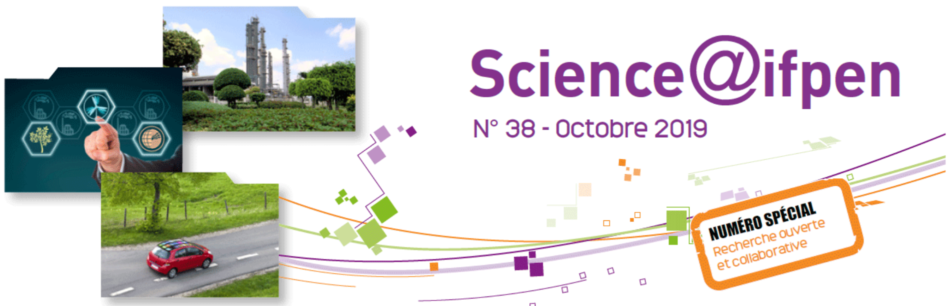


Written on 04 November 2019

15 minutes of reading

News

Fundamental Research

ces | Engineering sciences

As far as Rabelais was concerned, “Science without conscience is only ruin of the soul” but what can be said of science without sharing or cooperation?! Because while by its very nature scientific research is driven by knowledge already acquired and the analysis of previous work, incorporating outside expertise is essential to success.

IFPEN applies this principle in its fundamental research partnerships, tapping into the very dense research biotope in order to generate or further develop partnerships of strategic importance to its scientific policy. **Collaborative research programs are helping to overcome some fifty or so scientific challenges identified as obstacles** to research in its strategic areas: sustainable mobility, new energies, climate and the environment, responsible oil and gas. Of fundamental importance to research and innovation, this work takes the form of theses, post-doctoral research, scientific visitor secondments, collaborative projects and road maps formalized by a framework agreement.

These collaborative programs concerning research in various scientific fields and for diverse applications are illustrated in this issue. And they are all examples of the benefits of the open research IFPEN has been contributing to with conviction for many years.

Isabelle Morelon
IFPEN Scientific Division

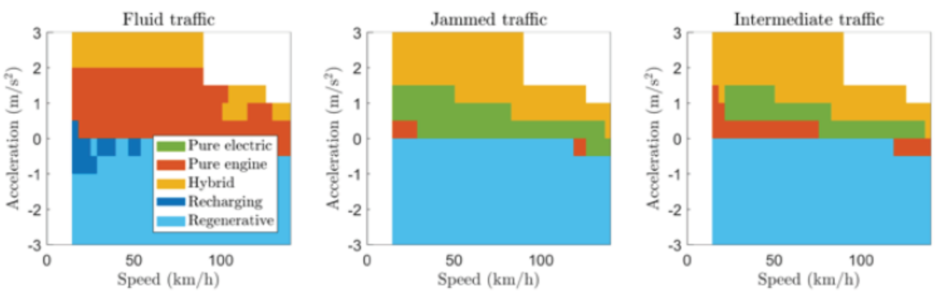
See the PDF of the letter

LES BRÈVES

The scientific cooperation agreement signed with INRIA in 2015 covers two fields: the “**digital and IT performance of simulato**rs” and the “**control and optimization of complex systems**”. A thesis carried out in the latter field (1) contributes to the optimized use of the energy on board hybrid vehicles, in such a way as to take full advantage of the potential offered by this technology in terms of **reducing CO_2 emissions**.

Striking the right balance between the Internal Combustion (IC) engine and the electric motor is dependent on an algorithm, known as the **energy management system** (EMS). However, this does not take into account the impact of traffic conditions, an important factor when it comes to consumption. As a result, the balance between the two sources is not optimized.

In the proposed approach, vehicle dynamics are modeled as a random process, sensitive to various topological road characteristics and different traffic conditions(2). This modeling is made possible thanks to massive mobility and traffic data flows, fed back from vehicles[a]. As a result, the new EMS will be able to implement control strategies based on stochastic dynamic optimization techniques. It will thus request a shift in the balance between IC and electric as a function of traffic conditions, as illustrated in the figure below.



Energy management law for a hybrid vehicle as a function of three different traffic scenarios on a section of road.

