
# Book of Abstracts

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# Organising committee

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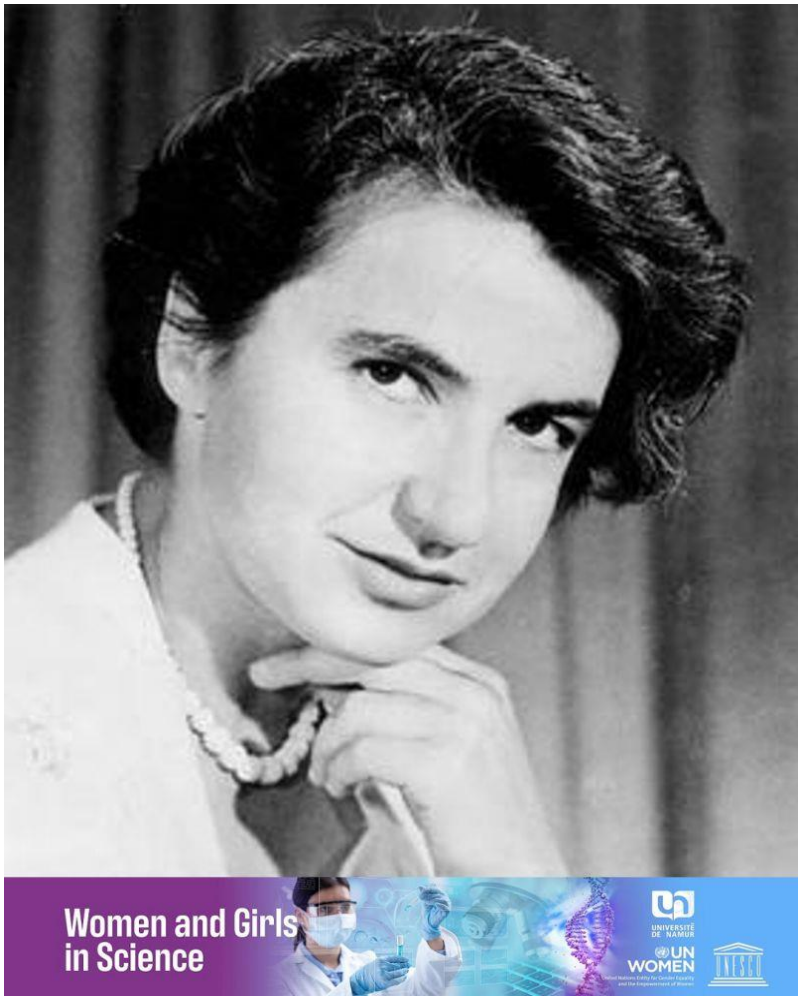
# Did you know?

The "Rosalind Franklin Auditorium" is the name of the auditorium in the Faculty of Science at University of Namur, where the Women in Science 2023 conference is taking place.
Rosalind Elsie Franklin (25 July 1920 - 16 April 1958) was a British chemist and X-ray crystallographer whose work was central to understanding the molecular structures of DNA, RNA, viruses, and graphite. Although some of her work was appreciated during her lifetime, Franklin's contributions to the discovery of the structure of DNA were largely unrecognised during her lifetime, leading to her being referred to as a ' forgotten heroine', a 'feminist icon' or the 'dark lady of DNA'.



