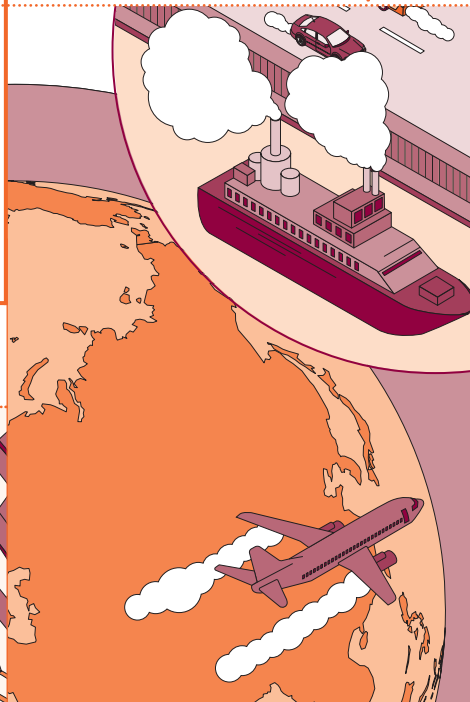
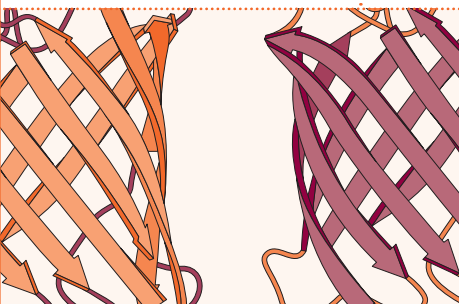
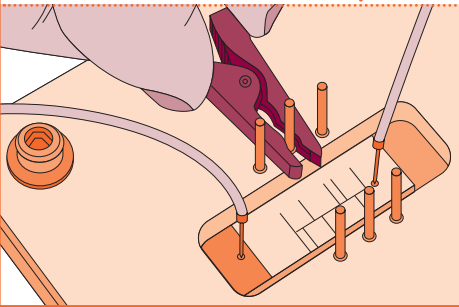
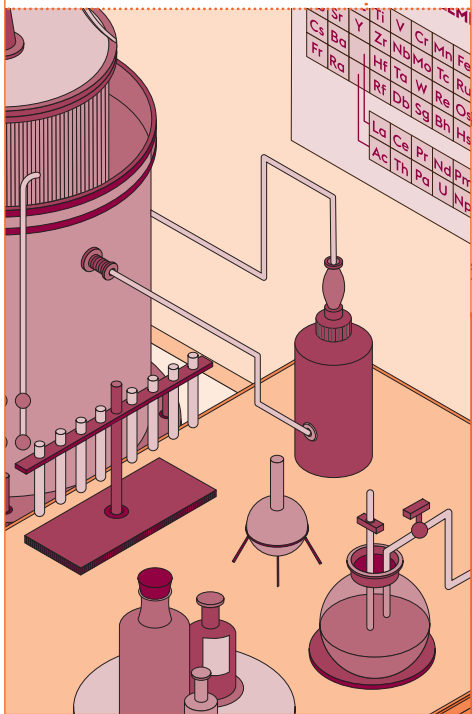
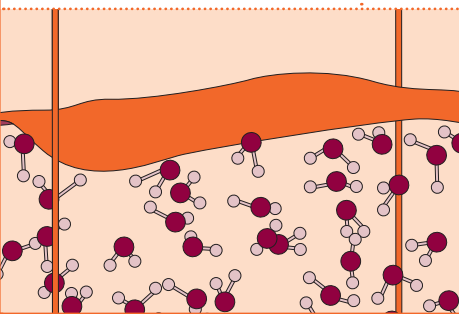


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AWARDS AND PRIZES



RESEARCHERS



© CEA-Didier Touzeau

Davide Audisio and **Frédéric Taran**, researchers at the i4C-Modelling Laboratory, part of the CEA Saclay Molecular Labelling and Bioorganic Chemistry Unit, received the **2019 research prize for chemistry** for their work on “click and release” approaches to chemistry.

Jan Borm, managing vice-president in charge of international relations at Université de Versailles – Saint-Quentin-en-Yvelines, was presented with a **PhD degree honoris causa** by the University of Lapland in Finland.



© HEPHAISTOS-Pharma

Martine Caroff, an internationally reputed specialist on endotoxins and longtime head of a research team at the Institute of Genetics and Microbiology, now known as the Institute for Integrative Biology of the Cell (I2BC – CNRS/ Université Paris-Sud), won the **2019 EU Prize for Women Innovators** for her startup LPSBioScience.

Aurélié Dudézert, a researcher at the economics and management lab specialised in the study of networks, spatial issues and globalisation (RITM – Université Paris-Sud), won the **Prix EFMD-FNEGE 2019 for the best book on management** in the “Essay” category in honor of her book “La transformation digitale des entreprises”.



© Inria-Photo G Scagnelli

François Fages, a senior researcher at the national research institute for the digital sciences (INRIA) at Saclay, was honoured with the **2019 Research award in the “Information Sciences” category** for his work on analog computation in natural and engineered biochemical systems.



© LSCE

Catherine Kissel, a researcher at the Laboratory for Sciences of Climate and Environment (LSCE – CEA/CNRS/Université Versailles – Saint-Quentin-en-Yvelines), received the **Petrus Peregrinus 2019 Medal** from the European Geosciences Union (EGU) for “outstanding contributions in paleomagnetism, applied to understanding the Earth’s magnetic field, paleoclimate, paleoceanography and the geodynamic evolution of the Mediterranean margins”.

Graham Nector, a researcher in plant biology at the Institute of Plant Sciences – Paris-Saclay, has been appointed **senior member of the French University Institute** for the exceptional quality of his research.

STUDENTS



© UPSud

Audrey Fels, a student at the Faculty of Medicine of Kremlin-Bicêtre (Université Paris-Sud), won the **gold medal at the 2019 national university championships for judo**.

The women’s soccer team from the **Department of Sciences and Techniques of Sports and Physical Activities** at Université Paris-Sud placed **third** in the Elite 8 of the national university championships.



© CentraleSupélec

Aviron CentraleSupélec Paris proved itself to be the best student rowing club from a “Grande École” at the 2019 national university championships.

PROJECTS/STARTUPS



CHIMACTIV, an interactive website co-developed by AgroParisTech, ENS Paris-Saclay and Université Paris-Sud offering digital educational resources relative to the chemical analysis of complex media, won a **2019 Digital Learning Excellence Award** in the “Education” category.



Néolithe, a startup supported by AgroParisTech and École Polytechnique, won the **Next Startupper Challenge** at VivaTechnology 2019. It has come up with an innovative fossilisation process to convert non-recyclable waste into building materials.



Spin-ION Technologies, co-founded by Dafiné Ravelosona of the Center for Nanosciences and Nanotechnology (CNRS/Université Paris-Sud), won the **2019 i-Lab Grand Prix** for its revolutionary process solution to increase the storage density of digital memory.

IUMTEK won the **2019 i-Lab** competition in the field of **Chemistry and Environment**. Specialised in industrial optical instrumentation in harsh environments, it designs and manufactures real-time in situ analysis equipment based on LIBS (Laser Induced Breakdown Spectroscopy) technology.

EverZom, **HEPHAISTOS-Pharma** and **Zi Surfaces** (Zero Surface Interference) won in the field of **Pharmacy and Biotechnology**. EverZom aims to produce and engineer “tailor-made” extracellular vesicles for the pharmaceutical and veterinary industries. HEPHAISTOS-Pharma is developing ONCO-Boost, an innovative immunostimulator to boost immunotherapy strategies in oncology. Zi Surfaces provides an innovative surface chemistry for biochips and enters the biosensor market.

HD Rain and **Teratronics** won in the field of **Electronics, Signal Processing and Instrumentation**. HD Rain is developing a precipitation measurement and forecasting solution for precision agriculture and insurance. Teratronics markets a non-destructive testing solution based on ultra-short terahertz (THz) pulses.

EDITOR'S LETTER



© UPSaclay

This beginning of the 2019-2020 academic year is under the best auspices for Université Paris-Saclay, its students, its partners and all the staff of its member institutions.

On July 10th, 2019, the new statutes of the university were approved with a large majority by the ComUE's board. This was done after similar votes by the boards of directors of all parties, i.e. Université Paris-Sud, which will merge in a few months' time with the current ComUE Paris-Saclay, the four schools (Agro-ParisTech, CentraleSupélec, ENS Paris-Saclay, Institut d'optique Graduate School) which will become component institutions of Université Paris-Saclay, and Université of Versailles Saint-Quentin-en-Yvelines and Université d'Évry, the two associate member universities which will also merge in 2025. The six partner national research organisations (CEA, CNRS, INRA, INRIA, INSERM, ONERA) and IHES did not have to formally vote on the statutes. However, some have done so with a comparable positive result.

From now on, and after the final stages of prior validation or consultation, the decree of creation will be published within two months, paving the way for the regulatory and administrative process that will lead, in January 2020, to the effective birth of the new Université Paris-Saclay. In other words: "here we are".

Summer is also the time when the Shanghai ranking (*ARWU, Academic Ranking of World Universities*) is published by Jiao Tong University. This publication has become an annual indicator of world-class research universities.

Whether awaited, criticised or coveted, this list of the 500 best institutions in the world mobilises each year around August 15th the attention of higher education and research stakeholders. The very good results of Université Paris-Sud, ranked 37th in the world this year, 9th in Europe and 1st in France, confirm its position as an intensive research university of international standing. They naturally raise many expectations for Université Paris-Saclay 2020, which will replace it, enriched by other higher education and research institutions – most of them were also present in this ranking with a positive dynamic – and partner organisations.

But until then, on the campus of Université Paris-Saclay, other projects are starting or delivering their first results. In this issue, you will discover the new Institute for Climate and Environmental Sciences (ICE), the new Agro Paris-Saclay campus dedicated to agronomy and agrifood, the 28 laboratories that bring together more than 1,500 key players in chemistry and a few noteworthy works on theoretical, molecular and ethical chemistry.

This issue is the last published under the aegis of Université Paris-Saclay in its current ComUE status.

The next one will come to you in January, as it has been for the past four years, and we will once again have many great initiatives to report and results to illustrate.

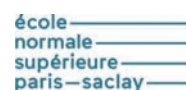
Thank you for your commitment. I wish you a very good beginning of the university year. See you soon.

Sylvie Retailleau,
President of Université Paris-Saclay



Chemistry

Members of Université Paris-Saclay



Title

Paris-Saclay's "excellence labs" offer chemistry doctoral students a broader range of training solutions



Playtime at the LERMIT LabEx summer school. © R. Diaz Lopez – UPSaclay

The Laboratories of Excellence (LabEx) of Paris-Saclay have set up and/or funded summer schools, tutorials and other types of additional training for university doctoral students.

Doctoral students from the CHARMMMAT LabEx (Chemistry of Multifunctional Molecular Architectures and Materials) had been eagerly awaiting this year's summer school on catalysis. Every two years since 2015, a three-day session of lectures and classes given by internationally reputed catalysis researchers has been held. The third edition ran from March 31 to April 3, 2019 in Cabourg, Normandy and was attended by 34 doctoral students from the LabEx. According to Arnaud Voiturier, a researcher at the Institute for the chemistry of natural substances (ICSN) of the French National Centre for Scientific Research (CNRS), "the idea is to expose students to the latest international findings on catalysis, one of the LabEx's main areas of study, along with materials."

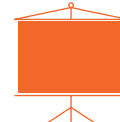
Mission accomplished! This year's four guest researchers, specialised respectively in organo-metallic catalysis, photocatalysis, biocatalysis and organocatalysis, each gave a lecture and

taught a two-hour class on their area of study. The pleasant seaside setting made the learning experience even more enjoyable. Fifteen oral reports and a twenty-poster session rounded out the scientific side of the programme, which also included a tour of a cider farm and a special dinner. "The number of participants is limited, which encourages discussion and allows them to get to know each other. The feedback has been excellent and some doctoral students have signed up for several editions. For them, the summer school is a golden opportunity to talk to world-famous researchers and get valuable advice regarding their thesis. In fact, one 2017 attendee is now doing postdoc research at the lab of one of that year's guest lecturers," observes Xavier Guinchard, who co-organised the event.

The summer school on catalysis, fully funded by the CHARMMMAT LabEx, was free of charge for students from affiliated labs. Open to internationals, the programme was taught in English, the summer school's official language. "This year, eight Chinese doctoral students signed up," notes Arnaud Voiturier. Completion of the summer school programme gives doctoral students credit for twenty hours of training. All eyes are already turning to the 2021 edition!