The results obtained from real data, gathered in three traffic scenarios over a few kilometers of highway, demonstrate a benefit in terms of overall energy consumption. The aim now is to validate this new control strategy over a wider geographic area.

a - This research used data provided by the Geco air smartphone app.

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(1) ***A. Le Rhun****, A stochastic optimal control for the energy management of a hybrid electric vehicle under traffic constraints, due to be defended in December 2019.*

(2) ***A. Le Rhun****, F. Bonnans,* ***G. De Nunzio****,* ***T. Leroy****, and P. Martinon, IEEE Transactions on Intelligent Transportation Systems, pp. 1–10, 2019.*
DOI : 10.1109/TITS.2019.2923292

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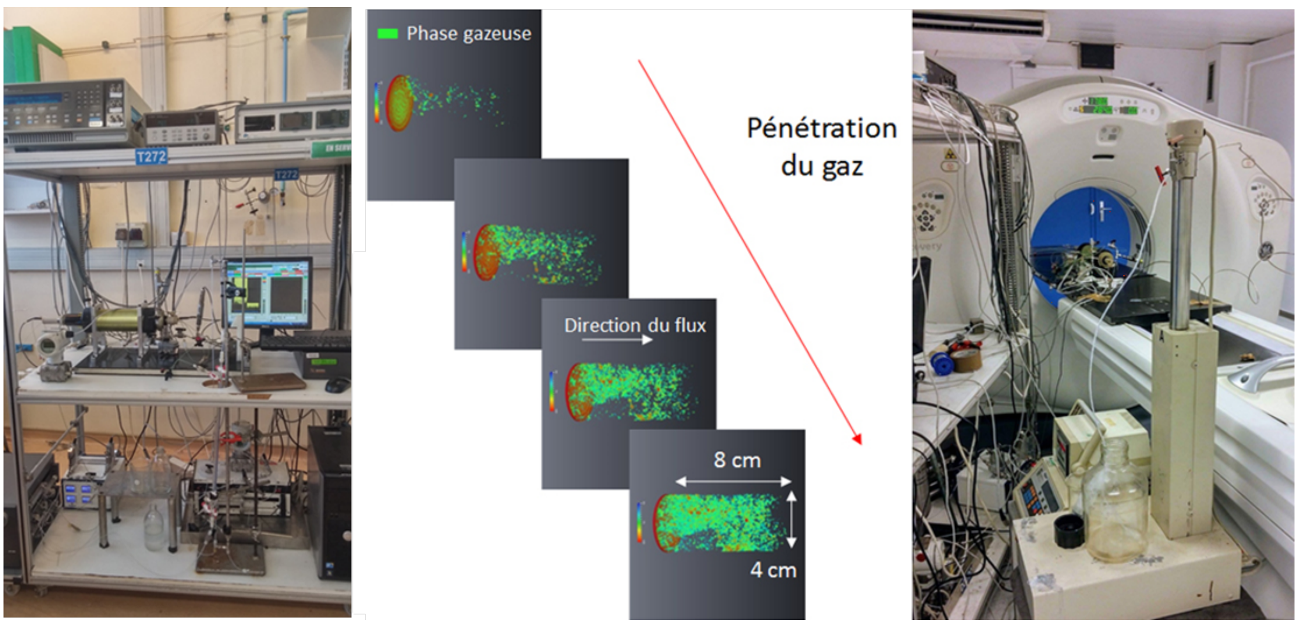
Hybrid vehicle energy management optimization within the framework of the partnership with INRIA

Over the past ten years, IFPEN has been conducting research on the **geochemical monitoring of the geological storage of CO_2**, in order to gain a better understanding of the **natural water flows** that may be impacted by any leaks in the **unsaturated zone** (UZ)[a]. IFPEN was also a partner in two ADEME projects[b] that led to the validation of a warning concept based on natural tracers associated with CO_2 [(1)].

Adrian Cerepi[c], who coordinated these two projects, was a scientific visitor at IFPEN between 2014 and 2016. He worked with **Bruno Garcia** (Geosciences Division) on reservoir rock characterization using **electrical measurements to determine, in real time, the petrophysical parameters required to characterize the surrounding rock**. This research led to a methodology and the development of a unique process for determining and monitoring, in real time, the relative permeability of a porous medium, based on electrical measurements and considering geochemical interactions, all using scanner imaging (figure).