# PROGRAMME

| | | |
|---|---|---|
| 08:30 | | Welcome and registration |
| **09:15** | | **Welcome words by Laurent Schumacher, Vice-rector for training and sustainable development** |
| **09:30** | **Keynote 1** | **Peeping at the Universe through a keyhole \| Prof. Stéphanie Roccia - Université Grenoble Alpes, France** |
| **10:15** | **Talk 1** | **Oil as an enabler for nanotomography analyses \| Dr. Céline Noël - IMEC, Belgium** |
| **10:35** | **Flash talks** | **Early-stage researchers - 3 minutes per talk** |
| 10:55 | | Coffee break |
| **11:25** | **Talk 2** | **Survival in extreme conditions \| Prof. Alice Dennis - UNamur, Belgium** |
| **11:45** | **Talk 3** | **Celestial mechanics and mathematical tools for space debris \| Prof Anne Lemaître - UNamur, Belgium** |
| **12:05** | **Talk 4** | **A serendipitous discovery – How some bacterial pathogens kill themselves, and why it matters \| Dr. Katy Poncin - UNamur, Belgium** |
| **12:25** | **Flash talks** | **Early-stage researchers - 3 minutes per talk** |
| **12:45** | | **A word by GSK** |
| 12:55 | | Lunch and Poster session |
| **14:30** | **Keynote 2** | **On relevance and responsibility - from piano to policy \| Prof. Cynthia Liem - TU Delft, The Netherlands** |
| **15:15** | **Talk 5** | **Building machines that learn and use language in a similar way than we do \| Prof. Katrien Beuls - UNamur, Belgium** |
| **15:35** | **Talk 6** | **Atmospheric trends of halocarbons derived from 15 years of IASI space observations \| Hélène De Longueville - ULB, Belgium** |
| 15:55 | | Coffee break |
| **16:25** | | **Panel session about the place of women and girls in science and how to make scientific careers easier for women** |
| **17:25** | | **Closing remarks \| Prof Carine Michiels - Vice-rector in charge of research, UNamur** |
| 17:30 | | Drink, networking and poster session |


# Flash talk program

| First session (10.35-10.55) | | |
|---|---|---|
| 1 | Yasmine Akaichi | A Consensus-based Framework for Federated Learning using Inductive Logic Programming |
| 2 | Blinera Juniku | Targeting the splicing factor TFIP11 in cancer by an intrinsically disordered protein-based drug design strategy |
| 3 | Davoud Alahvirdi | Autonomous Manager for Urban Traffic |
| 4 | Nora El Khalfaoui | Comparison of sensitivities between an indirect ELISA assay and clinical examination in ovine caseous lymphadenitis diagnosis |
| 5 | Alison Forrester | ER Exit Site Modulation and its Role in Cellular Homeostasis |
| 6 | Fabio Giovannercole | Characterization of the Translocation and Assembly Module (TAM) in Bacteroidetes |
| 7 | Antoine Honet | Electronic correlation effects on optical, electronic and magnetic properties of materials through model Hamiltonians and Green's functions |
| **Second session (12.25-12.45)** | | |
| 8 | Jelena Luyts | Environmental change, adaptations and gender in rural Senegal |
| 9 | Lucas Schoenauen | Usability of *C. elegans* as a model to investigate the FLASH effect in protontherapy |
| 10 | Candy Sonveaux | A state-feedback vaccination law for an age-structured SIRD model |
| 11 | Yathreb Naghmouchi | Quantum chemistry study of the second harmonic generation tensor in chloranilic acid-based crystals. |
| 12 | Gaetano Ricci | Designing organic emitters for next-generation Organic Light Emitting Diodes (OLEDs): a matter of symmetry and correlation |
| 13 | Sophie Fortz | Modelling Software Product Lines and their behaviour |