For an enlightened view on pharmaceutical development

Another recurring event is the "Drug Discovery" summer school programme, held annually since 2012 by the Laboratory of Excellence in Research on Medication and Innovative Therapeutics (LERMIT). This year's three-day session (July 10-12) took place at the Domaine de Saint-Paul in Saint-Rémy-lès-Chevreuse, southwest of Paris. The class, limited to thirty, included doctoral students, young researchers and researchers from pharmaceutical companies. Half of the class came from LERMIT-affiliated labs. Participants reviewed the steps involved in drug development (e.g. identification of the therapeutic target, toxicology, addressing, pharmacokinetics, animal modelling, clinical trials and commercialisation). They also discussed the socio-economic implications of therapeutic innovation for the regulatory environment, pharmacovigilance, the health economy and the organisation of the pharmaceutical industry, then tested their knowledge by playing a game ("L'Odyssée du Médicament" – The Drug Odyssey). "Our summer school provides a cross-cutting overview of pharmaceutical development and allows participants to build up their professional network," says Raquel Diaz Lopez, scientific project



manager for LERMIT. Many research collaborations got their start thanks to this type of training programme.

As for the twenty or so guest lecturers, half came from the pharmaceuticals industry and the private sector and most had direct experience with product development. *“The focus is on case studies about successful molecule development projects and startups, tracing innovations from discovery to clinical application and all the way to the patient,”* explains Raquel Diaz Lopez. Completion of this programme, funded by LERMIT (participants are only charged a token amount), gives doctoral students credit for twenty hours of training. *“LERMIT will to cease to exist at year-end 2019, but we’d like to see the summer school become a permanent fixture of the new Université Paris-Saclay,”* she adds.

A tutorial on digital simulation

This year, the annual deMon developers workshop was accompanied by a new tutorial at the Maison de la Simulation at the CEA Saclay research centre from May 20 to 25, 2019. The purpose was to familiarise participants with deMon2k and deMonNano software programmes used for density functional theory (DFT) calculations to simulate the dynamics of atoms, molecules, clusters and solids. *“When it comes to calculation speed, deMon is one of the best DFT programmes around,”* says Aurélien de la Lande, a researcher at the Physical Chemistry Laboratory (LCP – CNRS/Université Paris-Sud) and a member of the tutorial planning committee. *“In addition, it’s free of charge for academic researchers.”* The 23 tutorial participants – i.e. local or international master’s or doctoral students and researchers – all had a background in chemistry or physical chemistry.

The tutorial gave equal emphasis to lecture courses, the execution of small applicative tasks on computer and a short, guided project. It ended with a presentation of the projects done during the week by teams of two or three. *“Informed of the subjects ahead of time, participants could choose what they wished to work on,”* explains Fabien Cailliez, a researcher at the Physical Chemistry Laboratory and a member of the organising committee. *“They were asked to complete a short scientific assignment, e.g. to calculate the magnetic properties or absorption spectrum of molecules, or study the thermodynamic parameters of a chemical reaction.”*

The tutorial received support from a number of institutions, including PALM (LabEx on physics, atoms, light and matter), NEXT (nano, extreme measurements & theory project), the national agency for research, the

Federation of Physical Chemistry of Paris-Saclay, the chemistry department at Université Paris-Saclay, the Research Institute on Complex Atomic and Molecular Systems and the French Centre for Atomic and Molecular Computing, not to mention the Institute for Development and Resources in Intensive Scientific Computing (IDRIS) and the Maison de la Simulation. According to Fabien Cailliez, *“minimising the cost to participants was a priority. Their accommodation and meal expenses were covered almost entirely.”* Aurélien de la Lande concludes on this note: *“We think it vital to inform the younger generation about this quantum chemistry programme, one of the most effective to be found, whose potential is often underestimated.”*

<http://www.charmmmat.fr/fr/charmmmat/actualites/150-edec-2019>
www.labex-lermit.fr/fr/formation/ecole-d-ete
www.19thdemondeveloperswk.u-psud.fr/index.php/registration/tutorial/

Title

Secondary-level teachers get updated on chemistry research



Presentation by Raphaël Haumont. © VM-UPSaclay

On April 3, 2019, the French National Centre for Scientific Research (CNRS) held a training day in scientific culture in chemistry at the Orsay campus for secondary-level teachers. The CNRS partnered with the Maison d’initiation et de sensibilisation aux sciences (MISS), where the lectures took place. Marie-Pierre Fontaine-Aupart, a researcher at the Orsay Institute of Molecular Sciences (ISMO – CNRS/Université Paris-Sud), shed light on key advances in the chemistry of energy, materials, environmental science and health. Raphaël Haumont, a researcher at the Orsay Institute of Molecular Chemistry and Materials (ICMMO – CNRS/Université Paris-Sud), told some thirty local teachers how to cook up a storm using chemistry. Declaring that *“there’s nothing more molecular than cooking an egg!”*, he examined various possibilities for culinary

innovation relying on chemical principles (e.g. “no-cook” scrambled eggs, sugar-free orange marmalade and coffee in a flask frozen with liquid nitrogen). In her closing remarks, Marie-Pierre Fontaine-Aupart expressed the intent behind the event: *“Chemistry is a fascinating field of investigation. We’re ready to work with you in hopes that your students will choose careers in science and come work in our labs.”* During the afternoon, small groups of teachers toured the sophisticated laboratories and installations at ICMMO and the Physical Chemistry Laboratory (CNRS/Université Paris-Sud), and talked to the researchers there. According to teacher feedback, the content of the training day was varied and enriching, a source of inspiration for interesting experiments to do in class.

Title

CHIMACTIV: online self-study for experimental work

Chimactiv is an interactive website offering digital educational resources for the chemical analysis of complex media (e.g. food, drugs or biological media). It is intended for students in master’s degrees, engineers and pharmacists, chemistry and biochemistry teachers of these programs, and trainees and doctoral students in chemistry research laboratories. It was conceived and produced by a group of thirteen faculty members from three of the institutions that make up Université Paris-Saclay, namely AgroParisTech, École Normale Supérieure Paris-Saclay and Université Paris-Sud. The project is a good illustration of the open science culture in which Université Paris-Saclay firmly believes.

This website helps students prepare better for lab sessions and therefore make the most of their lab time and interact more effectively with teachers. What they learn on their own is subsequently reinforced during lab sessions. The idea is to have students propose methodologies, do experiments, discuss/interpret results and apply critical thinking skills in checking the validity of results.

The website has just received a Digital Learning Excellence Award in the Education category. This year’s judges liked several things about the site: its rich content, graphics, “open to all” approach and the English version for internationals.

<http://chimactiv.agroparistech.fr/fr>



Title

CURIOSITas festival: looking beyond appearances



© CURIOSITas2019

The CURIOSITas festival invites all audiences to an exhibition and shows blurring the boundaries between art and science. It will be held in Massy (Espace Liberté) from November 7 to 17, 2019.

The 20 works that will be exhibited over the ten days of the festival were co-created by artists and scientists from Université Paris-Saclay.

“For its fifth edition, CURIOSITas invites you to look *Beyond appearances*.”

They are entirely novel and have been selected by a jury. For its fifth festival, CURIOSITas invites you to look “Beyond appearances”, to escape and listen to the song of humpback whales, to dive inside a tree, where the cells and sap form the plant, to discover the power

of the stars and to go back in time to past climates... Plays and dance performances will also await you, dotted about the town.

In the act of co-creating, scientists and artists were able to change their perspective on their research topics, question themselves and, often, enrich each other's understanding. Ultimately, they have more in common than you would think.

A wide-scale public event that reflects the commitment of Université Paris-Saclay

Through CURIOSITas, organised by La Diagonale Paris-Saclay, the science and society service of Université Paris-Saclay, the university is accomplishing its mission to enhance culture and the interactions between scientists and society. For the public, this is an opportunity to discover the scientific research under way in France through artists' perceptive vision and questioning nature.

A festival for all inquiring minds

All week long and at the weekends, facilitators will guide the public in understanding the creators' process and intention. CURIOSITas will also hold workshops and entertainments for the whole family at the weekends. It will become possible for you to question the world, experiment and, why not, create an artwork. This November, be curious in Massy with CURIOSITas!

www.curiositas.fr

Title

Building the memory of the university: surprising treasures await!



© Inra

On the occasion of this anniversary year of Mendeleev's table, La Diagonale Paris-Saclay has organised a competition inviting staff to unearth old posters, instruments and other old objects linked to the chemical elements.

Two prizes worth €500 were awarded, one for the oldest object and the other for the most unexpected. The oldest was a work dating back to 1828, located by librarians Marina Pavlidès and Alain Bône from the Grignon National Institute for Agriculture's (INRA) EGER library: *Traité de chimie appliquée aux arts*, premier tome, Grignon (“Treatise of chemistry applied to art”, first volume, Grignon). The most unexpected was a ‘mass’ storage device that was used to store the coding results of the first IBM Personal Computer. It was showcased by Robert Sellem from France's National Centre for Scientific Research (CNRS).

Each winning institution will use its prize to finance a heritage mission. All the objects listed will be exhibited on a digital platform and accessible after the start of the 2019 European Heritage Days.

www.ladiagonale-paris-saclay.fr/nos-actions/tableau-periodique-patrimoine/

Title

Researchers in their elements

1869. The Russian chemist Dmitri Mendeleev organised the 60 or so known chemical elements. He arranged them in the columns and rows of what became the “Periodic table of elements” according to their physical-chemical properties.

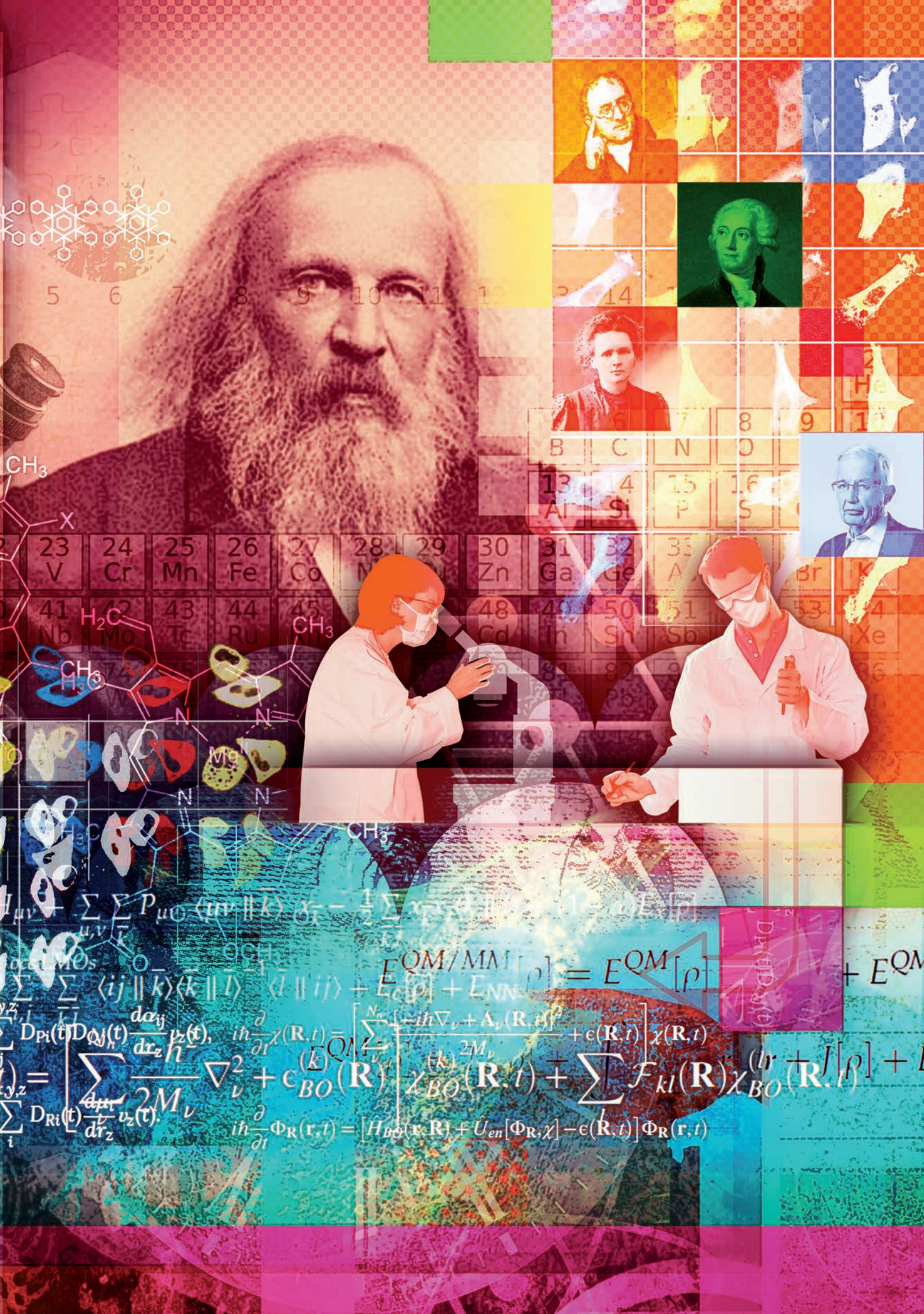
2019. Extended to 118 elements, this table still structures the way we perceive matter.