Experimental set-up for the combined measurement and observation of porous media permeability.

The two researchers also co-supervised a thesis with a significant impact[d] in this field[(2)].

Today, the partnership continues via the ADEME "Aquifer-CO_2 Leak 2019-2023" project to monitor the evolution of a CO_2 plume and associated tracers, in
the UZ but also in a subsurface aquifer. A methodology incorporating geochemical and geo-electrical measurements, as well as a real-time monitoring technology, will be developed and validated on a pilot site[e].

a - Section of the ground or underground located at the interface between the outermost layer (pedosphere) and the groundwater layer.
b - CO_2-Vadose (2009-2013) and DEMO-CO_2 (2013-2016), led by the University of Bordeaux.
c - Professor at ENSEGID (graduate school of environmental, geological and sustainable development engineering).
d - Three articles in peer-reviewed scientific journals and two patents.

e - Saint-Émilion pilot site.

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(1) ***B. Garcia****,* ***P. Delaplace****,* ***V. Rouchon****, C. Magnier, C. Loisy, G. Cohen, C. Laveuf, O. Le Roux, A. Cerepi. International Journal of Greenhouse Gas Control, vol. 14, (2013)*

(2) ***A. Chérubini****, The use of spontaneous and induced polarization methods for the detection of* CO_2 *in porous carbonate media. Thesis defended on 25 March 2019.*

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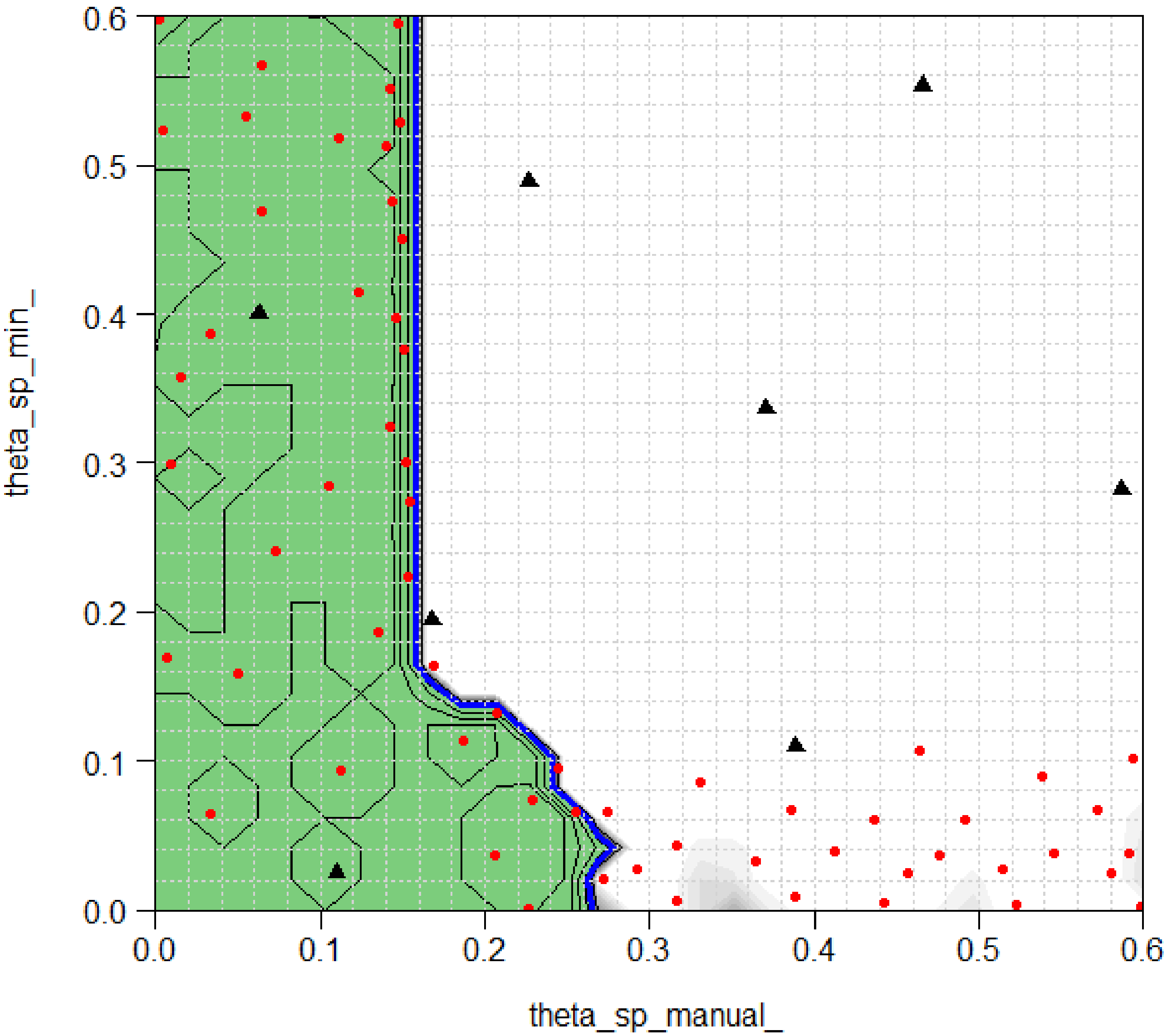
A scientific visitor helps improve the monitoring of CO2 storage facilities