# Posters

| | | |
|---|---|---|
| 1 | Cilya Oulmas | Development of an AlZnSnMg anode for the cathodic protection of steel in sea water |
| 2 | Valentin Goffinet | Metallic nanoparticle synthesis with silver thin layer irradiation |
| 3 | Xikun Zhang | Hydrogen Bond-Assisted Ultra-Stable and Fast Aqueous NH4+ Storage |
| 4 | Inès Bouriez | Impact of UVB-induced senescent keratinocytes on skin cancer cells |
| 5 | Chloé Matthys | Advancing esophageal adenocarcinoma treatments by resistant gene signature identification and venom testing |
| 6 | Yathreb Naghmouchi | Quantum chemistry study of the second harmonic generation tensor in chloranilic acid-based crystals. |
| 7 | Tanguy Colleu-Banse | Simulation of surface enhanced infrared absorption |
| 8 | Adriana Diaz Anaya | Intracellular localization of ABCB5, a transmembrane protein expressed in melanoma |
| 9 | Loris Chavée | Growth mechanisms and properties of magnetron sputtered $TiO_2$ thin films on complex 3D foam substrates |
| 10 | Laurelenn Hennaux | Refolding and biophysical characterization of the *Caulobacter crescentus* copper resistance protein, PcoB |
| 11 | Amira Khochtali | Characterization of the molecular role of PcoB in copper efflux in Caulobacter crescentus |
| 12 | Margaux Mignolet | Neuroinvasion of SARS-CoV-2 in SH-SY5Y cells can be partially blocked by using entry inhibitors |
| 13 | Marine Ote | Deciphering spatiotemporal regulation of antibiotic and copper coresistance in *C. crescentus* |
| 14 | Sarah Pinon | A Data Recommendation System for Decision-Makers |
| 15 | Lhorie Pirnay | Data-Driven Strategy Maps: A Hybrid Approach to Strategic and Performance Management Combining Hard Data and Experts' Knowledge |
| 16 | Pauline Tricquet | High-throughput screening for inhibitors of Elongator |
| 17 | Audrey Verhaeghe | Identification of the O-chain ligase in *Brucella abortus* |
| 18 | Liuxi Yang | Synthesis of Non-covalent porous materials |
| 19 | Pauline Castenetto | Effects of disorder on properties of two-dimensional $MoS_2$ |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|---|---|---|
| 20 | Guillaume Nguyen | Identification of Cyber Physical System (CPS) & Orchestration of fuzzing testing |
| 21 | Valentin Job | Investigation of the Antibacterial Properties of Silver-Doped Amorphous Carbon Coatings Produced by Low Pressure Magnetron Assisted Acetylene Discharges |
| 22 | Asena Aynaci | Consequences of the inactivation of the mannose-6-phosphate pathway on the growth, migration and drug sensitivity of HeLa cell |
| 23 | Marie Dorchain | Pattern reconstruction through generalised eigenvectors |
| 24 | Blinera Juniku | Targeting the splicing factor TFIP11 in cancer by an intrinsically disordered protein-based drug design strategy |
| 25 | Yasmine Akaichi | A Consensus-based Framework for Federated Learning using Inductive Logic |
| 26 | Joseline Flore Kenmogne Tchidjo | Investigating the Diels-Alder Reactions Combining Density Functional Theory with Bonding Evolution Theory (BET) |
| | Sébastien R. Mouchet | Linear and nonlinear optical response from the fluorescent photonic structures occurring in beetle integuments |
| | Hala Kasmo | Investigation of the bidirectional copper transport across the inner membrane of the free-living *Caulobacter crescentus* |
| | Lorena Ballesteros Ferraz | Tackling quantum algorithms using modular values |
| | Bruno Majérus | Plasmons in nanostructured and corrugated 2D materials |
| | Valérie Hoorne | L'accès des femmes aux sciences - Women Wavre 2023 |
| | Laurence Theunis | Digital4All - Pour une meilleure représentation des femmes dans le numérique |


# Book of abstracts

UNIVERSITÉ DE NAMUR
narilis NAmur Research Institute for Life Sciences
naxys Namur Institute for Complex Systems
NISM Namur Institute of Structured Matter
NADI Namur Digital Institute
EDT PANDA
UNIVERSITÉ DE NAMUR FACULTÉ D'INFORMATIQUE
UAR Unité d'appui à la recherche UNamur | Faculté des Sciences

# Invited speakers

# Peeping at the Universe through the keyhole

Stéphanie Roccia - Université Grenoble Alpes, France

The Universe and its history are at the same time very well understood and a big mystery. We have amazing tools from satellites to observatories to weight the universe as it is today and also as it was in the past. But the content of the Universe can simply not be explained by physicists. To get the full picture, we need to identify and understand the interactions at play throughout the life of the Universe. This is the meeting point between the infinitely small, the study of interactions with particles, and the infinitely big, the cosmology. I will guide you at this meeting point where the neutron, a very common neutral particle that is one of the main components of the human body, is used as a tool to understand why and when the matter prevailed over anti-matter. We are also starting to use it to probe extra-dimensions in the Universe … an idea that came from Namur.

https://wgis.unamur.be/programme/abstracts/view#autotoc-item-autotoc-0

https://www.scopus.com/authid/detail.uri?authorId=22935554500&fbclid=IwAR0srvnN1QRn-bBtWoAfHg_3ramCLd9C3FKzMRizAU1zGb3wEQTbeHi8cwc

**Celestial mechanics and mathematical tools for space debris**

# Oil as an enabler for nanotomography analyses

## Céline Noël – IMEC, Belgium

The ever-increasing complexity of semiconductor devices and the pervasive introduction of three-dimensional (3D) architectures require innovative three-dimensional materials characterization techniques for confined volumes.

