of Hydrogen Energy, 64, 583-598. doi:10.1016/j.ijhydene.2024.02.324
- Gonzato, S., Bruninx, K., Delarue, E. (2021). Long term storage in generation expansion planning models with a reduced temporal scope. Applied Energy, 298, Art.No. 117168, 1-15. doi:10.1016/j. apenergy.2021.117168
- Mertens, T., Bruninx, K., Duerinck, J., Delarue, E. (2021). Capacity credit of storage in long-term planning models and capacity markets. Electric Power Systems Research, 194, Art.No. 107070

- Kenneth Bruninx (kenneth.bruninx@kuleuven.be)
- Erik Delarue (erik.delarue@kuleuven.be)
- William D'haeseleer (william.dhaeseleer@kuleuven.be)



System modelling



Interfacial Engineering Research (iR)

KU Leuven – Bruges, Faculty of Engineering Science, Department of Materials Engineering

General expertise of the research group

The New Materials / iR group at KU Leuven – Brugge concentrates on the experimental development, using chemical synthesis methods and interface modification techniques, and characterization of novel functional (polymer) materials for sustainable solutions in various applications.

Specific hydrogen - related expertise & research topics

- Material surface area characterization by gas adsorption techniques
- Underground hydrogen gas storage in rock salt caverns
- Polymer membrane development
- Characterization of degradation of polymer membranes
- Electrochemistry

Available equipment/tools

- Electrochemical equipment (Metrohm Autolab potentiostat/galvanostat with impedance station and NOVA2 software)
- Electrosynthesis equipment (ElectraSyn)
- Automated film applicator
- Spin coater, dip coater, spray coater
- · Fumehoods and chemical synthesis equipment, autoclaves, ovens, centrifuge, etc
- Ultrasonic probe
- Tube furnace
- Ion chromatograph
- Viscometer
- · Pull-off adhesion tester

Participating in FL/B/EU funded projects with H₂ related research

 HYDE: Hydrogen technology for Defence applications, DEFRA Belspo. Partners: KU Leuven, VIVES Zuid, VIVES Noord, Solenco Power



Materials & components development



Main relevant publications

- Madhav, D., Shao, C., Mus, J., Buysschaert, F., Vandeginste, V. (2023). The effect of salty environments on the degradation behaviour and mechanical properties of Nafion membranes. Energies, 16(5), Art.No. 2256. doi:10.3390/en16052256
- Vandeginste, V., Ji, Y., Buysschaert, F., Anoyatis, G. (2023). Mineralogy, microstructures and geomechanics of rock salt for underground gas storage. Deep Underground Science and Engineering, 2 (2), 129-147. doi.org/10.1002/dug2.12039
- Xie, W., Wang, M., Vandeginste, V., Chen, S., Yu, Z., Wang, J., Wang, H., Gan, H. (2022). Adsorption behavior and mechanism of CO₂ in the Longmaxi shale gas reservoir. RSC ADVANCES, 12 (40), 25947-25954.
- Martin-Clave, C., Ougier-Simonin, A., Vandeginste, V. (2021). Impact of second phase content on rock salt rheological behaviour under cyclic mechanical conditions. Rock Mechanics and Rock Engineering, 54, 5245-5267.

Contact persons

Prof. Veerle Vandeginste (<u>veerle.vandeginste@kuleuven.be</u>)



Materials & components development



3.3.2. OCAS

Department of Applications and solutions

OCAS, R&D Centre

General expertise of the research group

Applied research and development of materials. Supported by a state-of-the-art lab, OCAS can perform decent metallurgical investigations and testing of materials in different environments with the ability to closely represent the operational circumstances. Solving questions of customers about material compatibility considering degradation, design life and safety aspects. Ranking of candidate materials, material selection and risk mitigation.

Specific hydrogen - related expertise & research topics

- Applied R&D on the interaction between hydrogen and materials
- Thorough knowledge and understanding of the metallurgical phenomena
- Testing, standard and non-standard test equipment, for determination and understanding of the effect of hydrogen on the material performance under specific conditions and w/o loading: unloaded, static or dynamic loading
- Determination of the behaviour of a material in an environment with presence of hydrogen at certain operating conditions
- Modelling of interaction between hydrogen and materials by empirical testing and numerical simulations. Models to optimise production processes, maintenance schedules and prediction of material/component lifetime in a hydrogen environment
- OCAS differentiates by focussing on large scale testing, test setups that cannot be performed in normal-sized labs, considering real operating conditions and safety aspects of the bigger industrial installations and infrastructure
- Building of specific test equipment for testing under high pressure (including hydrogen, pure or blend) exposing materials and/or components. This service comprises the design and assembly of tailor-made test rigs for multipurpose i.e. focussing on a specific component of which the fitnessforpurpose of the design is assessed with respect to a certain application, operating conditions and safety aspects
- Assessment of pass / fail criteria on re-purposing assets such as pipelines and pressure vessels towards using hydrogen as transport or storage medium
- Acceptance testing on fit for use aspects of seals (threaded metal-to-metal and other) in combination with different mixtures of hydrogen towards transmission, storage and end-use applications (e.g. downhole, pipeline, pressure vessel, gas bottle, connections, ...)



Materials & components development



Available equipment/tools

All analytical equipment for measuring hydrogen content, in and through materials. OCAS is accredited for a series of analyses and qualified to work with deuterium.

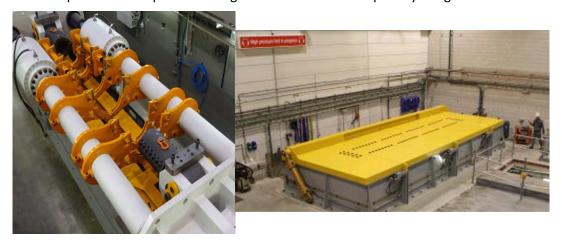
- See equipment as specified in section Metallurgy
- Specialised software and modelling tools
- Upscale fatigue bench for large scale components or structures
- Heavy testing bench with possibilities for external and internal loading (installed in pressure pit)
- New to build, tailor-made test rigs for customer dedicated

International collaborations

OCAS mainly works on a bilateral agreement between national or international customers. Different extends are possible, from a single measurement up to a dedicated research program. OCAS aims to accelerate the R&D at the customer, giving support by sharing competences and specific equipment.