The **OQUAIDO[a] applied mathematics chair**, launched in January 2016 and hosted by the École des Mines engineering school in Saint-Étienne, brings together academic and industrial partners[b] to tackle questions relating to the use of numerical simulators, such as **uncertainty quantification, inversion and optimization**. Its objective is to work on “upstream” research problems guided by practical applications.

A thesis(1) was carried out within the framework of this chair under the supervision of the Grenoble Alpes University, the École Centrale de Lyon and IFPEN. The application objective was to define the **parameters for a vehicle pollution control system in order to comply with pollutant gas emission standards**.

Of the many sources of uncertainty relating to the control of this system, the one that has the greatest impact is the variability of the driving cycle in real conditions. Hence in practice, compliance with standards is achieved by averaging, for a given sample of cycles, emission values estimated by a numerical simulator (figure).



For two control parameters, estimation (in green) of the NH3 emission standard compliance set (initial simulated points in black, points added via the iterative method in red).

Simulation calculation time was thus reduced, using an **approximation of the simulator via a Gaussian process** and a dimension reduction applied to the functional variable. Combining these techniques with an iterative uncertainty reduction method not only considerably reduced the number of required simulations, compared with state-of-the art methods, but it also made it possible to control estimation errors of the admissible set for the control system parameters[2].

a - From the French “Optimisation et QUAntification d'Incertitudes pour les Données Onéreuses”.

b - BRGM, CEA, CNRS, École Centrale de Lyon, IFPEN, IRSN, École des Mines engineering school in Saint-Étienne, Safran, Storengy, Grenoble-Alpes University, Nice Sophia Antipolis University, Toulouse Paul Sabathier University.

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*(1) **M. R. El Amri**, Uncertainty and robustness analysis for functional input and output models, Grenoble Alpes University PhD thesis, defended in 2019.*

*(2) **M. R. El Amri**, C. Helbert, **O. Lepreux**, **M. Munoz Zuniga**, C. Prieur, **D. Sinoquet**, Data-driven stochastic inversion under functional uncertainties, Statistics and Computing journal, 2019 Sept.*

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Research engineer / project leader in optimization
PhD in applied mathematics
A robust vehicle pollution control system thanks to the OQUAIDO chair

The rapid development of wind energy production depends, to a great extent, on improving its energy efficiency and its economic profitability. To maximize performance and operating life spans, the implementation of advanced and innovative control systems is a promising avenue explored by IFPEN as a member of the SmartEole (2015-2019) project, conducted by a consortium of public and private partners[a].

This project led to the development of the smart rotor concept to improve the operating conditions of wind turbines, incorporating new measurement systems, particularly a lidar[b] sensor mounted on the nacelle roof (figure), combined with innovative processing algorithms, developed at IFPEN.

Thus, a short-term forecast of wind properties at rotor plane was established from the lidar measurements[(1)], and then combined with an original wind turbine control strategy based on these reconstructed and predicted wind data[(2)]. The achieved solution prototype makes it possible to optimize the orientation of the nacelle and blades. The performance levels of this Lidar-assisted control, evaluated during simulation, herald a reduction in fatigue stresses of between 15 and 30%, depending on wind conditions, with a slight positive impact on power production.