To meet this demand, multiple atomic force microscopy (AFM)-based methodologies, using a slice-and-measure approach, often referred to as scalpel scanning probe microscopy (SPM) have been proposed to visualize tomographic information in confined volumes in a wide range of devices and bulk materials. They consist of scanning AFM probes that erode locally the sample's material at a relatively high load while sensing with the secondary AFM channel, thus accessing in-depth information compared to the standard surface-limited analysis.

Nonetheless, an overlooked aspect of scalpel SPM is the heavy debris accumulation at the tip apex and inside/around the scan area. As the high-pressure scan is performed, the etched particles pile up, coalesce, and eventually reattach to the surface. This is directly affecting the measurement quality and repeatability, contributing to the tip wear, and limiting the maximum 3D scan depth. These are the main reasons for the limited usability of scalpel SPM.

It is well known from the macroscopic and nanoscopic machining world that cutting fluids such as oils can significantly improve the cutting tool's lifetime and flush away debris from the cutting area. Here we explore the use of oil as a suitable medium to overcome the issue of scan debris accumulation while preserving the precise removal rate capability, and electrical AFM modes functionality.

# Survival in extreme conditions

Alice Dennis – University of Namur, Belgium

My research focuses on the evolution of adaptive traits. I am fascinated by the abilities of some organisms to survive in extreme and novel conditions, such as freezing temperatures. To understand this, I integrate physiological and molecular experiments with field work. I use physiological tests to understand survival of harsh conditions or how plasticity allows some species to better survive. I couple this with transcriptomic and genomic studies to identify the genes that have evolved to give greater adaptive abilities. By comparing close relatives, I try to understand how they have evolved in relation to past and present geographic ranges. I study not just freeze tolerance, but also greater tolerance of heat, pollution, and changes in diet. Today I will talk about two systems where I have used freeze tolerance to better understand where species live: intertidal snails in the USA and stick insects in New Zealand.

# Celestial mechanics and mathematical tools for space debris

Anne Lemaitre – University of Namur, Belgium

Six decades of space activities have led to a congested near-Earth environment, analogous to the 7-th continent of plastic waste in Earth's ocean. The space debris, uncontrolled remnants and hazards linked to human space activities, have dramatically increased in number over the years and some of them have « life expectancy » of thousands of years.
They clearly behave as natural bodies, and no more as controlled artificial satellites.
Three tools of celestial mechanics, traditionally developped for asteroids or particles in rings, were successfully adapted to space debris: symplectic integrations, resonances and chaos measurements, creating a first bridge of collaborations between two scientific communities. Moreover thanks to the creation of the research institute naXys, a second interdisciplinary bridge was developped with mathematicians: as results, the population of space debris has first been treated as a synthetic population, allowing simulations and predictions, and is now modelled on a dynamical network, with the links connected to the probability of collision.

# A serendipitous discovery – How some bacterial pathogens kill themselves, and why it matters

Katy Ponci – University of Namur, Belgium

*Neisseria gonorrhoeae* is the bacterium responsible for the sexually transmissible disease gonorrhea. It is exquisitely adapted to its human host and long-lasting immunity cannot be achieved, either naturally or through vaccines. Fortunately, there exist ways to study it *in vitro*, on petri dishes and in liquid media.

In their natural environment, bacteria have to compete against each other for resources, including space and food. To do so, they are equipped with different tools, such as harpoon-like apparatus and toxins. While looking for putative toxins that are only present in the genome of pathogenic *Neisseria* species, we found conserved cationic peptides of unknown function. Surprisingly, we realized that our hypothesis was wrong and that the peptides were instead involved in a suicide process called autolysis. Moreover, we found that the peptides have a direct effect on humans, by destroying red blood cells and playing on inflammation factors.

During this talk, I will therefore share with you the story of how this unexpected discovery was made.