Participating in FL/B/EU funded projects with H₂ related research

- Open to collaborate in funded projects
- HYWAY Multiscale Characterisation and Simulation for Hydrogen Embrittlement Assessment: Development of an Open Knowledge Platform to Foster Capability Integration - HORIZON-CL4-2023



Main relevant publications

See an excerpt of OCAS publications in section Metallurgy

- Steven Keyzer (steven.keyzer@ocas.technology)
- Philippe Thibaux (philippe.thibaux@ocas.technology)



Materials & components development



Department of Metallurgy

OCAS, R&D Centre

General expertise of the research group

Applied research and development of materials. Supported by a state-of-the-art lab, OCAS can perform decent metallurgical investigations and testing of materials in different environments with the ability to closely represent the operational circumstances. Solving questions of customers about material compatibility considering degradation, design life and safety aspects. Ranking of candidate materials, material selection and risk mitigation.

Specific hydrogen - related expertise & research topics

- Applied R&D on the interaction between hydrogen and materials
- Thorough knowledge and understanding of the metallurgical phenomena
- Testing, standard and non-standard test equipment, for determination and understanding of the effect of hydrogen on the material performance under specific conditions and w/o loading: unloaded, static or dynamic loading
- Determination of the behaviour of a material in an environment with presence of hydrogen at certain operating conditions
- Modelling of interaction between hydrogen and materials by empirical testing and numerical
- Simulations. Models to optimise production processes, maintenance schedules and prediction of material/component lifetime in a hydrogen environment
- Failure analysis. During such an analysis, investigation tries to clarify material damage, component failure due to hydrogen-related degradation mechanisms. Expertise on damage triggers such as hydrogen embrittlement and hydrogen induced cracking
- Material compatibility concerns. Advise on material selection, material degradation, corrosion and coating related to hydrogen. This advice may result in a dedicated material program that demonstrates material compatibility with respect to a certain goal. Notified bodies can be involved in such examinations
- Hydrogen testing in sour environment (OCAS dedicated H2S lab, NACE testing, qualification)
- National and international exchange on R&D, organisation of a series of international conferences Steelyhydrogen – 5th edition to be defined





Available equipment/tools

- All analytical equipment for measuring hydrogen content, in and through materials. OCAS is accredited for a series of analyses and qualified to work with deuterium.
 - Equipment for charging: electrolytical or autoclave
 - Equipment for H determination (hot and melt extraction)
 - Equipment for H diffusion and permeation
 - Thermal desorption
 - Equipment for Microstructural investigation
- Mechanical testing:
 - Constant load
 - Slow and high strain rate testing
 - Disc rupture testing
 - Fracture mechanics
 - Fatigue testing
- Equipment for NACE testing (H2S)

International collaborations

OCAS mainly works on a bilateral agreement between national or international customers. Different extends are possible, from a single measurement up to a dedicated research program. OCAS aims to accelerate the R&D at the customer, giving support by sharing competences and specific equipment.

Participating in FL/B/EU funded projects with H₂ related research

- Open to collaborate in funded projects
- FORGE Development of novel coating materials for a sustainable future (Evaluation of hydrogen pick up and hydrogen embrittlement) H2020-NMBP-ST-IND-2018-2020.
- HYDRO-REAL Study the sensitivity of ultra-high strength cold rolled steels to hydrogen embrittlement - RFCS-02-2019
- INiTiAl Advanced implementation of novel corrosion resistant high strength maraging steels with improved process robustness via tuned intermetallic nano-precipitation - RFCS-02-2017
- Charge & Load Hydrogen embrittlement and delayed fracture of advanced multiphase highstrength steels - RFSR-CT-2006-00025
- HYDRAMICROS Hydrogen sensitivity of different advanced high strength microstructures RFSRCT
 2010-00020
- SUPERHIGH In-use properties of Super High strength steels generated by a range of metallurgical strategies RFCS-PR-12161
- NOHENTRY Reuse of existing pipeline systems for H₂ transport via surface functionalisations inhibiting Hydrogen entry - ETF 2021
- SAFEH2PIPE Guidelines for material selection and qualification for safe transportation of H₂-NG mixtures in EU pipelines - RFCS 2022
- HYWAY Multiscale Characterisation and Simulation for Hydrogen Embrittlement Assessment: Development of an Open Knowledge Platform to Foster Capability Integration HORIZON-CL4-2023
- PILGRHYM Pre-normative research on integrity assessment protocols of gas pipes repurposed to Hydrogen and mitigation guidelines - HORIZON-JTI-CLEANH2-2023
- FEATHER Steel For nExt generATion H₂ cylinders RFCS 2022

Materials & components development

General





Main relevant publications

- Investigation of hydrogen trapping in retained austenite via deuterium charging at high temperature.
 L Moli-Sanchez, Z Zermout, L Duprez. Proceedings 3rd International Conference on Metals and Hydrogen, May 2018, Ghent, Belgium
- Hydrogen embrittlement of 4 martensitic steels with strength levels above 1000 MPa. L. Moli-Sanchez, Z. Zermout, L. Duprez, L. Malet. (Proceedings SteelyHydrogen 2014)
- Effect of in-situ hydrogen charging on the mechanical properties of advanced high strength steels. T.
 Depover, D. Pérez Escobar, E. Wallaert, Z. Zermout. International Journal of Hydrogen Energy. Vol. 39 (2014) pp. 4647–4656
- Hydrogen embrittlement in various steels with strength levels above 1000 MPa. L Duprez, M Arafin,
 F Van den Abeele, N Bernier. Joint HYDROGENIUS and I2CNER International Workshop on Hydrogen Materials Interactions 2012 Kyushu University
- Combined thermal desorption spectroscopy, differential scanning calorimetry, scanning electron microscopy and X-ray diffraction study of hydrogen trapping in cold deformed TRIP steel. D. Perez Escobar, T. Depover, L Duprez, K. Verbeken and M. Verhaege. (2012) ACTA MATERIALIA. 60(6-7). p.2593-2605
- Thermal desorption spectroscopy study of the interaction between hydrogen and different microstructural constituents in lab cast Fe-C alloys. D. Pérez Escobar, T. Depover, E. Wallaert, L. Duprez, M. Verhaege, K. Verbeken. Corrosion Science. Vol. 65 (2012) pp. 199-208
- Evaluation of hydrogen trapping in high strength steels by thermal desorption spectroscopy. D. Perez Escobar, K Verbeken, L Duprez, M Verhaege (2012) MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING. 551. p.50-58
- Internal and surface damage of multiphase steels and pure iron after electrochemical hydrogen charging. D Perez Escobar, C Minambres, L Duprez, K Verbeken, M Verhaege (2011) CORROSION SCIENCE. 53(10). p.3166-3176
- Selecting hydrogen embrittlement resistant materials by means of the disc rupture test. Elke Leunis,
 Lode Duprez. 18th World Hydrogen Energy Conference 2010, Essen / Germany