Optimization strategies for the management of an entire wind farm have also been developed, based on wake redirection techniques, with a view to minimizing interference between neighboring turbines and increasing overall production.

This numerical simulation research conducted using data measured on site has led to significant progress in terms of the approaches explored. Moreover, the results obtained have given rise to the emergence of several potential areas of application, such as the integration of lidar-assisted control on existing turbines (retrofit) and the optimized supervision of entire wind farms.

a - https://anr.fr/Projet-ANR-14-CE05-0034
b - Light Detection And Ranging.

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*(1) **F. Guillemin**, **H.-N. Nguyen**, **G. Sabiron**, **D. Di Domenico**, M. Boquet, Torque 2018, Milan.*

*(2) **D. Di Domenico**, **F. Guillemin**, **M. Laraki**, **G. Sabiron**, WindEurope 2017, Amsterdam.*

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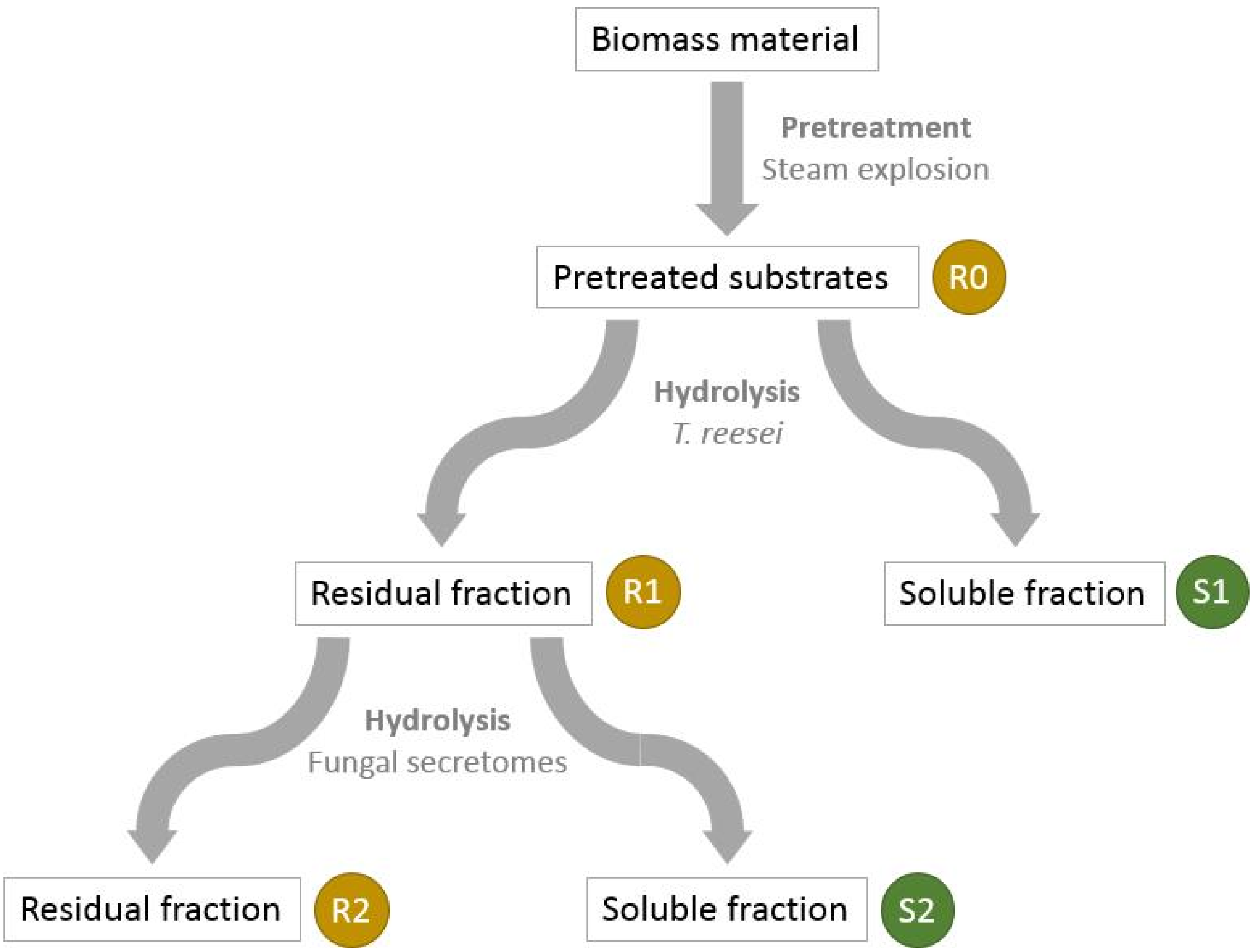
SmartEole project: making better use of wind through smart rotors