# On relevance and responsibility - from piano to policy

Cynthia Liem - TU Delft, The Netherlands

In this talk, I will present how my dual background in music and computing led to an unusual career trajectory. I will discuss how common assumptions and success criteria in the design of search engines and recommender systems were not compatible with my interests and needs as an artist, leading to my research interests in validation and validity of data-driven systems, and ways to still keep 'that what is not obvious' within reach in a world of digital information overload. Furthermore, I will highlight the importance of being able to communicate across disciplines, which has not only benefited me when working with artists and scholars in the humanities, but also in collaborations with social science researchers, and in matters of academic and tech policy.

Throughout the talk, I will touch upon more fundamental questions on what it means to 'have relevance'. While my take on this question has not been in line with traditional perspectives on the academic career, I will argue it is in line with values that academia upholds, and aligns well to increasing demands for transdisciplinary and public-interest research and education.

# Building machines that learn and use language in a similar way than we do

Katrien Beuls – University of Namur, Belgium

As human beings, we acquire our native languages by taking part in communicative interactions that are meaningful in the environment in which we grow up. On a fundamental level, there are two main cognitive mechanisms at play during language acquisition: intention reading and pattern finding. Intention reading refers to the capacity to hypothesise about the intended meaning of an observed utterance based on the situational context it is uttered in. Pattern finding refers to the ability to generalise over pairs of observed utterances and their hypothesised meaning, yielding form-meaning mappings of varying degrees of abstraction. The mechanisms through which humans acquire language are in sharp contrast with the methodologies that currently dominate the field of natural language processing (NLP). Indeed, unlike the linguistic systems of humans, large language models are learnt with an exclusive focus on linguistic forms (characters, words and sentences), in the absence of meaningful and intentional communicative interactions that take place in situated environments. In this talk, I will discuss recent advances in modelling language acquisition in a more human-like manner, and show how we can operationalise the processes of intention reading and pattern finding in artificial agents.

# Atmospheric trends of halocarbons derived from 15 years of IASI space observations

**Hélène De Longueville** [(1)], L. Clarisse [(1)], S. Whitburn [(1)], C. Clerbaux [(1, 2)] and P. Coheur [(1)]

[(1)] *Spectroscopy, Quantum Chemistry and Atmospheric Remote Sensing (SQUARES), Université libre de Bruxelles (ULB), Brussels, Belgium*
[(2)] *LATMOS/IPSL, Sorbonne Université, UVSQ, CNRS, Paris, France*

The chemical and radiative equilibrium of our atmosphere has been profoundly modified by the emissions of halocarbons, among which chlorofluorocarbons (CFCs), their hydrogenated derivatives (HCFCs, HFCs) and halons. These halogenated compounds are known to be powerful greenhouse gases and contribute, for chlorinated and brominated compounds, to the depletion of stratospheric ozone and to the development of the ozone hole. Therefore, the production of many of these anthropogenic gases is controlled since 1987 by the Montreal Protocol and its amendments. A continuous monitoring of CFCs and related halogenated substances is essential to evaluate the effectiveness of international regulations. Here we exploit measurements from the infrared satellite sounder IASI which offers the potential to robustly assess trends in the atmospheric abundances of trace gases owing to the stability and the consistency of the measurements made by three successive instruments over a period of more than 15 years.

Despite their weak spectral signatures, we have recently reported the detection of eight long-lived halocarbons in IASI spectra: CFC-11, CFC-12, HCFC-22, HCFC-142b, HFC-134a, $CF_4$, $SF_6$ and $CCl_4$. In this work we exploit the available record of continuous IASI measurements to determine the temporal evolution in atmospheric abundance of these species. Our results are validated with ground-based measurement networks and other remote sensors data. We conclude by assessing the usefulness of IASI and follow-on missions to contribute to the global monitoring of CFCs and their substitutes.