- Steven Keyzer (<u>steven.keyzer@ocas.technology</u>)
- Philippe Thibaux (philippe.thibaux@ocas.technology)





Department of surface engineering

OCAS, R&D Centre

General expertise of the research group

At the department of surface engineering, OCAS focusses on applied research and development concerning surface preparation, coating processes, morphologies, and other surface aspects such as corrosion. Supported by a state-of-the-art lab, OCAS can perform a full characterisation of surfaces besides several tools for testing surface properties and performing surface exposure and accelerated degradation tests. On the semi-industrial plating line (electrodeposition), OCAS can make samples for customers and assist in projects looking to, e.g.: alternative electrolytes, optimisation of process parameters or improvement of coating morphology including all related analyses thereof.

Specific hydrogen - related expertise & research topics

- Applied R&D on the interaction between hydrogen and materials
- Thorough knowledge and understanding of the metallurgical phenomena
- Modelling of interaction at the interface of hydrogen and substrate material: diffusion, adsorption kinetics, saturation
- Numerical simulations for prediction of lifetime in a hydrogen environment
- Coatings for H-barriers
- Corrosion testing in hydrogen related circumstances
- Hydrogen ingress during electrochemical coating processes (Process simulations on electroplating pilot line: https://vimeo.com/458463355)
- Hydrogen effusion from substrate materials during degassing
- Enamelling and hydrogen-related issues (fish scale)

Available equipment/tools

All analytical equipment for measuring hydrogen content, in and through materials. OCAS is accredited for this analysis and qualified to work with deuterium.

- See equipment as specified in section Metallurgy
- State of the art lab for surface characterisation
- Techniques for appearance, roughness, hardness, 2D/3D-topography, ...

International collaborations

OCAS mainly works on a bilateral agreement between national or international customers. Different extends are possible, from a single measurement up to a dedicated research program. OCAS aims to accelerate the R&D at the customer, giving support by sharing competences and specific equipment.



Materials & components development



Participating in FL/B/EU funded projects with H₂ related research

- Open to collaborate in funded projects
- FORGE Development of novel coating materials for a sustainable future (Evaluation of hydrogen pick up and hydrogen embrittlement) - H2020-NMBP-ST-IND-2018-2020
- NOHENTRY Reuse of existing pipeline systems for H₂ transport via surface functionalisations inhibiting Hydrogen entry - ETF 2021

Main relevant publications

See an excerpt of OCAS publications in section Metallurgy

- Steven Keyzer (<u>steven.keyzer@ocas.technology</u>)
- Philippe Thibaux (philippe.thibaux@ocas.technology)



Process development



3.3.3. UGent

Center for Microbial Ecology and Technology (CMET)

Ghent University, Faculty of Biosciences Engineering

General expertise of the research group

The Center for Microbial Ecology and Technology (CMET) is a part of the Faculty of Bioscience Engineering at Ghent University. CMET is specialized in the study and application of mixed microbial cultures or communities and the development of technology in a context of wastewater treatment, bioproduction and others. CMET researchers focus on the one hand on the optimal management of microbial resources, on the other hand (supporting) technologies such as (bio)electrochemical systems and monitoring systems are under development.

Specific hydrogen - related expertise & research topics

- Applied Microbial Ecology
- Microbial Monitoring
- Microbial CO₂ conversions
- H₂ upgrading
- Hydrogen driven microbiological processes: Exploring possibilities of the microbial hydrogen
 metabolism to produce microbial protein (feed and food for the future), to bioremediate pollutants
 in (waste)water, to remove nutrients for the enhancement of drinking water biostability, ...

Available equipment/tools

- (Online) microbial analysis, based on single cell and molecular principles
- Bacterial isolation, cultivation, characterisation and ecosystem assembly
- (Bio)Reactor systems
- Pilot scale systems
- Biomass synthesis
- Standard chemical analysis (GC, IC, HPLC, ...)

Participating in FL/B/EU funded projects with H₂ related research

- CO2Perate
- Baekelandt project
- FWO-SB and HEC scholarship on high-rate hydrogen-driven bioprocess for CO₂ bioconversions
- H2020 project Electra
- FWO-SB & SBO project Biostable on drinking water stability
- SBO project MicroDetox on micropollutant removal
- See website: research.ugent.be