Lignocellulosic biomass is an interesting raw material for the production of fuels and chemical intermediates because it is abundant and has a much smaller environmental footprint than fossil alternatives. On the other hand, its considerable structural and chemical complexity represents an obstacle to the development of viable conversion processes. The biochemical decomposition of sugar polymers thus requires a physicochemical pre-treatment to break down the structure of this complex substrate and thereby making it accessible to polysaccharide degrading enzymes (produced by the filamentous fungus **Trichoderma reesei**). However, their conversion via hydrolysis remains incomplete since parts of these polymers remain inaccessible.

The **F'Unlock project** (IFPEN, CNRS, INRA) sought to gain a better understanding of the reasons for this recalcitrance while seeking new, more effective enzymes to overcome it. The structural and physicochemical analysis of hydrolyzed samples, containing varying quantities of recalcitrant fractions, made it possible to find **relevant biodegradability markers**[a], in view of guiding enzyme selection. Moreover, new enzymes, from fungal biodiversity, were tested on partially hydrolyzed and more recalcitrant fractions R1 (figure) via a second enzymatic hydrolysis step[b].



Méthodologie d'hydrolyse enzymatique séquentielle des substrats.

In addition to its use for enzyme selection, marker identification has enabled a better understanding of the **cause of biomass recalcitrance**, paving the way for subsequent research(1). Moreover, since none of the enzyme mixtures tested were more efficient than the reference mixture, it appears that significant enzyme diversity is not essential. A more complete conversion of biomass may thus depend on some key catalytic activities, combined with effective pre-treatment.

a - Particularly lignin content, cellulose crystallinity, water adsorption capacity.
b - Giving rise to residual fractions R2 (figure).

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*(1) G. Paës, D. Navarro, **Y. Benoit**, **S. Blanquet**, B. Chabbert, **B. Chaussepied**, P. M. Coutinho, S. Durand, I. V. Grigoriev, M. Haon, L. Heux C. Launay, **A. Margeot**, Y. Nishiyama, S. Raouche, M. N. Rosso, E. Bonnin, J. G. Berrin. Biotechnol Biofuels. 2019 Apr 1; 12:76.*
DOI : 10.1186/s13068-019-1417-8

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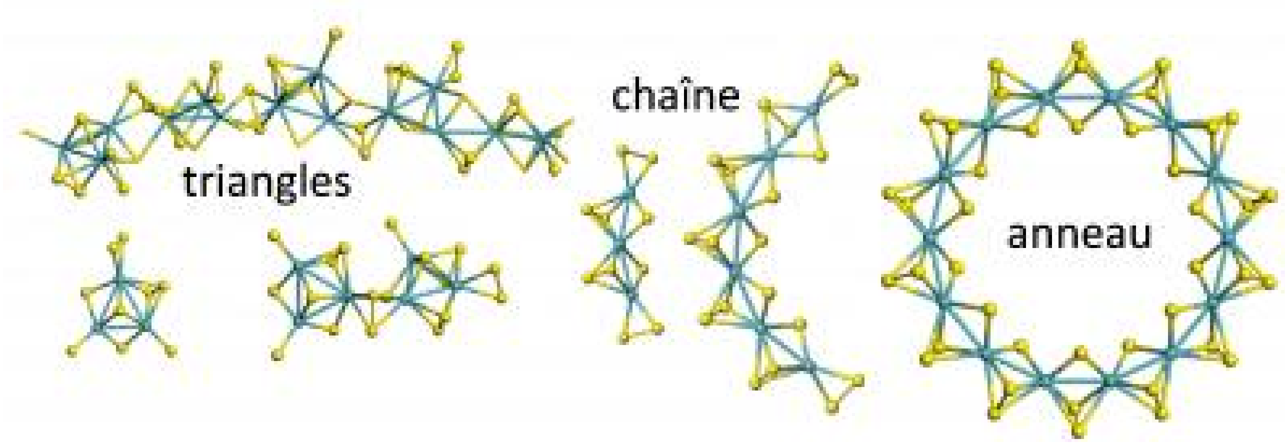
F’Unlock project: to unlock plant biomass hydrolysis using enzymes