By using it as a guide, the COMPAS (commu-

nication, outreach and scientific heritage) unit of the Orsay School of Sciences is issuing an invitation to discover some of Université Paris-Saclay's areas of research through a special exhibition. Each selected element ushers the public into a laboratory and helps researchers to unlock the secrets of matter, nature and life. A decidedly visual exhibition that will enable all to truly embrace the research topics addressed.

Soon to be inaugurated at Orsay University Library during the 2019 science fair, this exhibition will then be held at the Château du Val Fleury in Gif-sur-Yvette in January 2020, after which it will travel the country.

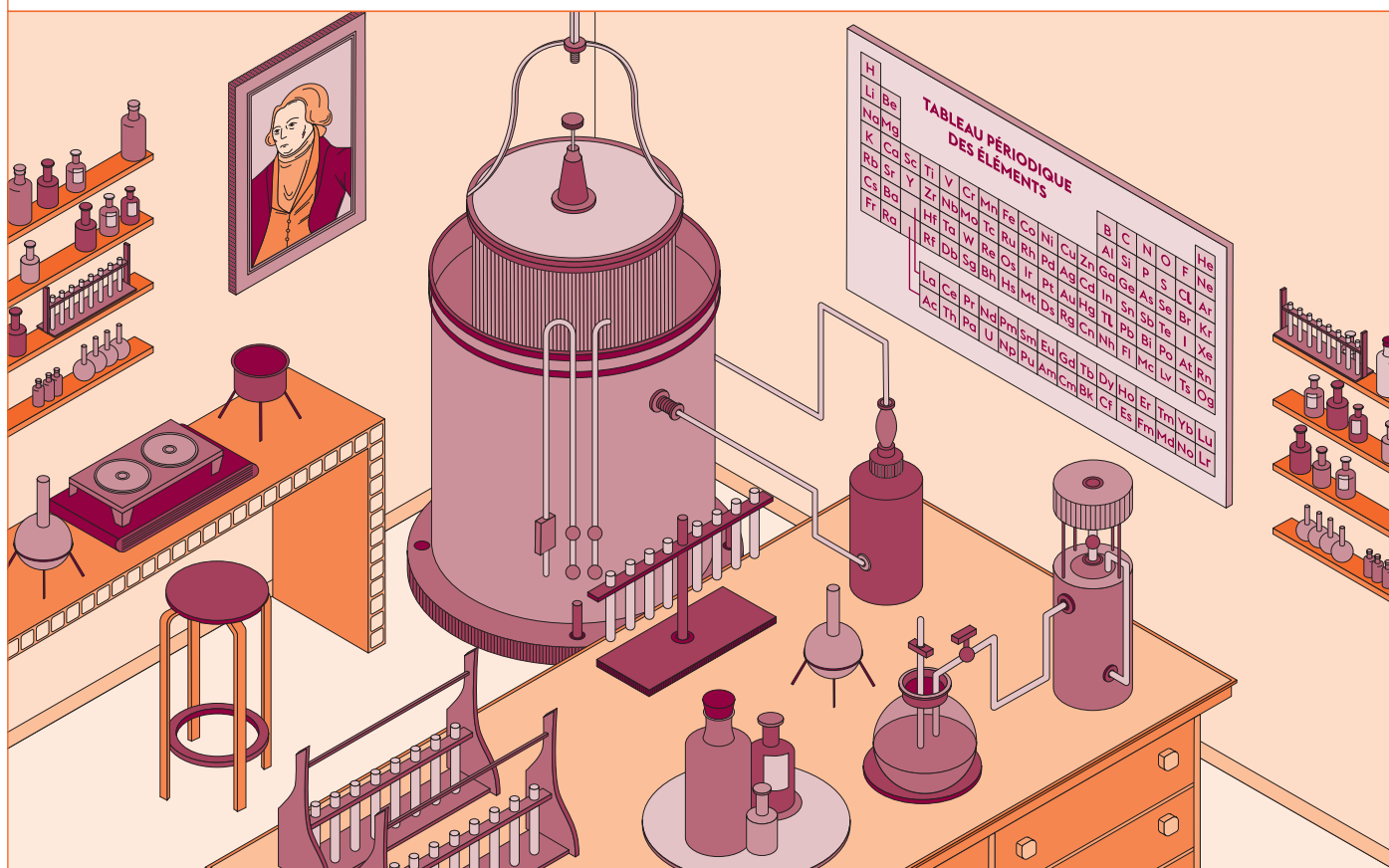
Illustrations
on the right page
and page 18:
Nini La Caille



$$I_{\mu\nu} + \sum_{\mu,\nu} \sum_{\vec{k}} P_{\mu\nu}(\vec{k}) \langle i\nu || \vec{k} \rangle \chi_{\vec{k}} - \frac{1}{2} \sum_{\vec{k}} \chi_{\vec{k}}^2 = \frac{1}{2} \sum_{\vec{k}} \chi_{\vec{k}}^2 + \frac{1}{2} \sum_{\vec{k}} \chi_{\vec{k}}^2$$
$$E_{QM/MM}[\rho] = E_{QM}[\rho] + E_{MM}[\rho] + E_{QM/MM}[\rho]$$
$$D_{Pi}(t) D_{Qj}(t) \frac{d\alpha_{ij}}{dr_z} v_z(t), \quad i\hbar \frac{\partial}{\partial t} \chi(\mathbf{R}, t) = \left[\sum_{\nu} \left[-i\hbar \nabla_{\nu} + A_{\nu}(\mathbf{R}, t) \right]^2 + \epsilon(\mathbf{R}, t) \right] \chi(\mathbf{R}, t)$$
$$\chi_{BO}^{(k)}(\mathbf{R}, t) = \frac{1}{\sqrt{2M_{\nu}}} \left[\chi_{BO}^{(k)}(\mathbf{R}, t) + \sum_{kl} \mathcal{F}_{kl}(\mathbf{R}) \chi_{BO}^{(kl)}(\mathbf{R}, t) \right] + I[\rho] + L$$
$$i\hbar \frac{\partial}{\partial t} \Phi_{\mathbf{R}}(\mathbf{r}, t) = [H_{BO}(\mathbf{r}, \mathbf{R}) + U_{en}[\Phi_{\mathbf{R}}, \chi] - \epsilon(\mathbf{r}, t)] \Phi_{\mathbf{R}}(\mathbf{r}, t)$$

Title

Chemistry, tell me your story



As 2019 was designated “Year of chemistry, from primary school to university” in France and the “International Year of the Periodic Table of Chemical Elements” by UNESCO, the historians of Université Paris-Saclay decided to set down the main changes for chemistry and its teaching over the centuries.

The child watched his father as he banged stones together, unleashing sparks. He memorised his actions and acquired the knowledge of the first men who had mastered fire. Fire was the first chemical transformation used by humans, more than 400,000 years ago. The child grew and took it into his head to heat earth, which, to his great surprise, changed colour and hardened. As well as improving food through cooking, fire made it possible to create new materials. The use of chemical transformations was thus based on knowledge and expertise that was passed on through learning. As well as that knowledge of the “chemical arts”, Greek philosophers began to speculate on the meaning of nature a few centuries before Christ. However, they did not conduct experiments, which they thought were too

susceptible to deception. They believed that the legitimate form of knowledge production should be based on common sense and knowledge that was accessible to all.

In about the 2nd century AD, alchemy developed in continuity with the practice of gold and silversmithing. Alchemists’ quest for the philosopher’s stone and a panacea distanced them from Greek rationalism. Their work led to the development of many techniques, instruments and laboratory protocols.

In Europe, it was only in the 17th century that a new, legitimate way of building knowledge emerged: experimentation. Alchemy gave way to chemistry as a rational scientific subject. Its aim was to understand the structure of matter and its transformations through a coherent theory. At the beginning of the 17th century, the first free, public chemistry class was established in the King’s garden, the ancestor of the current Museum of natural history, to complete the training of doctors and apothecaries. In the 17th and then 18th centuries, “chemists” turned to matters of analysis. They had before them a considerable variety of materials, which were essentially compounds, but did not have any way to separate their different components.

Virginie Fonteneau, director of the Laboratory for science and technical studies (EST) at Université Paris-Sud explained: “*Knowing how to analyse the products of a chemical transformation, whether solid, liquid or gaseous, was crucial for Antoine Lavoisier. The understanding of matter thus went hand in hand with the development of the tools necessary for chemical separations. Chemistry is taught through analytical means.*” Antoine Lavoisier was guillotined in 1794. Can you not hear the resonance of “*The Republic has no need of scholars*”? One of his most important discoveries was the role, in combustion, of what he called “oxygen”. Our understanding of matter and its transformations was shaken.

A new revolution was brewing. As Lavoisier had done his utmost to identify the components of chemical reactions, in England, in 1803, John Dalton (1766-1844) proposed an atomic theory to explain the difference in solubility of gases. “*This confronted chemists with a choice that divided them. Should they accept the atomic hypothesis even though they couldn’t prove it through an experiment? That hypothesis turned out to be heuristic for organic chemistry through the use of imagery enabling a ‘mental image’ of molecules, without knowing what*



actually linked the atoms,” Virginie Fonteneau stated. “At the time, chemists made great use of laboratory benches, while simultaneously calling on their imagination in a way that was simply unverifiable. Historians wondered, for example, how August Kekulé had imagined the cyclic compound benzene in 1865.”

“In Europe, it was only in the 17th century that a new, legitimate way of building knowledge emerged: experimentation.”

“The use of imagery is well-known in teaching,” she continued. “The French education system was then dominated by mathematics, which were the key to accessing the most prestigious schools. That predominance did not exist in England or Germany. In France, the idea of drawing and devising a visual for molecules was not considered good practice.” In France, atomic notation was not taken up in specialised education until 1882 and was only widely disseminated in textbooks in 1891!

Chemistry further developed in the 19th and 20th centuries, buoyed by the Industrial Revolution and the unprecedented progress made in knowledge and techniques. New branches of chemistry emerged, including quantum chemistry, supramolecular chemistry, which earned Jean-Marie Lehn the Nobel prize, biochemistry and the analysis of the macromolecules of life.

The child who learned to make fire by knocking flints together is now working on a chemistry PhD, as well as high performance computing using super calculators, but there is still that same gleam in his gaze as he works in the fascinating world of chemistry.

<http://www.est.u-psud.fr/>

» focus

The 150th anniversary of Mendeleev’s periodical table

In 1860, the theoretical chemist August Kekulé was 31. He and his peer Charles-Adolphe Wurtz decided to organise a major international congress, the first of its kind, and hold it in Karlsruhe,

Germany, to try to reach a consensus on crucial issues such as the definitions of the words “atom”, “molecule” and “equivalent”. Among the 140 chemists who attended were Dmitri Mendeleev (1834-1907), a young Russian professor, and Julius Lothar Meyer (1830-1895). They were both attempting to arrange the large number of known substances, which, at the time, were classed by element: hydrogen, followed by the substances containing hydrogen, oxygen, with the substances containing oxygen, and so on. It was a litany that was exceedingly tedious for students. They were looking for a different way to arrange the information, by detecting frequencies and grouping together elements that had similar chemical behaviours. Meyer developed the first classification system, which was published in 1862. For his table, Mendeleev also used atomic weights and tried to establish a general law. This led him to draw up a table with empty cells and predict the properties of the elements. His work and the presentation of the table, which was very different from the one we know today, were published in 1869, 150 years ago. It was one of the rare cases in which teaching directly fuelled research.

Title

Specific ethics for chemistry?

Through its links with industry and its impact on life, chemistry is a subject that inspires some of the liveliest reflections on ethics.

She got up, stretched and followed the coffee aroma that was permeating her flat. Today, she would go to work a little later than usual in her hybrid car... Coffee, smelling, digestion, the locomotion of living beings and machines... All of that is chemistry! It governs life and was probably even the origin of it. However, chemistry also has close ties to industry, which uses and develops it, particularly in pharmacology, the environmental sector, the food industry and the material-processing and energy sectors.

In the words of Karine Demuth-Labouze, teacher and researcher at the Research Ethics Department at Université Paris-Sud, “Justice,

dignity and benevolence’ are universal ethical principles that can conflict with the values at work in industry: ‘productivity, performance and competitiveness’. Chemistry has a greater stake in these dilemmas than other sciences because of its ubiquity in industry and because it offers one of the shortest paths between research and development”.