Main relevant publications

IIIIIII

GHENT UNIVERSITY

- See website: biblio.ugent.be
- De Vrieze J, Verbeeck K, Pikaar I, Boere J, Van Wijk A, Rabaey K, et al. The hydrogen gas bio-based economy and the production of renewable building block chemicals, food and energy. NEW BIOTECHNOLOGY. 2020;55:12-8
- Barbosa RG, van Veelen HPJ, Pinheiro V, Sleutels T, Verstraete W, Boon N. 2021. Enrichment of Hydrogen-Oxidizing Bacteria from High-Temperature and High-Salinity Environments. Applied and Environmental Microbiology 87. (Impact factor: 4,016; Quantile: Q1)
- Prévoteau A, Carvajal-Arroyo J, Ganigué R, Rabaey K (2020) Microbial electrosynthesis from CO₂: forever a promise? CURRENT OPINION IN BIOTECHNOLOGY, 62, 48-57. IF 2019: 8.288
- Hu XN, Kerckhof FM, Ghesquiere J, Bernaerts K, Boeckx P, Clauwaert P, Boon N. 2020. Microbial Protein out of Thin Air: Fixation of Nitrogen Gas by an Autotrophic Hydrogen-Oxidizing Bacterial Enrichment. Environmental Science & Technology 54:3609-3617. (Impact factor: 7,149; Quantile: Q1)
- Barbosa RG, Sleutels T, Verstraete W, Boon N. 2020. Hydrogen oxidizing bacteria are capable of removing orthophosphate to ultra-low concentrations in a fed batch reactor configuration. Bioresource Technology 311.(Impact factor: 6,669; Quantile: Q1)
- Ehsani E, Dumolin C, Arends JBA, Kerckhof FM, Hu XN, Vandamme P, Boon N. 2019. Enriched hydrogen-oxidizing microbiomes show a high diversity of co-existing hydrogen-oxidizing bacteria. Applied Microbiology and Biotechnology 103:8241-8253.(Impact factor: 3,67; Quantile: Q2)
- Ramio-Pujol S, Ganigue R, Baneras LI, Colprim J (2018) Effect of ethanol and butanol on autotrophic growth of model homoacetogens. FEMS MICROBIOLOGY LETTERS, 365 (10), fny084. IF 2017: 1.735
- Puig S, Ganigué R, Batlle-Vilanova P, Balaguer MD, Bañeras Ll, Colprim J (2017) Tracking biohydrogen-mediated production of commodity chemicals from carbon dioxide and renewable electricity. BIORESOURCE TECHNOLOGY. 228, 201 - 209. IF 2017: 5.807
- Matassa S, Verstraete W, Pikaar I, Boon N. 2016. Autotrophic nitrogen assimilation and carbon capture for microbial protein production by a novel enrichment of hydrogen-oxidizing bacteria. Water Research 101:137-146.(Impact factor: 5,528; Quantile: Q1)
- Matassa S, Boon N, Verstraete W. 2015. Resource recovery from used water: The manufacturing abilities of hydrogen-oxidizing bacteria. Water Research 68:467-478.(Impact factor: 5,323; Quantile: Q1)
- Hosseinkhani B, Hennebel T, Van Nevel S, Verschuere S, Yakimov MM, Cappello S, Blaghen M, Boon N. 2014. Biogenic Nanopalladium Based Remediation of Chlorinated Hydrocarbons in Marine Environments. Environmental Science & Technology 48:550-557. (Impact factor: 5,481; Quantile: Q1)

- Prof. Nico Boon (Nico.Boon@ugent.be)
- Prof. Ramon Ganigué (Ramon.Ganigue@ugent.be)





Centre for Sustainable Development (CDO)

Ghent University, Faculty of Political & Social Sciences

General expertise of the research group

GIIS is conducting research into six distinctive research areas in two overarching domains: security & foreign policy, and the development of the multilateral system.

At CDO, scientific researchers from different disciplines (political scientists, economists, educational scientists, (bio)engineers, sociologists, environmentalists, physicists, urban planners, etc.) work together to conduct research on sustainable development. Taking sustainable development in its multiple dimensions (economic, social, physical-ecological, institutional and ethical) as a guiding - though not determining - perspective, interdisciplinarity and transdisciplinarity are key aspects of research conducted at CDO.

Specific hydrogen - related expertise & research topics

- Geopolitics and international governance of H₂
- Political analysis, socio-technical system innovation, governance of transitions such as the transition of the energy-intensive industry

International collaborations

International Renewable Energy Agency (IRENA) – geopolitics of the hydrogen economy

The politics of the circular economy





Sustainable Cities



Science, Technology and Politics



Transitions and Future Studies





Materials & components development



Main relevant publications

- See website: biblio.ugent.be
- Dejonghe, M., Van de Graaf, T., & Belmans, R. (2023). From natural gas to hydrogen: Navigating import risks and dependencies in Northwest Europe. Energy Research & Social Science, 106, 103301
- Dejonghe, M. (2023). Risky Business? Evaluating Hydrogen Partnerships Established by Germany, The Netherlands, and Belgium. Sustainability, 15(24), 16876
- Van de Graaf, T. (2022). Hydrogen's Decade. Finance and Development, 59(4), 21-23
- IRENA (2022). Geopolitics of the Energy Transformation: The Hydrogen Factor. Abu Dhabi: IRENA. (Lead author: T. Van de Graaf)
- Van de Graaf, T. (2021). "Clean Hydrogen: Building Block of a New Geopolitical Landscape," Energy and Geostrategy, Spanish Institute for Strategic Studies
- Van de Graaf, T. (2021). "The next prize: geopolitical stakes in the clean hydrogen race," In Oxford Energy Forum (No. 126, pp. 30-34)
- Van de Graaf, T., Overland, I., Scholten, D., & Westphal, K. (2020). The new oil? The geopolitics and international governance of hydrogen. Energy Research & Social Science, 70, 101667.)

- Prof. Thijs Van de Graaf (<u>Thijs.VandeGraaf@UGent.be</u>)
- Prof. Erik Paredis (Erik.Paredis@UGent.be)
- PhD. Marie Dejonghe (TMarie.Dejonghe@UGent.be)







Centre of environmental & energy law

Ghent University, Faculty of Law Criminology, Department of European, Public and International Law

General expertise of the research group

Energy Law is the part of the law that regulates the human acting dealing with production/exploitation, transports an use of energy. The contemporary Energy Law is very recent. Especially the European liberalisation and Climate change have led to a juridification of the traditional technical approach of "the energy business" and to an appearance of Energy law. Energy Law is extremely technical and complex, fast evoluating Law Branch.

The Centre for Environmental and Energy Law has built a specific expert's centre regarding Energy Law. This unit works within Ghent University together to bound research, valorization and cooperation with other research groups of Energy Law.

Specific hydrogen - related expertise & research topics

- The division of competence in the field of hydrogen and green molecules
- Certification of hydrogen and green molecules

Participating in FL/B/EU funded projects with H₂ related research

See website: research.ugent.be

Main relevant publications

- See website: biblio.ugent.be
- Vandendriessche F, Claeys P. "Target setting" in het Europese energie- en klimaatbeleid : het "Clean Energy Package." TIJDSCHRIFT VOOR MILIEURECHT. 2019;(3):262-83.
- Maes T, Van Eetvelde G, De Ras E, Block C, Pisman A, Verhofstede B, et al. Energy management on industrial parks in Flanders. RENEWABLE & SUSTAINABLE ENERGY REVIEWS. 2011;15(4):1988–2005.