The 1st industrial chair within the IdexLyon project[a], **ROAD4CAT** (RatiOnAl Design for CATalysis), launched in June 2018, brings together IFPEN and the Chemistry Laboratory at École Normale Supérieure Lyon(1). Its holder **Pascal Raybaud**, a researcher in the Catalysis, Biocatalysis and Separation Division, delivers Master's level lectures in the relevant themes.

The chair's scientific strategy is based on an **innovative research approach to computational chemistry on a quantum level**, applied to the rational design of heterogeneous catalysts, as well as the precise understanding (on an atomic scale) of the mechanisms at work, from their preparation (active phase genesis) through to their operation (key properties) in reaction conditions. The research will mobilize ten researchers from the partner teams (IFPEN, ENSL, UCBL, CNRS), four PhD students and five postdoctoral researchers for a period of five years.

Ongoing research conducted by the first two PhD students and first two postdoctoral researchers has delivered promising results that will appear in scientific publications:

- the quantum simulation of structural, electronic and spectroscopic properties provides a **better understanding of the amorphous MoS_3 phase** (figure), a key intermediate for the activation mechanisms of the MoS_2 phase, which is likely to be employed in the hydrodesulfurization reaction, in the photoreduction of CO_2 or in the hydrogen evolution reaction;
- the interaction of inorganic additives with the alumina-gamma support employed for industrial catalysts is described by a **combined quantum modeling/NMR spectroscopy approach**;
- the use of advanced quantum methods also improves the **prediction of optical properties and charge mobility within the molybdenum oxysulfide materials**. The potential of solar fuels, produced by photocatalysis, is thus being explored.



Various amorphous MoS3 phase nanoclusters identified by quantum simulations.

This research will have an environmental and societal impact associated with the improvement in the eco-efficiency of catalytic processes and the reduction in the quantity of metallic atoms employed in catalysts.

a - ANR-16-IDEX-0005 excellence institute.

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(1) IFPEN 2018 activity report, page 35

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Researcher in Molecular Modeling applied to Catalysis
The ROAD4CAT chair one year in

To support the development of innovations for the energy transition, the CNRS, École Normale Supérieure Lyon, IFPEN, Sorbonne University, Claude Bernard Lyon 1 University and the University of Strasbourg have created a **joint research laboratory** (JRL). **CARMEN** is a five-year venture in which the partners are pooling their expertise and know-how in the field of the characterization of materials for new energies. The objective is **to reinforce knowledge on molecular and/or colloidal transport in porous substrates** and develop new methodologies for the detailed analysis of these materials.

The latter, like catalyst supports and soils, have numerous applications in the fields of catalytic biomass conversion, adsorbents for the reduction of contaminants and renewable energy storage. Their optimization for new energy technologies depends on the identification of the relationships between their structural and chemical properties, on the one hand, and their physicochemical properties (transport, mechanical resistance, etc.), on the other. The research conducted by the CARMEN JRL will thus focus on the multi-scale characterization of their structure in operating conditions as close to reality as possible -operando-, in order to relate them to their transport properties as well as their reactivity.

By bringing together three outstanding academic teams at sites in Lyon (the Very High Fields RMN Center), Paris (the PHENIX Physicochemistry of Electrolytes and Interfacial Nanosystems laboratory) and Strasbourg (Strasbourg Institute of Physics and Chemistry of Materials) with IFPEN teams, the **CARMEN JRL forms a consortium that is unique in the world.** In addition to the complementary nature of the assembled expertise, it will make it possible **to pool high-performance equipment and mobilize numerous characterization techniques**, including innovative operando approaches such as low field and high field NMR as well as imaging techniques combined with modeling.

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