Beyond the general ethical challenges involved in research, which are addressed in the work of Université Paris-Saclay’s Research Ethics and Scientific Integrity Council (POLÉTHIS), chemistry, and particularly biochemistry, is the science that is closest to life, as well as industry. Karine Demuth-Labouze added that “In the time of biomedicine, chemistry is contributing to technicising medicine, which is changing our relation to illness, clinics and care, and which sometimes tends to treat illnesses rather than care for people”.

“I am currently working on the medicalisation of behavioural problems in children, and particularly attention deficit hyperactivity disorder (ADHD). In this area, chemistry makes it possible to alleviate symptoms, but it cannot cure them. This ‘biologising’ of the problem raises typical bioethical issues. While we can curb the inattention, impulsivity and hyperactivity of children with a synthetic compound and combat undesirable effects with additional medication, is it right to do so, without considering and resolving the underlying psychological conflicts? In the psychiatric field, the fact chemistry can rapidly change behaviour has relegated other approaches, including psychoanalysis, to the background. That means we are neglecting to treat the essential causes of patients’ suffering.” The promise, hope and progress brought by scientific research will never rule out the need for ethical reflection.

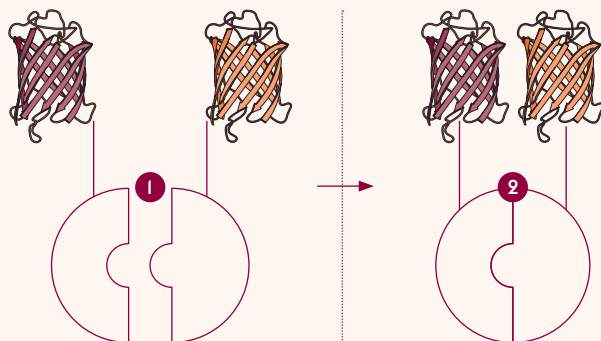
<https://www.universite-paris-saclay.fr/fr/actualite/lengagement-ethique-a-luniversite-paris-saclay>

Title

Reporter molecules lead the way in molecular labelling and detection

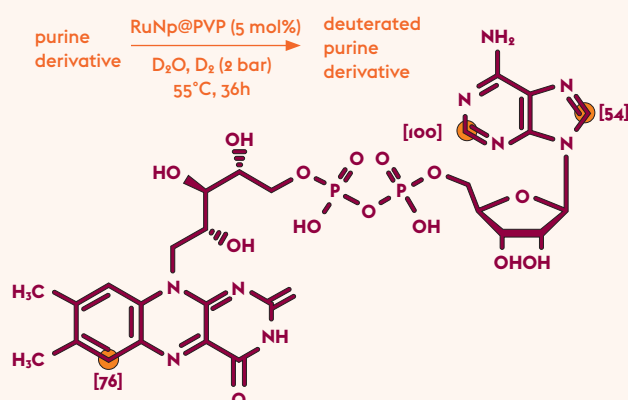
FRET APPROACH

- 1 – Couple of fluorescent proteins from the GFP family grafted onto different proteins
- 2 – The protein-protein interaction brings the fluorophore couple closer together and yields to FRET

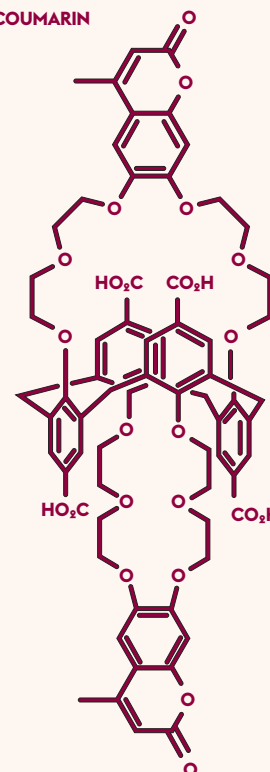


METHOD AND EXAMPLE OF DEUTERIUM ISOTOPIC ENRICHMENT OBTAINED ON FLAVIN ADENINE DINUCLEOTIDE (FAD)

● deuterium incorporation site
[X] isotopic enrichment measured by NMR



CALIXARENE MOLECULE COUPLED WITH COUMARIN



There are many different types of molecular tags and strategies employed to facilitate detection of a molecule in a sample or cell environment or to identify its partners. For an overview, read on!

A variety of biochemical and bioanalytical techniques are used to explore the chemistry of living things. At the Chemistry and Physics Laboratory (LCP – CNRS/Université Paris-Sud), the team of Fabienne Mérola and Marie Erard is developing genetically coded fluorescent probes that are grafted to proteins of interest and specifically addressable in the cell.

These tags rely on green fluorescent proteins, because GFPs possess the property of emitting fluorescence at an appropriate wave length after excitation. By chemically modifying the chromophore or its environment, it has been possible to obtain a vast array of optical biosensors that vary in color as well as performance. “The quantity of fluorescence emitted by the fluorophore (i.e. the fluorescent molecule) upon excitation to return to its fundamental state, its lifetime and its emission spectrum give us information about the environment and the

reactions to which it was exposed in the cell,” explains Marie Erard.

Fluorescence resonance energy transfer (FRET), i.e. the transfer of energy between fluorescent molecules, is one of the techniques used to decipher interactions between proteins or changes in the conformation of a single protein. “We measure the perturbation of a fluorophore’s fluorescence signal due to the presence of another fluorophore, at a certain distance,” reports Fabienne Mérola.

Towards the structural characterisation of NADPH oxydase in vivo

Recently, the team collaborated with Oliver Nüsse’s group from the same lab, combining FRET with spectromicroscopy to develop a new analytical strategy in order to elucidate the interactions and topology of the three cytosolic subunits of NADPH oxydase of phagocytic cells in a cell context. This protein, a key element of the immune system, produces superoxide anions ($\text{O}_2^{\cdot -}$) that are precursors of oxygen-reactive species, critical for host responses to microbial infections.

Once activated by a pathogen, the three cytosolic subunits undergo structural changes and

associate themselves with two membrane subunits and Protein G to form an enzyme complex with six subunits. Not only is NADPH oxydase required to mount a defense against pathogens, but it is also responsible for chronic inflammatory phenomena in certain individuals. The development of specific inhibitors would be of great therapeutic interest.

“But conventional structural approaches have only partially succeeded in characterising this type of highly ‘flexible’ protein,” says Marie Erard. “By attaching fluorescent tags to either end of each of the three cytosolic subunits, we were able to determine how the latter organise themselves in their native environment.”

Fluorescent molecule cages to detect water pollution

Considering the diversity of micropollutants in natural environments, their presence in trace amounts and their toxicity for organisms, the detection and quantification of these substances in natural environments has become a major analytical and public health challenge. Guided by the Directive 2000/60/EC establishing a framework for Community action in the field of water policy, Isabelle Leray’s research team at the Supramolecular and



Molecular Photophysics and Photochemistry Laboratory (PPSM – ENS Paris-Saclay) is working on detecting polluting species in tap water.

For this investigation, the team developed molecular sensors linking a fluorophore (e.g. coumarin, rhodamine or dansyl amide) with a calixarene, creating a molecule "cage" able to trap heavy metals in ionic form (cations) in its hydrophobic cavity. *"During complexation of the cation by the sensor, the fluorophore undergoes modifications of its photophysical properties and the fluorescence changes"*, explains Isabelle Leray.

Several improvements have been made in this method, proven to be highly sensitive in detecting ions of lead (Pb^{2+}), aluminum (Al^{3+}), mercury (Hg^{2+}), cadmium (Cd^{2+}) and cesium (Cs^{2+}). Implemented in a microfluidic system equipped with optical fibers and electroluminescent diodes, it has also been tested with optical resonators.

An alternative to existing detection systems based on electrochemistry or mass spectrometry, this system is portable and can be used directly in the field. Today, the team is focusing on the detection of pesticides, such as glyphosate (Gly^{2-}). *"We are working with metallic complexes that can trap this dianion by means of hydrogen bonds."*

Using isotopic exchange to label nucleic bases

Fluorescence is not the only labelling method available and sometimes researchers opt for radioactive tracers instead. At the Tritium Labelling Laboratory, part of the Molecular Labelling and Bioorganic Chemistry Department (SCBM) at the CEA Saclay research centre, Sophie Feuillastre and Alberto Palazzolo – in partnership with the Pharmacology and Immunoanalysis unit at CEA Saclay and the Laboratory of Physics and Chemistry of Nano-Objects in Toulouse – have devised an innovative approach to facilitate the labelling of nucleic bases.

Nucleic bases – belonging to the family of purines or pyrimidines – enter into the composition of nucleic acids, i.e. DNA and RNA. They also enter into the composition of many pharmaceutical drugs. Monitoring them in living organisms represents great interest for the evaluation of their efficacy or toxicity.

Isotopic exchange, a commonly used labelling method, involves replacing one or more hydrogen atoms with one of its isotopic variants (having the same number of protons and electrons but a different number of neutrons). An exchange involving the stable isotope – deuterium – or the radio-

active isotope – tritium – allows researchers to either quantitatively analyse the molecule's presence in a sample or monitor it in vivo without changing its interactions.

But it is not easy to achieve both a chemical transformation of the nucleic bases without adversely affecting their integrity and a good isotopic enrichment, especially given the temperatures higher than 80°C required by these processes.

The method developed by the researchers at the SCBM lab uses ruthenium nanoparticle catalysts and is compatible with a wide array of solvents and lower temperatures (under 55°C). *"The reaction takes place at the surface of the nanoparticle by activation of the substrate's C-H bond,"* points out Alberto Palazzolo. Sometimes bound within a polymer matrix, sometimes stabilised by organo – or hydrosoluble carbenes, these nanoparticles lead to an isotopic enrichment ranging from 50 to 99%.

"The method works with many substrates (e.g. nucleosides, nucleotides and oligonucleotides). Today, we're studying the compatibility of other metals with pyrimidine bases."

Publications

· Cornelia S. Ziegler et al., Quantitative live-cell imaging and 3D modeling reveal critical functional features in the cytosolic complex of phagocyte NADPH oxidase. *J. Biol. Chem.* (2019) 294(11) 3824–3836.

· Xuan Qui P. et al., New water-soluble fluorescent sensors based on calix[4]arene biscrown-6 for selective detection of cesium. *Journal of Photochemistry and Photobiology A-Chemistry*, 2018, 364, 355–362.

· Alberto Palazzolo et al., Efficient Access to Deuterated and Tritiated Nucleobase Pharmaceuticals and Oligonucleotides using Hydrogen-Isotope Exchange. *Angew.Chem.Int.Ed.* 2019,58,4891–4895.

» focus

Fluorinated peptidomimetics: from phytosanitary to medicinal chemistry research

The team headed by Sandrine Ongerî at the BioCIS Laboratory (CNRS/Université Paris-Sud) specialises in designing therapeutically active fluorinated amino acids and peptidomimetics. Currently, it is participating in two collaborative projects funded by the European Commission under the Horizon 2020 Programme.

The purpose of the FET-Open NoPest project, launched in January 2019, is to find alternatives to the copper salts used massively to fight the oomycetes responsible for grapevine downy mildew.

"Although this pesticide is accepted for use in organic farming, it's highly toxic for aquatic organisms, contaminates groundwater and has been mentioned in association with the appearance of cancers or neurodegenerative diseases," reports Sandrine Ongerî. Five partners (four academic and one industrial) are joining forces to develop innovative technologies for the detection of parasites on grapevines, identify enzymes key for their survival, model and synthesise their peptide inhibitors, and do market studies. *"We're designing and synthesising peptidomimetics that are more effective and more stable."*

The TubInTrain project, an innovative training network in the field of medicinal chemistry, will start in October 2019 and focus on the microtubule degradation associated with neurodegenerative diseases. This consortium is composed of seven beneficiaries and fourteen partners (including ten industrial firms). *"Our team is developing peptidomimetics to inhibit the interactions or aggregation of the alpha-synuclein and tau molecules."* Mainly oriented towards doctoral training, the project is to recruit thirteen doctoral students in first quarter 2020, including three to work at the BioCIS lab.

www.h2o2onopest.org
www.tubintrain.eu

» focus

"Click and release" reactions: bioorthogonal chemistry for controlled drug release in vivo

Developing chemical reactions compatible with biological environments is a major scientific challenge. One such reaction between a iminosynnone and a cycloalkyne, described in 2017 by researchers at the SCBM Unit at the CEA Saclay research centre, is used to trap molecules by ligation, then release them by cleavage. In a recent report, researchers showed that this in vivo strategy has big potential for applications. Using a bioorthogonal cleavage reaction, they succeeded in controlling the release of fluorescent molecules contained in tumor-targeting micelles, only once they were inside the cancer cells.