Contact persons

Prof. Dr. Frederik Vandendriessche (<u>Frederik.Vandendriessche@UGent.be</u>)



Soete Laboratory

Ghent University, Faculty of Engineering and Architecture, Department of electromechanical, Systems and Metal Engineering

General expertise of the research group

At Soete Laboratory, we are pushing the boundaries in fracture mechanics and tribology. As researchers we are active in both experimental and numerical research on fatigue, fracture, friction, wear, reliability and durability of machine parts and mechanical constructions.

Within Soete Laboratory, the fatigue & fracture mechanics research group is headed by Prof. Wim De Waele and Prof. Stijn Hertelé. The activities of the group can be divided into three topics: Fatigue lifetime analysis, joining and additive manufacturing (Prof. De Waele) and quasi-static fracture and damage mechanics (Prof. Hertelé).

Specific hydrogen - related expertise & research topics

- Effects of hydrogen on mechanical properties of steel (embrittlement), mostly in a transport/storage context (pipelines)
- Effect of hydrogen on accelerated rolling contact fatigue failure of roller bearings

Available equipment/tools

- Universal test rigs for small- and large-scale mechanical testing (up to 8 MN)
- In-house test procedures for advanced mechanical testing (e.g. low-constraint fracture toughness testing)
- Development of material models involving hydrogen diffusion, hydrogen assisted degradation and resulting material damage

Participating in FL/B/EU funded projects with H₂ related research

- FWO research project on hydrogen embrittlement
- SIM SBO MaSiWEC
- See website: research.ugent.be



Materials & components development





Main relevant publications

- See website: biblio.ugent.be
- Depover T, Hertelé S, Verbeken K. The effect of hydrostatic stress on the hydrogen induced mechanical degradation of dual phase steel: a combined experimental and numerical approach. ENGINEERING FRACTURE MECHANICS. 2019;221.

Contact persons

Prof. Stijn Hertelé (Stijn.Hertelé@ugent.be)



Materials & components development

General



Sustainable Materials Science (SMS)

Ghent University, Faculty of Engineering and Architecture, Department of Materials, Textiles and Chemical Engineering

General expertise of the research group

The research group Sustainable Materials Science is part of the Department of Materials, Textiles and Chemical Engineering (MaTCh) and has a large amount of experimental and characterization facilities at its disposal. Experimental work is complemented with simulations and modelling efforts. Main research expertise is the study of the interaction of metallic materials with hydrogen and how hydrogen impacts the performance of these metals. Apart the work on hydrogen induced degradation, the groups also study the degradation of metals resulting from interaction with their environment (corrosion processes) and high-temperature metallurgical processes (pyrometallurgy).

Specific hydrogen - related expertise & research topics

The research group has internationally recognized expertise in generating high impact research based on developing experimental methodologies related to hydrogen embrittlement which are going beyond the state-of-the-art. The strategy is to design innovative experimental set-ups e.g. by combining different sets of equipment, while keeping in mind the very specific nature of hydrogen/microstructure interaction such as the low hydrogen solubility and high hydrogen diffusivity in BCC-steel, whereas hydrogen has a high solubility and low diffusivity in FCC-alloys. For the moment 10 PhD students and two postdocs are working on hydrogen related research topics.

Specific research topics are focusing on the interaction of hydrogen with amongst others wire steels, pipeline steels, bearings, additive manufactured alloys, titanium, tungsten, duplex stainless steels, austenitic stainless steel, automotive steel grades (first, second and third generation advanced high strength steels). Both fundamental and application-oriented aspects are highlighted.

The group has a vast amount of knowledge on high-end material characterization techniques, alloy development and offers an in-depth understanding and expertise on all metallurgical phenomena.



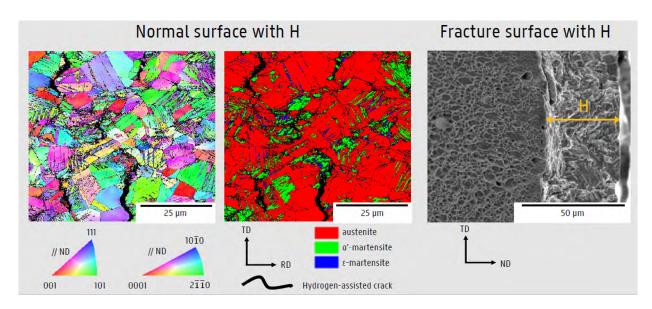
Available equipment/tools

- Thermal desorption spectroscopy
- Various equipment and set-ups for electrochemical hydrogen charging and gaseous hydrogen charging via autoclaves
- Electrochemical hydrogen permeation, incl. applying mechanical load during permeation test demonstrating effect of mechanical load on hydrogen diffusion coefficient
- Diffusion based models
- Hot and melt extraction to determine hydrogen content of metal
- Various set-ups for in-situ mechanical tests (performing mechanical test while material remains in contact with hydrogen environment). Tests include slow strain rate tensile tests, constant load tests, bending tests, single edge notch tensile tests
- Advanced microstructural characterization tools (e.g. for crack initiation and propagation, phase transformation, role of hydrogen on deformation mechanism, identification of hydrides) such as scanning electron microscopy, transmission electron microscopy, electron backscatter diffraction,
- Micro-tensile device inside scanning electron microscopy

International collaborations

The group is involved in multiple international collaborations with academic partners and research institutes. Demonstrated examples are found in joint work with among others colleagues from NTNU (Norway), MCL Leoben (Austria), TU Graz (Austria), University of Queensland (Australia), Ecole des Mines Saint-Etienne (France), Paristech (France), TUEindhoven (The Netherlands), RWTH Aachen (Germany), Max-Planck Institute fur Eisenforschung (Germany). Curtin University (Australia), Kyushu University (Japan),...

Multiple collaborations are ongoing with international industrial partners. Due to NDA's, names can however not be revealed.