# Flash talks

# **Abstract entitled :** A Consensus-based Framework for Federated Learning using Inductive Logic Programming

Yasmine AKAICHI

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Nowadays, the data used by artificial intelligence systems are often dispersed across the world on various heterogeneous, and non-secure platforms. It can also reside on static machines as well as mobile devices. Federated learning is an emerging machine learning paradigm involving multiple clients, e.g., mobile phone devices, with an incentive to collaborate in solving a machine learning problem coordinated by a central server. The traditional Federated Learning framework is recognized as poorly resilient to attacks that can de-anonymize sensitive data when exchanging the model updates between clients and central servers. As an alternative approach to that end, we investigate the use of inductive logic programming. It uses both techniques from machine learning and logic programming with the objective of inducing theories, as sets of logical rules, that generalize the given training examples. Theories will therefore be exchanged between nodes, which solves many security concerns. However, learning in that way on different nodes requires to unify different theories, which we plan to obtain through the development of consensus techniques.

**Keywords:** Federated learning , Inductive logic programming, machine learning, logic programming.

# *Targeting the splicing factor TFIP11 in cancer by an intrinsically disordered protein-based drug design strategy*

**Blinera Juniku[1], Denis Mottet[2], Catherine Michaux[1]**

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The spliceosome is the main cellular machinery guiding the splicing reactions of pre-mRNA. Recent studies have revealed that cancer cells survival is highly dependent on that splicing function. These findings have resulted in a growing interest in targeting splicing regulatory proteins in the treatment of cancer.[1,2] In this project, we consider the human splicing factor TFIP11 (Tuftelin Interacting Protein 11). Its depletion was recently shown to alter cell cycle progression and to induce apoptosis in cancer cells, pointing up TFIP11 as a potential target for cancer therapy.[3]

TFIP11 belongs to a particular class of proteins called intrinsically disordered proteins (IDPs). Unlike globular proteins, IDPs lack a well-defined tertiary structure and exist as conformational ensembles. Their various context-dependent conformations allow them to interact with multiple partners. About 30% of the TFIP11 sequence is predicted disordered, especially two regions within the N-terminal extremity. They were shown to be crucial for TFIP11 protein-protein interactions (PPIs) and for spliceosome correct assembly.[3]

The aim of this research is to decipher TFIP11's behavior and to identify hit molecules able to block TFIP11's disorder (closely linked to its multi-functionality) or its PPIs. A rational drug design approach, challenging in the context of IDP, will be applied.[4,5] For that purpose, we combine *in vitro* and *in silico* approaches using spectroscopic (intrinsic fluorescence, circular dichroism, dynamic light scattering, …) and computational (molecular dynamics and virtual screening) methods. Further developments including lead molecules optimization, *in vivo* assays,... will then be required to achieve safe and effective anti-cancer drugs.

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2. Rahman MA, Krainer AR, Abdel-Wahab O. *Cell*. 2020, 180(1):208-208.e1.

3. Duchemin A. *et al*. *Nat. Commun*. 2021, 12, 1–20.

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**Autonomous Manager for Urban Taffic**

Davoud Alahvirdi

The AUTOMATic project aims to develop and to test, in a simulation environment, a content-aware urban traffic management system relying on a swarm of unmanned aerial vehicles (UAVs). Urban traffic refers to the movement of public and private vehicles as well as of pedestrians in an urban road network. With the term content-aware system for traffic management, we refer to a set of artificial devices that, by extracting data describing urban traffic and by operating ground based units, can autonomously and automatically: i) evaluate the traffic current status; ii) predict its future; and iii) mitigate or avoid undesired developments (e.g., congestion).

# Comparison of sensitivities between an indirect ELISA assay and clinical examination in ovine caseous lymphadenitis diagnosis

**Nora El Khalfaoui[1,2*], Bouchra El Amiri[2], Nathalie Dubois[1], Mouad Chentouf[3], Marianne Raes[1], Tanguy Marcotty[1], Nathalie Kirschvink[1]**

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## Abstract

Caseous lymphadenitis (CL) is an infectious cosmopolitan disease that affects small ruminants. It is clinically characterized by suppurative necrotic inflammation of the superficial and internal lymph nodes or organs and it is caused by a facultative intracellular bacterium, *Corynebacterium pseudotuberculosis*. The mean clinical prevalence of CL superficial abscesses in sheep flocks is 34.6% in Settat province in Morocco, where superficial CL form affects principally young sheep between 6 and 24 months. CL causes significant economic losses to ovine breeders. CL diagnosis is based on characteristic clinical symptoms. The isolation and bacterial identification of *C. pseudotuberculosis* which is considered as diagnostic gold standard is performed with caseous content of drained abscesses. Serological tests appear as advantageous when abscesses are not clinically detectable. In this work, sensitivity of clinical and serological diagnosis is compared using data from sheep in Settat province in Morocco.