Publication · Karine Porte et al., Controlled Release of Micelle Payload via Sequential Enzymatic and Bioorthogonal Reactions in Living Systems. *Angewandte Chemie Int. Ed.* (2019)

BUSINESS & INNOVATION

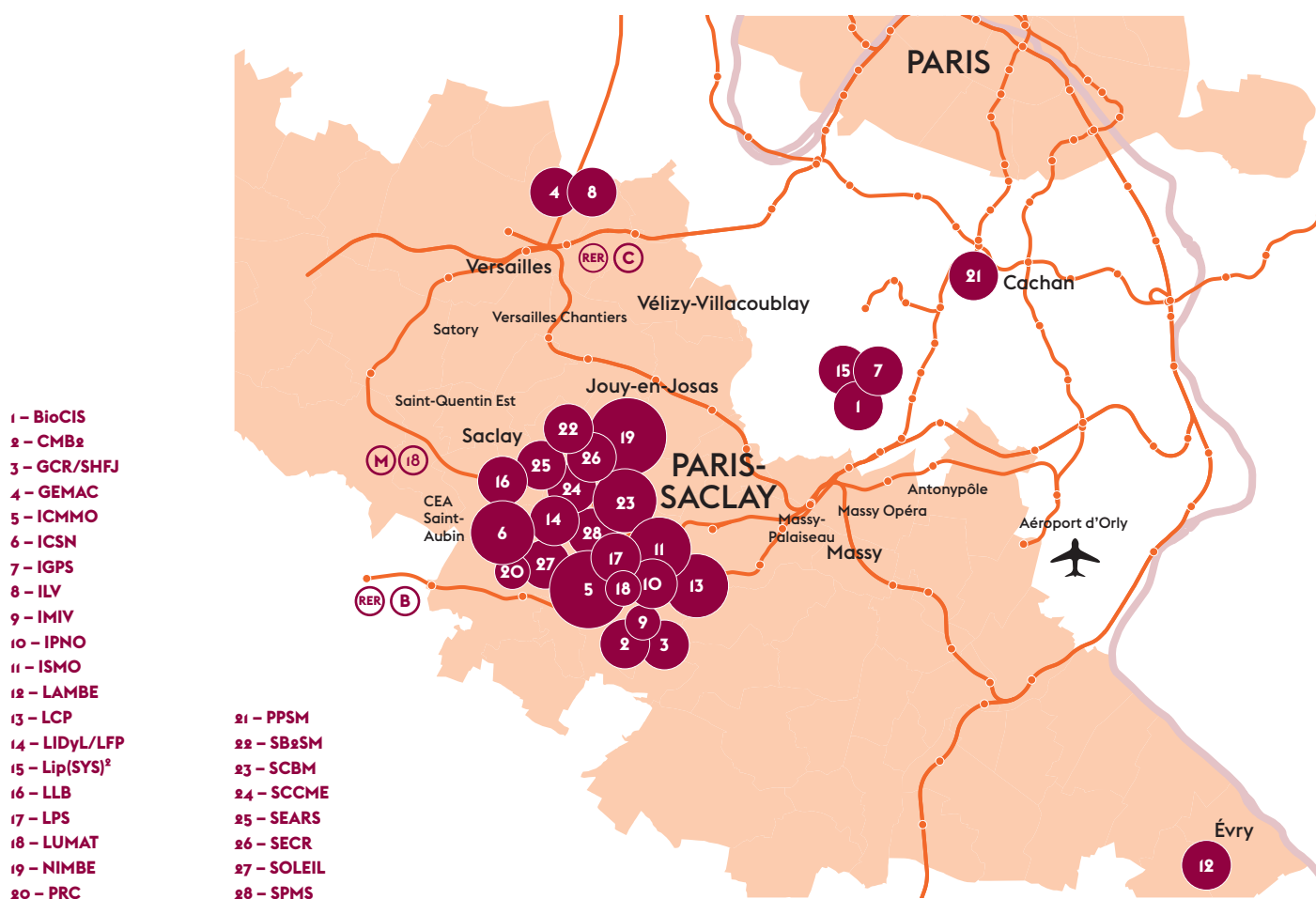
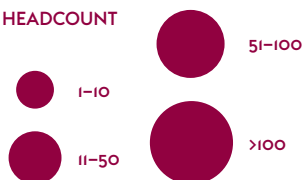
Chemistry – PATTOX – C@PS – microRNA
microfluidic detection – Bichromatics

Title

Chemistry at Université Paris-Saclay

Université Paris-Saclay has true strengths in chemistry, both scientific and educational. It can thus make a real contribution to society's major challenges: energy, environment, information, innovation, health and scientific outreach.

HEADCOUNT



28
research
units

1 150
researchers,
teachers/
researchers,
engineers and
technicians

Our major, cross-cutting research areas:

- From the study of elementary reactions to analytical methods in physical chemistry
- Chemistry of materials, interfaces and nano-objects

- Molecular architecture
- Chemistry and physical chemistry of and for living beings
- Multiscale theory and simulations, developments and applications
- Platforms and large instruments

Four laboratories of excellence (LabEx)

- CHARMMMAT
- LERMIT
- NanoSaclay
- PALM

Chemistry courses
at Université
Paris-Saclay

300
Master's students

400
PhD students

4 first-year Master's degrees:

- Chemistry
- Chemistry - Frédéric Joliot-Curie track
- Bidisciplinary chemistry and biology
- Chemistry - international track (SERP+)

12 second-year Master's degrees:

- Inorganic chemistry- molecules, surfaces and nano-objects
- Organic chemistry
- Pharmaceutical chemistry
- Physical chemistry- instruments, concepts and applications

- Higher education chemistry training
- Chemical and biomolecular engineering
- Instrumentation and methods of molecular analysis
- Chemical pollution and environmental management

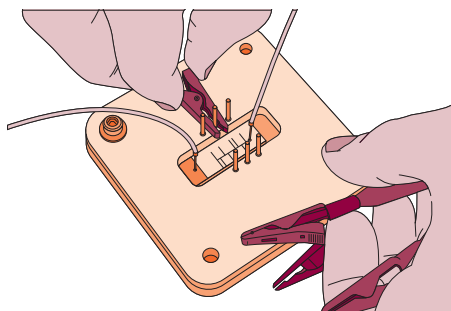
- Science, technology and societies
- Research and development for analytical strategies
- Molecular chemistry and interfaces
- Industrial and medical applications of radiation (SERP-Chem)

Three PhD schools:

- Chemical science: molecules, materials, instrumentation and biosystems
- Basic to applied therapeutic innovation
- Interfaces



The search for biomarkers



Microfluidics, a technology enabling the handling of small volumes of fluid, is a rapidly expanding research field, particularly regarding the analysis of biomarkers. A team from the Centre for Nanoscience and Nanotechnology (C2N – CNRS/Université Paris-Sud) patented a miniaturised device that can quickly detect microRNAs circulating in blood. MicroRNAs are biomarkers that show great promise for the early detection of the muscle injuries behind different illnesses (cardiovascular illnesses, haemorrhages, cancerous lesions). The device uses hyperthermia and electrochemical detection technology. It is so sensitive that it can detect the conditions at a very early stage. The analysis takes less than three hours, whereas older technology such as polymerase chain reactions (PCR) takes more than twice that long.

The proof of concept is based on a change of paradigm with regard to PCR. It combines phases of magnetic capture, release (magnetic hyperthermia) and electrochemical detection. It was validated for synthetic microRNAs (miR-122) involved in liver cancer. Other applications outside the field of medical diagnostics could be considered, for instance in health inspections.

www.c2n.universite-paris-saclay.fr/fr

Bichromatics will astonish you

Bichromatics is a startup founded on two researchers' wonder at colour and the unexpected visual effects generated by gold particles. Olivier Pluchery is a physics professor at Sorbonne Université and Hynd Remita a senior researcher at the Physicist Chemistry Laboratory (LCP – CNRS/Université Paris-Sud). "Everyone knows that metallic gold is yellow. However, we also know how to condition it to give it a far more varied colour palette," explained Hynd Remita. "The collective oscillations of the electrons of a gold nanoparticle – plasmons – can be excited by a

light wave. They depend on the size and shape of the nanoparticle, its environment and the polarisation of the light." The gold is then imbued with many colours.

Bichromatics has thus created 100% gold and silver-based liquid pigments with astonishing colours. These pigments are plasmonic, non-organic and inalterable. The patented technology, upon which the start-up was built, also has other uses such as creating an orange-hued film that projects a blue shadow! Bichromatics won the Cosmetic Victories in 2018.

www.bichromatics.com

PATTOX: quickly and inexpensively detecting agri-food contaminants

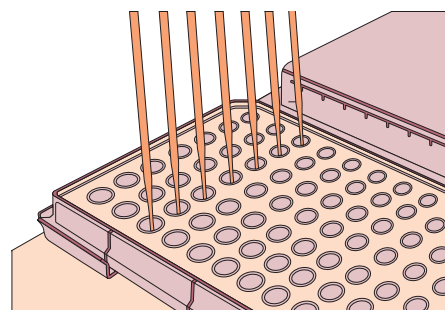


Established in autumn 2019, PATTOX is a start-up that is developing a portable device for biological analyses and diagnoses based on an electrochemical biosensor, which can detect pathogens and toxins in agri-food products. The patented technology is the result of research conducted by Hafsa Korri-Youssoufi and her team at the Orsay Institute of Molecular Chemistry and Materials (ICMMO – CNRS/Université Paris-Sud). Once a sensor specific to the microorganism under study is selected, the device works by measuring the electrochemical response to the target biomarker. "If the sample is contaminated, the link between the sensor and the biomarker generates an electrical current – so a positive signal – proportional to the quantity of target molecules contained in the sample," explained Hafsa Korri-Youssoufi. The test, which is inexpensive, straightforward, reliable and fast, taking only a matter of minutes, can detect even very low concentrations of microorganisms.

The first target audience is the wine market and its stakeholders (oenologists, wine-growers, winemakers, wine merchants, etc.). Nawel Mejri-Omrani, former PhD student at the ICMMO and current CEO of Pattox, commented: "The device can detect *Brettanomyces*, a yeast that can develop in wine at any stage of its production. It causes an irreversible loss

in quality." The startup will then turn to the milk sector to detect bacteria such as *Listeria*, and then, the medical sector, for the early detection of illnesses such as cancer and tuberculosis.

An IBISA platform for identifying biologically active molecules



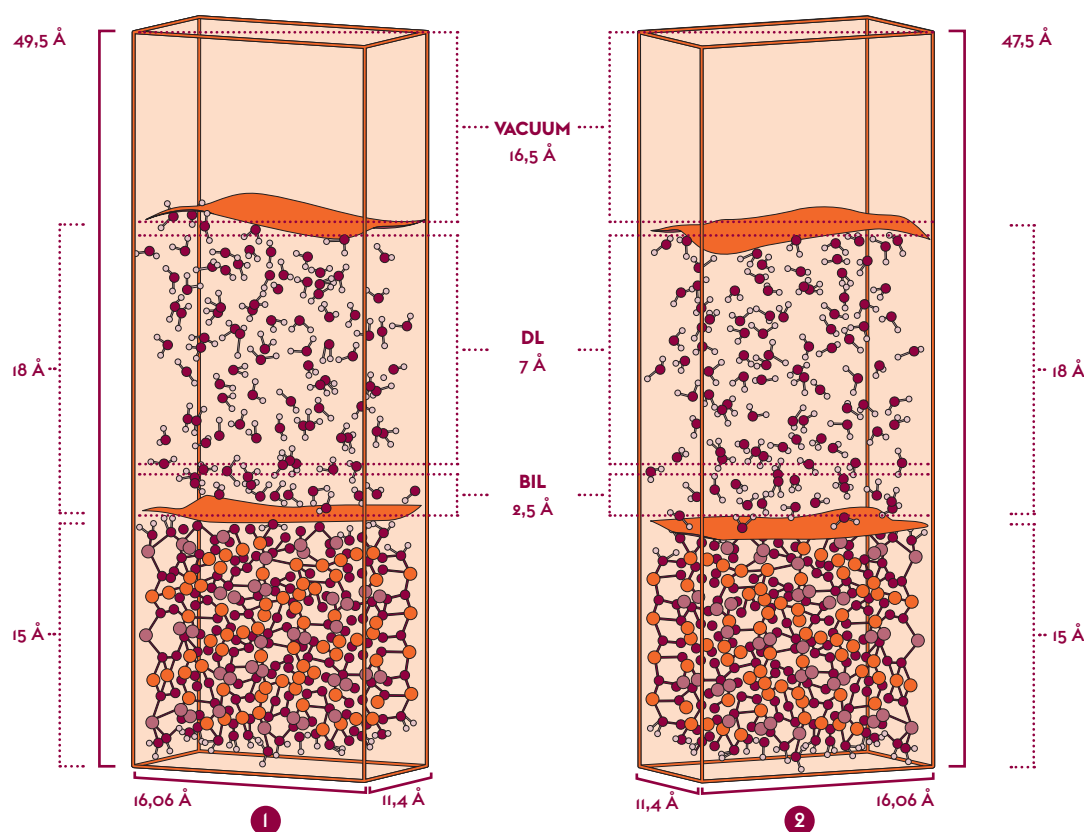
Chemists are able to create tens of thousands of drugs. As of yet, the biological activity of many of them is still unknown. How can we study these drugs and determine their effects so we can produce new treatments? If such work was carried out drug by drug and illness by illness, it would take centuries. That is where high-throughput screening robotics come in. They perform thousands of repeatable operations each day to test the activity of the different drugs on biological targets.