Materials & components development

General



Participating in FL/B/EU funded projects with H₂ related research

For the moment, 10 PhD students and 2 postdocs are working on hydrogen related research. Topics include the interaction of hydrogen with amongst others pipeline steels, bearing steels, additive manufactured alloys, titanium, wire steels, duplex stainless steels, austenitic stainless steel, automotive steel grades (first, second and third generation advanced high strength steels). This work is funded by a wide variety of funding schemes including FWO, SIM, UGent, Vlaio and EU funding

See also website: research.ugent.be

Main relevant publications

- Via the following links for more info as the research group as over 100 relevant papers
 - Https://research.ugent.be/web/person/kim-verbeken-1/publications?1
 - Https://www.ugent.be/ea/match/sms/en
- The potential of the internal friction technique to evaluate the role of vacancies and dislocations in the hydrogen embrittlement of steels, L Vandewalle, M Konstantinovic, T. Depover, K. Verbeken, Steel Research International, 2021, 2100037
- EBSD characterization of hydrogen induced blisters and internal cracks in TRIP-assisted steel, A
 Laureys, M. Pinson, T. Depover, R. Petrov, K. Verbeken, Materials Characterization, 159, 2020,
 110029
- Critical assessment of the evaluation of thermal desorption spectroscopy data for duplex stainless steels: a combined experimental and numerical approach, L Claeys, V Cnockaert, T. Depover, I. De Graeve, K. Verbeken, Acta Materialia, 186, 2020, 190-198
- Microstructural based hydrogen diffusion and trapping models applied to Fe-C-X alloys, A Drexler, T.
 Depover, S Leitner, K. Verbeken, W Ecker, Journal of alloys and compounds, 826, 2020, 154057
- Qualification of the in-situ bending technique towards the evaluation of the hydrogen induced fracture mechanism of martensitic Fe-C steels, M Pinson, T. Depover, H. Springer, K. Verbeken, Materials Science and Engineering A, 792, 2020, 139754
- The detrimental effect of hydrogen at dislocations on the hydrogen embrittlement susceptibility of Fe-C-X alloys: an experimental proof of the HELP mechanism, T. Depover, K. Verbeken, International Journal of Hydrogen Energy, 43, 2018, 3050-3061
- Understanding the interaction between a steel microstructure and hydrogen, T. Depover, A Laureys,
 D. Perez Escobar, E. Vanden Eeckhout, E Wallaert, K. Verbeken, Materials, 11, 2018; 698
- Effect of deformation and charging conditions on crack and blister formation during electrochemical hydrogen charging, A Laureys, E Van den Eeckhout, R Petrov, K Verbeken, Acta Materialia, 127, 2017, 192-202
- Fractographic analysis of the role of hydrogen diffusion on the hydrogen embrittlement susceptibility of DP steel, T. Depover, E. Wallaert; K. Verbeken, Materials Science and Engineering A, 649, 2016, 201-208
- The effect of TiC on the hydrogen induced ductility loss and trapping behavior of Fe-C-Ti alloys, T. Depover; K. Verbeken, Corrosion Science, 112, 2016, 308-326,

- Prof. dr. ir. Kim Verbeken (<u>Kim.Verbeken@ugent.be</u>)
- Prof. dr. ir. Tom Depover (<u>Tom.Depover@ugent.be</u>)



Sustainable Systems Engineering (STEN)

Ghent University, Faculty of Bioscience Engineering, Department of Green Chemistry and Technology

General expertise of the research group

The Research Group Sustainable Systems Engineering (STEN) aims at designing and evaluating systems in a sustainability context, relying on engineering principles. Products, processes, supply chains, and production and consumption patterns are studied with:

- A focus on resources, i.e. resource footprint and resource efficiency
- A lifecycle thinking approach, e.g. operationalized through MFA and LCA
- Thermodynamic principles, relying on the second law: exergy and exergetic life cycle analysis

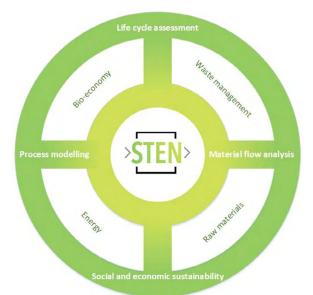
The research is in close collaboration with national and international universities, research centres, policy makers and industry in areas of the following nature: chemical, pharma, primary raw materials, waste-as-aresource, agro-bio-food ...

Specific hydrogen - related expertise & research topics

- LCA of e-fuels
- Resource footprint
- Resource efficiency

Participating in FL/B/EU funded projects with H₂ related research

- S2Chemicals (NL)
- **CCU Hub**
- See website: research.ugent.be





System modelling



Main relevant publications

- See website: biblio.ugent.be
- Huysman S, Sala S, Mancini L, Ardente F, Freitas de Alvarenga R, De Meester S, et al. Toward a systematized framework for resource efficiency indicators. RESOURCES CONSERVATION AND RECYCLING. 2015;95:68-76.
- Buchmayr A, Verhofstadt E, Van Ootegem L, Sanjuan Delmas D, Thomassen G, Dewulf J. The path to sustainable energy supply systems: proposal of an integrative sustainability assessment framework. RENEWABLE & SUSTAINABLE ENERGY REVIEWS. 2021;138.

Contact persons

• Prof. Jo Dewulf (<u>Jo.Dewulf@ugent.be</u>)







3.3.4. VITO

Techno-economic assessments and LCA analysis

VITO/EnergyVille – Unit SCT and SEB

General expertise of the research group

VITO, one of Europe's leading research centres with 1,300 employees, turns scientific insights into groundbreaking technological innovations, AI solutions, and policy advice. We do so with a single objective: to help the world thrive for at least 1,000 more years.

As a science-to-technology partner, we support companies, governments, and society in their sustainability transition. With our multidisciplinary approach and unique lab, scale-up, and testing infrastructure, we create practical technological innovations. We accelerate progress towards a regenerative economy that reinforces planetary boundaries (prioritising electrification and circularity), smart climate solutions for resilient and secure ecosystems, and a healthy living environment harmonising humans, industry, agriculture, and nature.

At VITO, we harness the power of science, engineering, digitalisation, and collaboration to implement sustainable solutions globally, enabling the continued integration of well-being and prosperity. Within several units VITO combines the competences to perform techno-economic assessments and life cycle assessments (LCA and LCC) of the hydrogen value chain. With our developed models we can execute these assessments on the micro/meso/macro scale from a specific project/technology and upscale to the energy system covering energy supply and demand sectors.