A total of 701 sera were collected at 2 months intervals between February 2021 and July 2022 during a longitudinal follow-up of 170 sheep belonging to six flocks in Beni-Meskine, Settat province. The clinical data of superficial abscesses were recorded at each serum collection, by palpation of superficial lymph nodes. Serum was analysed by an indirect ELISA assay using ELITEST CLA kit (Hyphen BioMed, France, Ref CK105A). By considering a 100% fixed specificity of clinical and serological diagnostic approaches, Bayesian analysis was carried out to compare sensitivity between clinical and serological diagnosis. Data were first analyzed ignoring age categories and, subsequently, repeated separately for two age categories: lambs (<6month, 307 observations from 81 animals) and older sheep (>6 months, 394 observations from 89 animals).

Among 701 clinical observations, 191 displayed superficial abscesses (106 in lambs and 85 in older sheep). The number of seropositive cases were 416 (122 in lambs and 294 in older sheep). The Bayesian analysis indicated that the sensitivity of serological test was higher in older sheep with a median of 85.4% (95% credible interval: 73.6%-96.2%) versus 59.3% (95% CI: 39.9%-76.3%) in lambs. On the contrary, the sensitivity of clinical examination was lower in older sheep with a median of 24.9%% (95% credible interval: 19.4%-31.0%) versus 51.7% (95% CI: 34.4%-67.5%) in lambs. This could be explained by the fact that older animals develop more internal abscesses (not seen at clinical examination) while the production of specific antibodies may be lower after a first exposure, compared to subsequent infections (explaining a lower serological response in lambs).

*This study is part of a cooperation research project and is funded by ARES CCD.*

**ER Exit Site Modulation and its Role in Cellular Homeostasis**
**Alison Forrester**

In the early secretory pathway, Endoplasmic Reticulum (ER) Exit Sites (ERES) are specialised areas of the ER deputed to sorting cargo into COPII coated carriers, for transport from the ER to the Golgi apparatus. This is a highly dynamic process, carefully regulated by the orchestration of a number of proteins on the cytosolic side of the ER membrane. The first pharmacological inhibitor of ERES, Retro-2, has been described for its role as an inhibitor of Shiga toxin retrograde trafficking (Stechmann B. et al. Cell 2010). Counterintuitively to its effects on retrograde trafficking, the target of Retro-2 has been identified as ERES component Sec16A (Forrester A. et al. Nat Chem Biol 2020).

Targeting Sec16A using Retro-2, caused a specific but partial decrease in ER to Golgi trafficking of SNARE protein Syntaxin-5 (Syn5). This consequently caused a loss of the novel Syn5-GPP130 interaction, that we found was crucial for retrograde trafficking of Shiga toxin from early endosomes to the *trans*-Golgi Network. Through this mechanism, Retro-2 protects against the toxic effects of Shiga toxin.

Using Retro-2 as a tool to study acute ERES inhibition, and a proof of principle that ERES can be targeted, this work forms the foundations of a new research program, pursuing three key directions: 1) How does the target of Retro-2, ERES component protein Sec16A, mediate ERES function and cargo selection? 2) What is the effect of acute ERES modulation on organelle and cellular homeostasis? 3) What is the potential for ERES modulation in physiologically relevant disease models?

Using fundamental cell biology and interdisciplinary approaches, my group will build fundamental knowledge on the homeostatic effects of ERES modulation, along with the identification of novel compounds and the cargoes whose secretion can be affected by their treatment, with a view to targeting diseases of aberrant secretion.