The high-throughput screening platforms of the Saclay plateau's chemical libraries have gathered under a single banner, taking up the name of C@PS (Criblage sur le plateau de Saclay – high-throughput screening at Plateau de Saclay). At the end of 2018, C@PS acquired the IBISA (infrastructure for biology, health and agricultural science) label, earning national recognition. It combines the skills of several platforms: the Saclay French Alternative Energies and Atomic Energy Commission's (CEA) CCCHD, which specialises in combinatorial chemistry and high-throughput screening, the Institute for the chemistry of natural substances' (ICSN) high-throughput screening CIBI/CTPF in Gif-sur-Yvette and Université Paris-Sud's CIBLOT (high-throughput screening, biology-chemistry interface and operational transfer laboratory) in Châtenay-Malabry. C@PS provides the only offer of its kind in France, with radioactive high-throughput screening (³H, ¹⁴C, ³⁵S), thermal high-throughput screening, high-throughput in ovo screening and AlphaScreen-based high-throughput screening, as well as the screening of organelles and tumoroids.

<https://www.ibisa.net/plateformes/detail.php?tri=&srch=&q=582>

Title

Modelling Complex Molecular Systems



DFT-MD SIMULATIONS OF AN INTERFACE BETWEEN COBALT OXIDES AND WATER

1 – 352 solid atoms and 120 water molecules.

2 – 320 solid atoms and 120 water molecules.

Adapted from Marie-Pierre Gaigeot et al., DFT-MD of the (110)-Co₃O₄ cobalt oxide semiconductor in contact with liquid water, preliminary chemical and physical insights into the electrochemical environment. *J. Chem. Phys.* 150, 041721 (2019).

By means of computation and simulation, the theoretical chemists at Université Paris-Saclay decipher the processes, chemical properties and molecular dynamics of systems in cases where the time scale or complexity remain inaccessible to experimentation.

“A few years ago, theoretical chemistry entered a glorious period,” says Marie-Pierre Gaigeot, head of the Theory and Modelling team at the Laboratory of Analysis and Modelling for Biology and the Environment (LAMBE – CNRS/Université d’Évry/Université Cergy-Pontoise/CEA). “Thanks to today’s supercomputers, we’ve seen steady progress in simulation opportunities.” David Lauvergnat, head of the Theory and Simulation (ThéoSim) group at the Chemistry and Physics Laboratory (LCP – CNRS/Université Paris-Sud), adds: “The tremendous advances made in software and computing power allow us to carry out increasingly long simulations and deal with increasingly complicated and realistic systems, even if hardware architecture often evolves faster than programmes do.”

Theoretical chemistry applies the principles and basic equations of quantum mechanics to

the study of the structural, dynamic or spectroscopic properties of matter or those relative to its chemical reactivity. This field has several branches – e.g. quantum chemistry, digital (computational) chemistry and modelling as well as molecular dynamics and mechanics – whose respective methods are now crossing over between them. “Previously, if we wanted to study a molecule that was a bit large, we would treat certain parts of it schematically to simplify the qualitative analysis. Today, we can study larger systems by applying a combination of techniques to a single computing operation. We can treat the electronic structure with greater precision using, say, the density functional theory (DFT) – a particular quantum computing method – and the environment with less precision using a molecular mechanics method,” explains David Lauvergnat.

Far from abstract, the problems dealt with in theoretical chemistry are often inspired by difficulties encountered during experiments. Researchers doing simulations engage in ongoing give-and-take with their colleagues in the lab. “Simulations make it possible to investigate phenomena occurring at time scales incompatible with experimentation, measured in picoseconds (10^{-12} s), femtoseconds (10^{-15} s)

“Today, we can study larger systems by applying a combination of techniques to a single computing operation.”

David Lauvergnat

or even smaller units of time,” comments David Lauvergnat. “Today’s theoretical chemistry methods are sufficiently mature to be able to couple experiments, data analysis and digital computations confirming or infirming a model, then obtain a detailed description of a system.” Marie-Pierre Gaigeot agrees, adding that “Often, the people doing experiments ask us to help them rationalise their results.”

A hard-to-investigate solid/liquid interface

At the LAMBE lab, Marie-Pierre Gaigeot is looking for approaches combining ab-initio molecular dynamics and vibrational spectroscopy to apply to matter in all states (e.g. molecules, gas-phase clusters and complex interfaces). She is especially interested in the



electrolysis of water (“splitting” water) to generate dihydrogen – a clean, sustainable vector of energy – and finding the best catalysts for the reaction. More specifically, she is investigating the role played by the area at the interface between a material (solid) and water (liquid). Little is known about the structure or dynamics of this interface, which still has many mysteries to be elucidated. How do water molecules organize themselves at the surface of a material? Which atoms are present and which surface sites are key to the reaction? What is the surface’s state of oxidation-reduction and protonation? *“It’s very hard to answer these questions by means of experimentation. Working at atomic scale with very short reaction times considerably limits the number and type of feasible experiments.”*

She and her team recently used simulation to evaluate the degree of a silica surface’s hydrophobicity or hydrophilicity. She showed that, although the material was hydrophilic at the macroscopic level, it presented hydrophobic areas at the microscopic level, inducing a particular structural organisation of water at the interface. *“The resulting structural and molecular dynamic properties could yield a different chemical reactivity,”* points out the researcher. *“By adapting the design of the surface, one could influence its hydrophobicity or hydrophilicity, hence modulate the reaction.”* The team has also been working to characterise the structural organisation and dynamics of water at the interface with semiconductors of cobalt oxide, a material that is potentially more durable, economical and eco-friendly than those typically used to split water.

Exploring biological processes

The LCP lab team, headed by David Lauvergnat, also does work of a cross-cutting nature. Aurélien de la Lande, a member of the ThéoSIm research group, is interested in the processes and effects of ionising radiation (e.g. protons, alpha particles, X-rays and gamma rays) – which releases a great deal of energy – on living biological material. *“During irradiation, the ionising rays dislodge electrons from molecules, very quickly inducing a violent chemical reaction and greatly destabilising the molecules, which become denatured. This can lead to premature aging or cancer, depending on the type of molecule irradiated (e.g. DNA, protein or from the lipid layer).”* Working with teams from the LCP lab, he carries out digital simulations to establish what happens in the first instants of irradiation on a time scale measured in femtoseconds or even attoseconds (10^{-18} s). *“The idea is to describe the movement of electrons affected by the ionising rays and understand how energy deposited on a molecule is transmitted to the nuclei of atoms, helping it dissipate into the environment. For now,*

using fairly large pieces of DNA, we’ve managed to simulate the effect of localised irradiation on a base, then the displacement of charges within the molecule.” Currently, Aurélien de la Lande has high hopes regarding the development of analytics tools.

This team is also exploring electron transfers in biomolecules, cryptochromes and photolyases and their possible involvement in magnetoreception in migrating species. Fabien Cailliez explains: *“When these proteins absorb blue light, a cofactor – flavin – is excited, triggering a cascade of electron transfers between the molecule’s tryptophan amino acids. According to the current hypothesis, this cascade, one of the fastest ever known in a biological environment, may be what enables species to get their bearings in the earth’s terrestrial magnetic field in the course of their migration.”* With the help of this double representation combining quantum chemistry and molecular mechanics, Fabien Cailliez was able to better understand events on the atomic scale and validate his model by comparing his results with the experimental data obtained by the team of Pavel Muller and Klaus Brettel from the Institute for Integrative Biology of the Cell (I2BC – CEA/CNRS/Université Paris-Sud). Verdict: *“We gained temporal resolution!”* In the near future, a thesis co-supervised with the University of Exeter will be shedding further light on the subject.

While theoretical and digital methods have lifted the veil on a number of mysteries, there remain many more to be plumbed.

Publications

- Marie-Pierre Gageot *et al.*, Molecular hydrophobicity at a macroscopically hydrophilic surface. *PNAS*, January 29, 2019, vol. 116, no. 5, 1520–1525.
- David Lauvergnat *et al.*, H₂, HD, and D₂ in the small cage of structure II clathrate hydrate: Vibrational frequency shifts from fully coupled quantum six-dimensional calculations of the vibration-translation-rotation eigenstates. *J. Chem. Phys.* 150, 154303 (2019)
- De la Lande A. *et al.*, Molecular Simulations with in-deMonk QM/MM, a Tutorial-Review. *Molecules*. 2019 Apr 26;24(9).
- Fabien Cailliez *et al.*, Quantum effects in ultrafast electron transfers within cryptochromes. *Phys Chem Chem Phys*. 2016 Aug 21;18(31):21442–57.

» focus

Quantum dynamics and approximation methods

The state and observable properties of a quantum system (atom, molecule, molecule cluster or macromolecule) are determined by the molecular wave

function. *“To describe these systems on computer and understand their reactivity, we sometimes have to simplify the wave function by making approximations,”* remarks Federica Agostini, who works at the Chemistry and Physics Laboratory (LCP – CNRS/Université Paris-Sud). For instance, the Born-Oppenheimer approximation is heavily used in molecular dynamics and quantum chemistry. *“Here, we assume that the electrons are moving very quickly and remain in a given electronic state and that the nuclei, much heavier than the electrons, move very slowly.”* In some cases – e.g. when a molecule absorbs light containing enough energy to trigger an electronic transition – the approximation breaks down. The nuclei of the excited molecule move very quickly, which calls for new theoretical approximations, such as the Born-Huang and Exact-Factorization representations, both of which constitute effective approaches.

Publication · Federica Agostini *et al.*, Different flavors of nonadiabatic molecular dynamics. *WIREs Comput Mol Sci*. 2019;e1417.

» focus

A center for HPC (high-performance computing) simulation

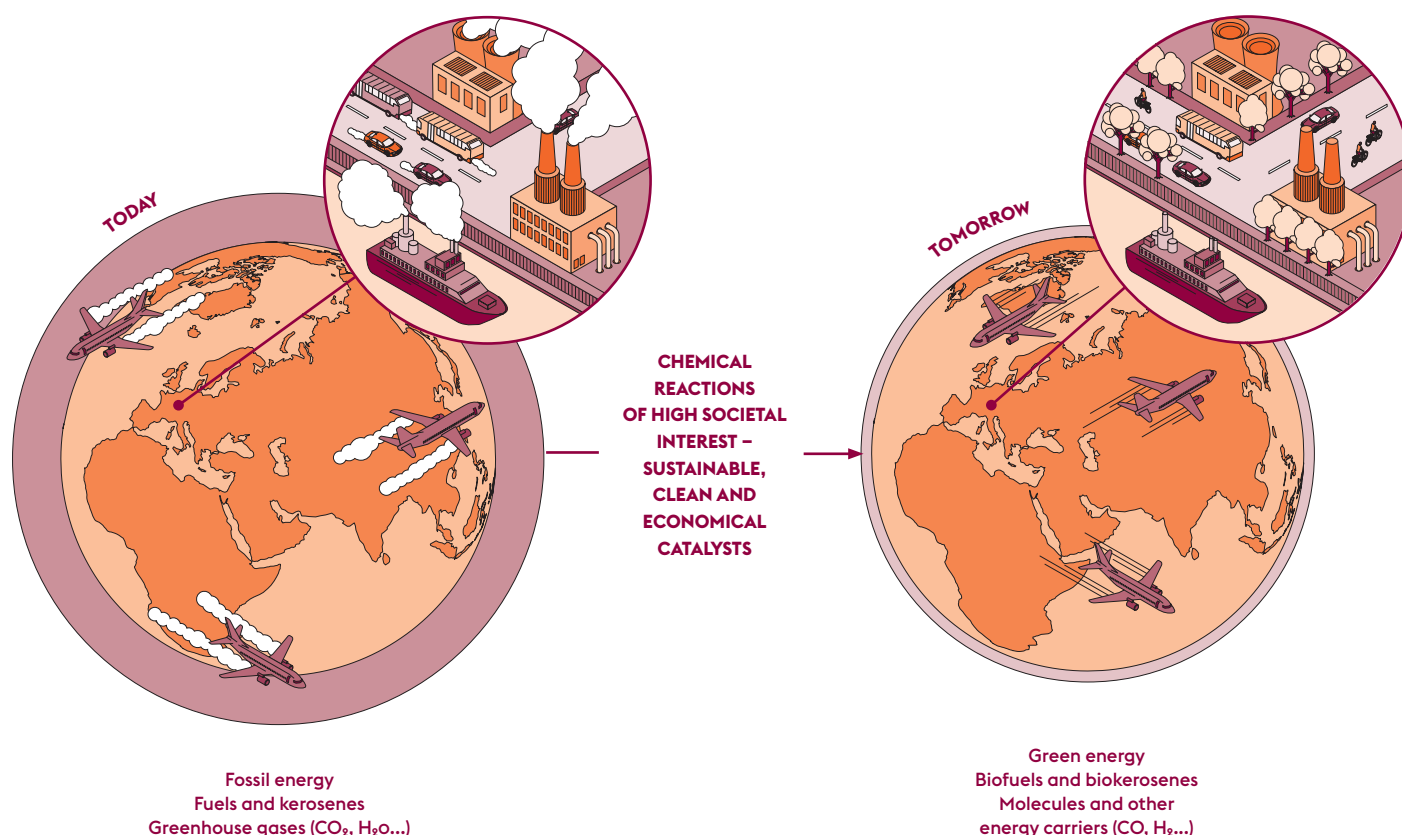
The Maison de la Simulation (Simulation House) is a laboratory co-run by the Alternative Energies and Atomic Energy Commission, the National Centre for Scientific Research, Université Paris-Sud and Université Versailles Saint-Quentin-en-Yvelines. It aims to promote the emergence of a national HPC community and get French researchers to optimise their use of national and European computing resources. The idea is to adapt programming models and software to existing – and future – machines and prepare users to make the best possible use of them.