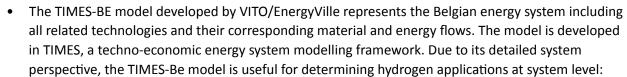
Specific hydrogen - related expertise & research topics

- Techno-economic analysis model focusing on the electrocatalytic production of hydrogen; the model is dynamic considering that changes in the technical parameters are translated into the economic metrics to give an indication of the economic feasibility under different circumstances; moreover, the model integrates hourly load variations and storage needs; the levelized cost of hydrogen (LCOH) can be derived for different scenario's
- PhD research project (BE-HyFE) focusing on the development of an investment and operational optimization modelling framework for the future hydrogen infrastructure. The model represents the hydrogen-related supply technologies and pure hydrogen gas flows with high spatial resolution (in the level industrial clusters) to deliver some insights on the cost-optimal required hydrogen backbone capacity, and how different policies can affect the industrial hydrogen production and demand



General





- TIMES will indicate the cost-optimal route in terms of technology investments. Due to the high level of industrial process detail, the model allows for hydrogen applications to be compared to its possible future competitors
- The TIMES-BE model has an integrated system approach, meaning that the interaction between sectors is considered in the analysis. The TIMES-BE model was developed under close collaboration between industry and researchers, allowing for detailed insights regarding industrial needs

Available equipment/tools

- Techno-economic assessment model
- LCC models
- LCA models
- Long-term energy system optimisation model: TIMES (co-development within IEA-ETSAP technology collaboration programme)

International collaborations

vito

- During 2023/24 a study with objective: "Making Indian Ports Infrastructurally Ready for Green Hydrogen Transition", a techno-economic feasibility analysis for green hydrogen storage and transportation has been carried out by VITO in partnership with Rocky Mountain Institute (RMI); final report will be published soon
- VITO NDC Support Center: the NDC Support Center provides support to increase capacity of
 African countries to improve their National Energy Information Systems and their energy modelling
 expertise, to prepare climate communication and to improve policymaking in the framework of
 commitments as set for the Paris Agreement; The NDC Support Center is currently active in Malawi,
 Mozambique, Uganda, and Morocco
- Horizon Europe Water-Energy-Food Nexus: WEF Energy Planning and Modelling through Integrated Assessment of Climate-Land-Energy-Water Nexus in Sub-Saharan Africa: The Cases of the Volta and Tana River Basins

Participating in FL/B/EU funded projects with H₂ related research

- Energy transition funds projects PROCURA, TRILATE and HEFAISTOS focus on the role of hydrogen production, import and infrastructure in the industrial and energy system
- The frequently referenced Paths2050 study, which went live during December 2022, will publish a new version during Q1 2025, of the cost optimal pathways for the Belgian energy system, including the role of hydrogen. Several large (industrial) organisations are meanwhile member of the Paths2050 coalition where low carbon energy scenarios are being developed and insights shared (visit www.perspective2050.energyville.be)







Main relevant publications

- Martinez, G. E., Degens, R., Espadas-Aldana, G., Costa, D., & Cardellini, G. (2024). Prospective Life Cycle Assessment of Hydrogen: A Systematic Review of Methodological Choices. Energies, 17(17),
- Www.perspective2050.energyville.be contains the most relevant TIMES related results of the past year, including a topic on hydrogen

Contact persons

✓ vito

- LCA: Giuseppe Cardellini (giuseppe.cardellini@vito.be)
- TEA (Miet.Vandael@vito.be)
- Long-term modelling (Pieter.Lodewijks@vito.be)
- Pieter.vingerhoets@energyville.be





3.3.5. VUB

Electrochemical and Surface Engineering (SURF)

Vrije Universiteit Brussel, Faculty of Engineering, Department of Materials and Chemistry

General expertise of the research group

The Electrochemical and Surface Engineering group (SURF) has a long tradition in research on electrochemical systems, and is internationally recognized for its expertise in unravelling mechanisms of electrochemical processes related with corrosion and protection, passivation of metals, localized corrosion, surface treatments and coatings. The multidisciplinary research strategy of the group is employed based on complementary macroscopic and local electrochemical methods, own developed computational software for process simulation and in-situ/ex-situ surface analytical techniques. SURF is in the unique position of having advanced research technology in-house and has own infrastructure of about 6 million euro. SURF has a large network of companies supporting the research.

Specific hydrogen - related expertise & research topics

- Study of the hydrogen-steel interactions from a SURFACE perspective: influence of surface state, oxide types, on the hydrogen-steel interaction mechanisms
- Use and development of electrochemical methods to study hydrogen-metal interactions at the H-steel surface/interface, based on voltammetry, local methods (e.g. Scanning Kelvin Probe Force Microscopy) etc
- Electrochemical modelling of the hydrogen-steel interactions (FEM modelling, in-house developments)
- Electrochemical analysis of new electrode materials for hydrogen fuel cells

Available equipment/tools

- Materials' surface analyses: XPS, FEG-AES, Tof-SIMS, FEG-SEM/EDX/WDX, Raman, Ellipsometry, FTIR, nano-IR / EIS combination, AFM
- Electrochemical experimental analyses:
 - Macroscopic: polarisation methods (OCP, CV, ...), Impedance spectroscopy (in-house developed ORP-EIS), climate chamber...
 - Microscopic: AFM, SKPFM, SVET, SECM
- Electrochemical FEM modelling (own developed approaches & expertise)

International collaborations

- Industrial:
 - APERAM
 - TOYOTA
 - AIRBUS
- Academic:
 - Prof. Fréderic Christien, Ecole des Mines, Saint-Etienne, France, for collaboration on Scanning Kelvin Probe Force Microscopy
 - Dr. Lars Jeurgens, EMPA, Switserland, for micro-capillary cell analysis



Participating in FL/B/EU funded projects with H₂ related research

- AVN Association Vinçotte Nuclear, PhD projects, on Surface state impact of hydrogen-steel interactions
- SBO project DeMoPreCi, SIM Maduros program, on electrochemical permeation modelling
- FWO fundamental research PhD grant, on Hydrogen in Duplex SS steel
- Industrial research with Aperam, Toyota, Airbus