In the fields of chemistry and materials, the Simulation House is currently lending its support to research teams seeking to develop HPC methods and codes for electrochemistry and energy, investigate solvation phenomena or study high pressure hydrogen phases, providing a complete quantum description of the nuclei and electrons.

www.maisondelasimulation.fr/index.php

Title

Moving towards the substitution of oil with alternative energy



The chemists of Université Paris-Saclay have taken an interest in new, cleaner and more sustainable energy sources, in order to free ourselves from oil while reducing the levels of greenhouse gases (GHGs) in the atmosphere.

Oil, a fossil fuel that is heavily exploited by humankind, is still the main raw material used as fuel for current means of transport. The environmental problems caused by oil and its contribution to climate change through the GHGs produced by its combustion call for its progressive but inevitable replacement by cleaner, more sustainable, alternative forms of energy.

Biofuels, which come from renewable, organic plant matter (sugar, vegetable oils, agricultural and forest waste, etc.), are now used, in varying proportions, in almost all the liquid fuels used for cars. Aware of its own environmental impact, the aeronautics sector is also taking an interest in biokerosene as an alternative to Jet A-1 fossil kerosene.

“In the aviation sector, this type of kerosene is a reference,” explained Mickaël Sicard, senior

research fellow with the Chemistry of Energetic Materials, Emissions and Environmental Impact (CMEI) research unit within the Multi-Physics Department for Energy (DMPE) at ONERA, France’s aerospace lab. *“It meets very strict specifications and performance needs, to ensure the optimal performance of plane.”*

On the proper functioning of biokerosene in the aeronautics sector

Described according to its chemical composition (concentration in aromatic compounds, sulphur, etc.) and properties (density, viscosity, freezing point, etc.), biokerosene must comply with Jet A-1 standards. Some procedures have now been certified by ASTM International, a standards organisation for materials, products, systems and services. However, biokerosene is permitted only as a blend with Jet A-1, making up a mere 10 % to 50 % of the fuel.

In its laboratories, ONERA is evaluating the proper functioning of the entire fuel system, from the tank to the emissions, with regard to the alternative fuels provided as part of national or European projects. Mickaël Sicard commented, *“For instance, the aim of the European programme JETSCREEN is to connect chemical composition and properties: what impact will*

the concentration of the fuel’s aromatic compounds have on the swelling of the seals and the emissions? How will the fuel behave when it’s cold as opposed to when it’s hot?” Using test beds, ONERA is simulating the working conditions of the fuel and engine system so it can describe the fuel as accurately as possible.

Water, an underestimated greenhouse gas?

There is another problem: vapour trails, the famous white plumes that sometimes linger in the sky long after planes have vanished. Weeded Ghedhaïfi, research engineer in the same ONERA unit, explained that *“Depending on climate conditions – temperature, ambient humidity, pressure, etc. – these trails, which are made up of ice crystals, can turn into high-altitude cirrus clouds. This cloud cover changes the Earth’s radiation balance, causing it to warm up or cool down. We suspect that its impact could exceed that of carbon dioxide (CO₂), although we don’t know its exact value.”*

The main culprits behind the formation of ice crystals are the soot and aerosols emitted by plane engines, as they serve as condensation nuclei. The water molecules emitted by the engine and those in the ambient air settle on



those surfaces, then, depending on thermodynamic conditions, can form ice crystals.

"We're studying the emissions, dispersion, chemical evolution and interactions of the different compounds emitted by aeroplanes, from the engine until a few kilometres further on," Weeded Ghedhaïfi commented. In her research, she uses parametric studies and digital simulations. Among other parameters, these take into account the type of fuel, motorisation, plane, strategy and flight efficiency, just like PHYWAKE, the national programme backed by France's Civil Aviation Authority (DGAC). *"In time, our ambition is to provide recommendations to limit their environmental impact."*

Molecular catalysts to produce dihydrogen

Producing sufficient quantities of a fuel that could compete with oil while reducing the concentration of GHGs already in the atmosphere is not a trifling matter. In search of a virtuous cycle, the chemists of Orsay Institute of molecular chemistry and materials (ICMMO – CNRS/Université Paris-Sud) are banking on the capture and recycling of the molecular culprits, as well as the use of other energy carriers.

They are currently interested in some chemical reactions of high societal value requiring the use of catalysts. These are generally noble metals such as platinum. They are costly and global stocks are dwindling. That is why researchers are developing new, more sustainable catalysts that contain no trace of precious metals and are less expensive.

Loïc Assaud and his colleagues are particularly interested in the generation of dihydrogen (H_2) through the electro(photo)lysis of water using molecular catalysts. The team is developing complexes using transition metals, the electroactive centre of which contains an atom of iron, nickel or cobalt. They are also grafting on organic ligands to improve the catalysts' redox properties.

Recently, the team developed an electrocatalyst based on cobalt clathrochelates and evaluated its electrocatalytic activity, either dissolved in the acidic electrolyte or functionalised at the surface of a working electrode. *"We observed that electrocatalytic activity was exacerbated when the catalysts were immobilised at the surface of the electrode. By tweaking their molecular chemistry, we optimised our deposition technique for covalent, robust, lasting electrografting and maximal electrocatalytic activity,"* commented Loïc Assaud. The emissions output of H_2 amounted to nearly 80 % and its performance came close to those of platinum catalysts.

The next step is to take the operation to the industrial scale. *"We now have to implement that system over greater surfaces, reaching 600 cm²."*

When nature becomes a Muse

Inspired by biology, the new catalyst developed by Ally Aukauloo at the ICMMO and Winfried Leibi's team at the Institute for integrative cell biology (I2BC – CEA/CNRS/Université Paris-Sud) reduces the CO_2 in water to CO. Ally Aukauloo commented, *"The CO_2 molecule is extremely stable. To break the C=O bonds, you have to tackle the central carbon atom and its electrons and protons, which, thermodynamically and kinetically speaking, is a very constrained process. If we deform the molecule a little through the interplay of hydrogen bonds, activation becomes easier. Catalysis is a three-dimensional problem!"*

"Catalysis is a three-dimensional problem."

Ally Aukauloo

Made of iron porphyrin, a cyclically structured molecule containing an iron atom in its central cavity, their catalyst imitates the active site of carbon monoxide dehydrogenase (CODH), an enzyme found in bacteria. *"By examining the active site of CODH, we noticed that two amino acids were pointing towards the metallic centre – the "electron source" – of the enzyme, creating hydrogen bonds with the CO_2 substrate. When we added urea groups to iron porphyrin, that is what we recreated."* It is noteworthy that this catalyst does not require the addition of an external acid. *"The H_2O molecules go into the catalyst with the substrate and supply the protons needed for the reaction."* Stable, sustainable, effective and energy-efficient, this new catalyst shows promise. *"We must now deepen our understanding of the internal mechanisms through a photochemical approach,"* concluded Winfried Leibl.

Publications

- Jourmada Al Cheikh et al., Engineering a cobalt clathrochelate/glassy carbon interface for the hydrogen evolution reaction. *Applied Catalysis B: Environmental*. Volume 250, 5 August 2019: 292-300.
- Gotico P. et al., Second-Sphere Biomimetic Multipoint Hydrogen-Bonding Patterns to Boost CO_2 Reduction of Iron Porphyrins. *Angew Chem Int Ed Engl*. 2019 Mar 26; 58(14): 4504-4509.
- Mickaël Sicard et al., Explic Program - Impact Of Aromatic Types And Quantities On O-Ring Polymers, 15th International Symposium On Stability, Handling And Use Of Liquid Fuels, Rome 2017.
- J.C. Khou et al., CFD simulation of contrail formation in the near field of a commercial aircraft: effect of fuel sulfur content. *Meteorologische Zeitschrift* Vol. 26 No. 6 (2017): 585 – 596.

» focus

Innovations in catalytic science based on renewable carbon sources

"Faster, cleaner, more efficient." That could be the motto for Université Paris-Saclay's catalytic research. *"Catalysis is actually one of the 12 principles of green chemistry,"* said Damien Prim, researcher at the Institut Lavoisier de Versailles (CNRS/Université de Versailles – Saint-Quentin-en-Yvelines) and coordinator of the Paris-Saclay Institute of catalytic science for sustainable chemistry (ISC²D). This virtual institute, labelled a strategic research initiative, has rallied several scientific communities, including those of Université Paris-Saclay's catalytic, human, social and environmental sciences, to develop innovations in catalytic science from renewable carbon sources.

"It is now becoming imperative to take into account the entirety of a product's value chain, from its design and sourcing in raw materials to its recycling or final destruction. The challenge is to develop new catalytic procedures that are sustainable and based on permanent, renewable resources, with a minimal environmental impact. The idea would thus be to replace manufactured products obtained through oil processing with bio-based products. For that to happen, we need to develop the tools."

www.universite-paris-saclay.fr/fr/isc2d





Seen from

Tsuyoshi Kawai,
of NARA Institute of Science
and Technology (NAIST),
Japan

© Tsuyoshi Kawai-NAIST



Rémi's research and mine are very complementary. He has very good skills, background and knowledge in ultrafast spectroscopy and very nice achievements in microscopy. I have a good background in compounds and chiral chemistry.

This motivated us to start the collaboration. We thought that our research dreams could come true! We want to get more evidence of the role of circularly polarised light, like possibly in plant growth, and make cheap procedures to create this

light. We need to design new molecules and compounds that could have a strong circularly polarised light emission and to characterise them.

Professor at NAIST, Tsuyoshi Kawai is in charge of the Photonic Molecular Science Laboratory. His research focuses on the study of molecules, polymers, compounds and low-dimensional nanomaterials that actively interact with photons and present advanced photofunctionality.

The collaboration that currently links his team to that of Rémi Métivier, of the Laboratory of Supramolecular and Macromolecular Photophysics and Photochemistry (PPSM) at ENS Paris-Saclay, focuses on photochromic materials and molecules capable of changing colour under the influence of ambient light, supramolecular fluorescent systems (nanofibers) and luminescent chiral molecules, i. e. circularly polarised light emission. Beyond the fundamental interest of understanding these mechanisms, this research also points to promising and emerging applications in the fields of cosmetics, smart agriculture, biological imaging, document security or optical information storage.

The teams of Tsuyoshi Kawai and Rémi Métivier have known each other and have been working together for several years now. The meeting dates back to their joint participation in the International Research Group Photo-switchable Organic Molecular Systems & Devices (GDRI PHENICS), which ran between 2008 and 2015. At the end of it, the two teams

began to work together more closely, notably through the Photosynergetics consortium, to which NAIST belonged. In January 2018, the signature of the Associate International Laboratory (LIA) Nano-Synergetics (Photo-active Nanomaterials with Cooperative and Synergetic Responses), led by ENS Paris-Saclay and its Vice-President of Research Keitaro Nakatani, established a formal framework for the collaboration for the period 2018-2021. Many student exchanges were set up and intensified between the two teams, supported by mobility grants from the French and Japanese governments. Nowadays, doctoral students of one of them regularly carry out a post-doctoral fellowship in the other's laboratory. A double-degree PhD programme will also begin in October 2019 between the two laboratories, providing funding for three years.