Main relevant publications

- B. Ozdirik, K. Baert, T. Depover, J. Vereecken, K. Verbeken, H. Terryn, I. De Graeve, 'development of an electrochemical procedure for monitoring hydrogen sorption/desorption in steel', journal of the electrochemical society 164(3) (2017) c747-c757.
- B. Ozdirik, T. Depover, I. Vecchi, K. Verbeken, H. Terryn, I. De Graeve, 'comparison of electrochemical and thermal evaluation of hydrogen uptake in steel alloys having different microstructures', journal of the electrochemical society 165 (11) (2018) c787-c793.
- B. Ozdirik, T. Suter, Ulrik Hans, T. Depover, K. Verbeken, P. Schmutz, L. P. H. Jeurgens, H. Terryn, I. D. Graeve, 'study of the hydrogen uptake in deformed steel using the microcapillary cell technique', corrosion science doi:10.1016/j.corsci.2019.04.029.
- L. Vecchi, Darja Pečko, et al. H. Terryn, 'numerical interpretation to differentiate hydrogen trapping effects in iron alloys in the devanathan-stachurski permeation cell', corrosion science doi:10.1016/j. corsci.2019.04.008.
- L. Vecchi, et al. H. Terryn, 'modelling of hydrogen permeation experiments in iron alloys: characterization of the accessible parameters part i the entry side', electrochimica acta 262 (2017) doi: 10.1016/j. electacta.2017.12.172.
- L. Vecchi, et al., 'modelling of hydrogen permeation experiments in iron alloys: characterization of the accessible parameters part ii the exit side', electrochima acta 262 (2018) 153.
- L. Claeys, T. Depover, I. De Graeve, K. Verbeken, 'electrochemical hydrogen charging of duplex stainless steel', corrosion 75(8) (2019) p.880-887.
- L. Claeys, I. De Graeve, T. Depover, K. Verbeken, 'impact of hydrogen and strain rate on the martensitic transformations and mechanical properties of 304l stainless steel: hydrogen embrittlement or hydrogen enhanced ductility?', acta materialia accepted msa_140079.

Contact persons

Iris De Graeve (<u>iris.de.graeve@vub.be</u>)





Mobi research centre - EVERGi

Vrije Universiteit Brussel - Faculty of Engineering, Department of Electric Engineering and Energy Technology

General expertise of the research group

EVERGI focuses on developing holistic models that include all aspects of the energy and mobility sector for an integrated approach: ELECTRICITY, MOBILITY, HEAT, COOLING, WATER, DATA, HYDROGEN, E-FUELS ...

Sustainable Energy Communities connect renewable energy generation with advanced multi-energy systems, including storage and prosumers.

EVERGI has special attention to the inclusion of key technologies to enable the energy transition, such as electric powertrains for vehicles, automation, bidirectional charging infrastructure, digitalisation, Internet-of-Energy, artificial intelligence (machine learning) and cryptocurrency.

Specific hydrogen -related expertise & research topics

- Design, optimisation and techno-economic assessment of Multi-Energy Systems that include Hydrogen as an energy vector
- Life cycle assessment, life cycle optimisation and techno-environmental evaluation of Multi-Energy Systems that include Hydrogen as an energy vector
- Energy management systems for Multi-Energy Systems including multiple Hydrogen assets

Available equipment/tools

- Tools:
 - Design and optimisation framework for techno-economic and environmental assessment of Multi-Energy Systems including Hydrogen as an energy vector
- Equipment/assets to be installed:
 - Electrolyzer
 - Fuel-cell
 - Storage
 - Gas mixer

International collaborations

- Ongoing joint PhD with Kobe University, Japan
- Research ex-change with University of Zaragoza, Spain
- Inycom, Spain. Doctoral Internship



Participating in FL/B/EU funded projects with H₂ related research

• Reformers:

UNIVERSITEIT

BRUSSEL

- Renewable Energy Valleys to increase energy security while accelerating the green transition in Europe
- Horizon Europe Project
- Together with 28 European partners from 12 different countries
- Renewable energy valley in Alkmaar, Netherlands and 6 replication valleys in Europe

• Smart dHYstrict:

- Hydrogen as a vector in semi-autonomous local energy systems
- Interreg FL project
- Together with WaterstofNet (NL/BE), PRIVA, Fluvius, Solhyd

Main relevant publications

- Techno-economic assessment on hybrid energy storage systems comprising hydrogen and batteries:
 A case study in Belgium, A. Martinez Alonso, D. Costa, M. Messagie, T. Coosemans, International
 Journal of Hydrogen Energy, 2023, ISSN 0360-3199, https://doi.org/10.1016/j.ijhydene.2023.06.282.
 (https://www.sciencedirect.com/science/article/pii/S0360319923032615)
- Multi-state optimal power dispatch model for power-to-power systems in off-grid hybrid energy systems: A case study in Spain, A. Martinez Alonso, G. Matute, J.M. Yusta, T. Coosemans, International Journal of Hydrogen Energy, 2023, ISSN 0360-3199, https://doi.org/10.1016/j. ijhydene.2023.06.019. (https://www.sciencedirect.com/science/article/pii/S036031992302832X)
- Phasing out steam methane reformers with water electrolysis in producing renewable hydrogen and ammonia: A case study based on the Spanish energy markets, A. Martinez Alonso, N. Naval, G. Matute, T. Coosemans, J.M. Yusta, International Journal of Hydrogen Energy, 2023, ISSN 0360-3199, https://doi.org/10.1016/j.ijhydene.2023.07.347. (https://www.sciencedirect.com/science/article/ pii/S0360319923039009)

- Professor Thierry Coosemans (thierry.coosemans@vub.be)
- Hydrogen modelling Ander Martinez Alosono (ander.<u>martinez.alsonso@vub.be</u>)
- Infrastructure/lab Lennert Callebaut (<u>lennert.callebaut@vub.be</u>)

WaterstofNet

Open Manufacturing Campus Slachthuisstraat 112 bus 1 2300 Turnhout Belgium

T +32 (0)14 40 12 19 Contact person: Stijn Meel

E-mail: Stijn.Meel@waterstofnet.eu

Office The Netherlands

Automotive Campus 30 5708 JZ Helmond The Netherlands