<https://mswebs.naist.jp/LABs/kawai/english/index.html>

» focus

New d'Alembert chairs at Université Paris-Saclay

Through the "Jean d'Alembert" fellowship programme, Université Paris-Saclay enables each year highly-qualified foreign scientists from all disciplines and countries to stay from 6 to 12 months in one of its 275 laboratories. Since 2018, the arrival of the "fellow" researcher has given rise to an inaugural lesson, filmed and then available on the Youtube channel of the university.

Recently, Professor Frédéric Frézard, an expert in drug delivery systems of the Department of Physiology and Biophysics at Minas Gerais University (Brazil), joined Professor Philippe Loiseau's "Antiparasitic Chemotherapy" team at BioCIS laboratory (CNRS/Université Paris-Sud) in Châtenay-Malabry. The objective would be to provide therapies and vaccines for leishmaniasis, a parasitic disease too often neglected. Michele Vallisneri, a theoretical physicist at NASA, and Filippo Vernizzi of the Institute of Theoretical Physics at CEA Saclay, are interested in the use of gravitational waves to study dark energy and the expansion of the universe. "Paris-Saclay has become a second scientific home for me", Professor Vallisneri likes to say.

www.youtube.com/user/UParisSaclay
www.youtube.com/playlist?list=PLyHq-UkjFkVtSJmcWdyoNIXcPBfy-hpn

Journal

**Cameroon
tribune**

Title

UNIVERSITY COOPERATION: PERFECT AGREEMENT BETWEEN DOUALA AND PARIS-SACLAY

Employability and professional integration on the agenda of the partnership signed in the Cameroonian economic capital.

www.cameroon-tribune.cm/article.html/24929/fr.html/cooperation-universitaire-accord-parfait-entre-douala-paris-saclay

Title

ICE, a building for climate and environmental sciences

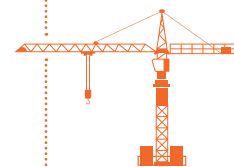
The brand new white building of the Climate and Environmental Sciences Laboratory (LSCE – CEA/CNRS/Université Versailles – Saint-Quentin-en-Yvelines) stands at the entrance of the CEA's site in Saint-Aubin. Delivered at the end of August 2018, this Infrastructure for Climate and Environmental Sciences (ICE) of 10,500 m² brings together almost all the staff (300) and scientific instruments of the LSCE, previously spread out between the CNRS campus in Gif-sur-Yvette and the CEA in Saint-Aubin. *“It has been obvious since the creation of the LSCE in 1998 that the staff needed to be gathered in a unique place,”* says Elsa Cortijo, director of the lab. Only two teams still remain in their former premises. *“We are discussing with our supervisors the possibility of a complementary real estate project.”*

The move, which took place between September 2018 and March 2019, has since given way to a gradual appropriation of the premises. *“The good conformity of the building, particularly in its technical aspects, is being assessed.”*

With a total budget of 36 million euros, the construction, carried out by Demathieu Bard, was supported by internal financing, the General Investment Commission and local authorities. The architectural design was entrusted to the architectural firm Celnikier & Gabli. Particular attention has been paid to the building's energy efficiency: North-South orientation, glass surface to solid surface ratio, exterior insulation, green terrace, natural lighting favoured by large patios... *“However, given the technical constraints required for experiments, it was not possible to go beyond the RT 2012 regulations.”* In fact, the building houses among other things a casemate for very low radioactivity measurements, a laboratory to analyse the vertical structure of the atmosphere, clean rooms and mass spectrometers, a non-magnetic chamber to be isolated from the earth's magnetic field, an experimental terrace to measure greenhouse gases and air quality. *“The specificity of LSCE is that it brings together researchers who study climate and the environment on past, present and future time scales, analyse field data, and perform numerical modelling. This building makes it possible to raise new scientific questions even more dynamically than in the past.”*

www.lsce.ipsl.fr





Title

AgroParisTech and INRA in Palaiseau: the Agro Paris-Saclay Campus



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At the beginning of 2021, the 66,000 m² Agro Paris-Saclay campus will bring together 2,000 students and 1,350 staff members of AgroParisTech and France's National Institute for Agricultural Research (INRA). This includes 920 academic and research staff members.

The work began in January 2019 on a 4.2 hectare plot on the western edge of the joint development zone of the École polytechnique in Palaiseau. The project will concentrate in a single location the training, research and innovation activities carried out at AgroParisTech's sites in the Paris region in close collaboration with the INRA. This represents twelve joint research units in life and environment sciences and engineering.

Designed by architects Marc Mimram and Jean Baptiste Lacoudre/Patriarch, this campus will be divided into eight buildings. The entrance building will open up to a large garden, surrounded by five buildings dedicated to teaching and administration, and two research buildings.

Title

It is time to submit your Globetalkers and Campus Life projects!

Through its Globetalkers and Campus Life calls for projects, Université Paris-Saclay supports projects (events, operations, sports competitions, etc.) of its students and staff that promote its influence and develop its identity. In 2018/2019, the university supported 25 Globetalkers projects and 52 Campus Life projects, with budgets ranging from 500 to 8,000 euros. For example, students of the AgroVéloCity Asia project went from Bangkok to Hong Kong by bicycle while making a documentary and collecting data on urban agriculture in Asia. And "Paris Saclay's Got Talent" gathered students for a talent competition during a great evening of celebration...

www.universite-paris-saclay.fr/Globetalkers
www.universite-paris-saclay.fr/aap-vie-de-campus2020

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PAST EVENTS			DON'T MISS			NOVEMBER		
JULY			OCTOBER			Dates	Place	Host
7 - 12	Paris	IUPAC	5-13	The Paris-Saclay campus	Université Paris-Saclay	12-15	Orsay	Université Paris-Sud
47TH WORLD CHEMISTRY CONGRESS OF THE INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY (IUPAC) Theme: "Frontiers in chemistry: Let's create our future! 100 years with IUPAC". IUPAC sought to emphasize its universality by welcoming chemists from all over the world to this event, along with scientists from industry and academia that attend the regular colloquia. www.iupac2019.org			"FÊTE DE LA SCIENCE 2019" The theme of this year's science festival is "Talking Science, Imagining the Future" and its slogan is "See you tomorrow!" www.fetedelascience.fr/pid35363/ile-france.html			7TH MEETING OF THE FRENCH SOCIETY OF ISOTOPES (SFIS 2019)  In line with the SFIS mission statement, this meeting aims to help scientists working in different disciplines share knowledge about isotopes and isotopic measurements to cross-fertilize applications in a broad range of fields. www.sfis.eu/7eme-congres-de-la-sfis-sfis2019/		
AUGUST			THE 1ST SYMPOSIUM ON SCIENTIFIC INTEGRITY, RESEARCH ETHICS AND SOCIAL RESPONSIBILITY The point of this day-long event is to discuss issues relative to conflicts of interest and conflict-of-interest ties and take the thought process beyond the normative to cover socio-epistemological concerns. www.ymw5bq70.evenium.net			INTERNATIONAL CONFERENCE "Vulnerability" and "resilience" Seeking to update existing approaches to development and the environment, this conference is being organised by the Centre for Study on Globalisation, Conflicts, Territories and Vulnerabilities (CEMOTEV). The goal is to conduct a forward-looking assessment of the concepts of vulnerability and resilience almost 20 years after they began to circulate in academic research as well as development and environmental policies. https://vr2019.sciencesconf.org/		
QUANTUM FUTURE ACADEMY 2019 Participants in this week-long Franco-German program learned about various fields of application of quantum technologies as they developed their skills and increased their knowledge of quantum physics. The Academy offered participants an opportunity to explore the relationship between quantum physics and the development of new technologies while networking with an international, interdisciplinary group of researchers, entrepreneurs and students. www.universite-paris-saclay.fr/fr/quantum-academy			SYMPOSIUM "Socially responsible organizations and territories in the face of social and environmental challenges" This event is designed to have senior management and executives working for local authorities, businesses and other organisations engage in give-and-take with researchers in the humanities and social sciences. The goal is to ponder the social and societal responsibility of organisations as well as to study and highlight the importance of socially responsible territorial projects. www.uvsq.fr/symposium-organisations-et-territoires-responsables-face-aux-enjeux-sociaux-et-environnementaux-413210.kjsp?RH=1507821125055			DECEMBER		
SEPTEMBER			JUNIOR CONFERENCE 2019 – JDSE2019 This data science and engineering conference was for students in their first year of a PhD programme, a Master 2 course or their third year of engineering at Université Paris-Saclay. It gave participants a chance to present their first scientific research and sharpen their critical thinking skills. The innovative "junior conference" format consisted of a dense scientific programme of international guest speakers, oral reports, poster sessions and software demonstrations. https://jdse-paris.github.io/jDSE2019			A FESTIVAL TO SHARE KNOWLEDGE ABOUT TRANSPORTATION, MOBILITY AND URBAN PLANNING  The 1 st "Doctilien" festival invites Paris-Saclay PhD students in any discipline to share their research with a public of students, businesspeople and residents of the greater Paris area, not to mention the entire Paris-Saclay scientific community, transporting their audience to the city of tomorrow! www.openagenda.com/agendas/86184123/embeds/6268688/events/90157157?lang=fr		
12-13 Gif-sur-Yvette Centrale Supélec			17 Paris Université de Versailles – Saint-Quentin-en-Yvelines			5 Gif-sur-Yvette Centrale Supélec		
14 Paris Poléthiis			14 Paris Poléthiis			13, 14, 15 Guyancourt Université de Versailles – Saint-Quentin-en-Yvelines		
24-31 Sites in France and Germany Université Paris-Saclay and partners			14 Paris Poléthiis			13, 14, 15 Guyancourt Université de Versailles – Saint-Quentin-en-Yvelines		
21 Gif-sur-Yvette Inra			21 Gif-sur-Yvette Inra			21 Gif-sur-Yvette Inra		

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READING HIGHLIGHTS

THE CONVERSATION

A new way to heal fractures

Jérôme Grenier, PhD student in biomedical engineering at Université Paris-Saclay, presents the possibility of using hydrogels as an effective treatment in bone regeneration.

www.theconversation.com/une-nouvelle-piste-pour-guerir-les-fractures-119337

20th anniversary of the law on palliative care: a founding text with insufficient results

Emmanuel Hirsch, professor of medical ethics at Université Paris-Saclay, revisits the law of 9 June 1999, which aimed to guarantee the right to access palliative care.

www.theconversation.com/la-loi-sur-les-soins-palliatifs-fete-ses-20-ans-un-texte-fondateur-mais-un-bilan-insuffisant-118517

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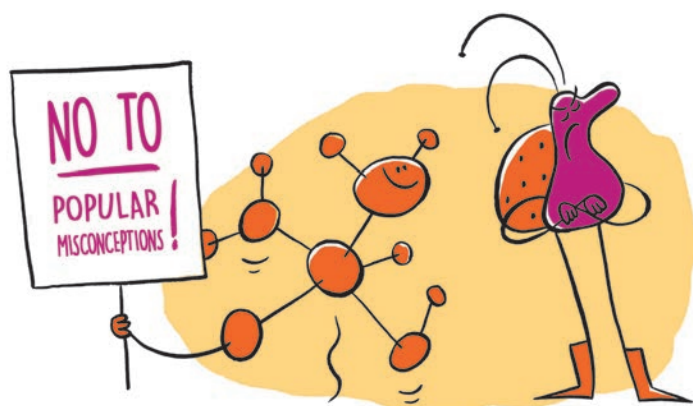
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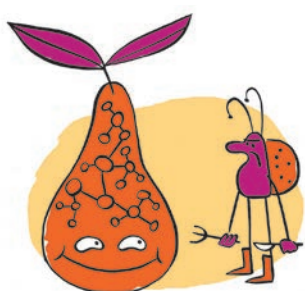
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NO TO POPULAR MISCONCEPTIONS IN CHEMISTRY!



At a time when climate, the environment and the protection of our planet are finally taking centre stage, Université Paris-Saclay, which has a large community of chemists with its researchers and students, has chosen to focus on chemistry. This exciting discipline, which studies the composition, properties and transformations of matter, suffers from a negative public image. The time has come to correct the stereotypes that overshadow the variety and wealth of the fields of chemistry, covered by research, training and professions. It is also time to shed light on the way chemistry contributes to major societal issues. "NO to popular misconceptions in chemistry!": a series of deliberately quirky illustrations that we hope will spark a debate!



"I don't want any chemical substances in my plate!"



"Natural products are better than chemical products!"



"Chemistry is not for me, it's too complicated!"



"Chemists are mad scientists who act as they please!"



"A chemical compound with a long name is necessarily dangerous!"



"A natural perfume is a perfume made without chemistry!"



"Chemistry is dangerous for your health!"



"Cosmetics are bad and full of chemical substances!"



"Chemistry is plastic waste!"



"Chemistry is an old and outdated science!"

<https://www.universite-paris-saclay.fr/en/news/no-to-popular-misconceptions-in-chemistry-13>