# Characterization of the Translocation and Assembly Module (TAM) in Bacteroidetes

Fabio Giovannercole
University of Namur, Belgium

The Translocation and Assembly Module (TAM) is a nanomachine mainly known to transport and insert virulence factors in the outer membrane (OM) of Proteobacteria. This complex is composed of the OM-embedded protein TamA, a BamA homolog, and of the inner membrane-anchored protein TamB.
In Bacteroidetes, TamA is replaced by a lipid-anchored variant named “TamL”, whose function is completely unknown. Furthermore, in two Bacteroidetes species, *i*) *Capnocytophaga canimorsus* (*Cc*), an oral commensal bacterium of cats and dogs and an accidental human pathogen, and in *ii*) *Flavobacterium johnsoniae* (*Fj*), an environmental bacterium, we recently found that TamL- and TamB-encoding genes are essential, in high contrast with their homologs in Proteobacteria. This suggests a phylum-related function that deserves further investigation.
Based on the above, we aimed at elucidating the essentiality of the TAM complex in Bacteroidetes using *Cc* and *Fj* as model organisms. To this aim, we envisaged a biochemical and a genetic approach. In the former, we performed TamL and TamB pull-down assays, coupled with mass spectrometry (MS) analyses, to identify proteins TamL and TamB interact with. In the latter, we depleted TamL and TamB to characterize the effect of their depletion on cell viability, morphology, and OM homeostasis.
Our preliminary results show that the depletion of TamL and TamB has a detrimental effect on cell viability, and that TamL depletion leads to morphological abnormalities, which may indicate an effect on OM integrity. Altogether, these results pave the way to fully elucidate the biological function of TAM in Bacteroidetes.

# Electronic correlation effects on optical, electronic and magnetic properties of materials through model Hamiltonians and Green's functions

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[2] Engineering Science and Mechanics Department, Pennsylvania State University

*Optical or magnetic properties from materials can be deduced from their electronic properties. Among numerical techniques for electronic structure calculations, the most popular are ab initio techniques such as Density-Functional Theory. Besides model Hamiltonians that are parametrized and thus (semi-)empirical keep a huge interest. Indeed, the computational cost is reduced by several order of magnitudes, rending possible to model larger nanosystems or to account for effects that are usually set aside in ab initio computations, such as correlation.*

*We present here a Green's functions formalism applied to model Hamiltonians that allows for computing electronical, optical and magnetic properties of nanoparticles, including correlation, through the GW approximation of the Hubbard model. Optical properties of small polycyclic aromatic hydrocarbons have been previously investigated and compared to experiments (see Ref. 1). We show fundamental effects of correlation for very small systems [2] as well as preliminary results on the magnetic states of graphene nanoribbons (GNRs) that are extensively studied these last years, both numerically and theoretically (mostly within mean-field theory, neglecting correlation effects). These GNRs are now foreseen as potential building blocks for new electronic and spintronic devices.*

*Fundamental effects of correlation on electronic, optical and magnetic properties are still misunderstood while they are playing an important role in collective phenomena such as plasmons.*

[1] A. Honet, L. Henrard, V. Meunier, "Semi-empirical many-body formalism of optical absorption in nanosystems and molecules", Carbon Trends 4, 100073 (2021).

[2] A. Honet, L. Henrard, V. Meunier, "Exact and many-body perturbation solutions of the Hubbard model applied to linear chains", AIP Advances 12, 035238 (2022).

# Flash talk – Abstract

*Jelena Luyts*

My flash talk will give a general overview of my research: why is it interesting? What am I looking for? How am I doing my research?

Senegal is a region which underwent, undergoes and will undergo major changes in its environment, whether it be due to climate change or induced by humans. Local populations mainly live of agriculture, livestock or fishing, activities highly dependent on the environment. Therefore, the populations are forced to continuously adapt.

To better understand who adapts, when and how, I went to meet with men and women, and asked about the changes they perceived in their environment, how it impacted their lives and how they adapted to these changes.

Taking a gendered perspective, my thesis tries to give an overview on the adaptation journeys, identify family dynamics, and maybe identify chronologies of adaptation. Hopefully my thesis will give some clues to accompany the populations facing environmental change in their adaptation process.

# Usability of C. Elegans as a model to investigate the FLASH effect in protontherapy.

**Background:** UHDR irradiations show healthy tissues sparing effect known as the FLASH effect. Since 2014, the FLASH effect is investigated worldwide to understand how it works and how to trigger it. Recent work suggest that the beam structure is an important parameter to trigger the FLASH effect but there is, to our knowledge, no investigation on the beam structure effect with fixed other parameters such as dose rate, dose or the biological model used. The C. Elegans is a well-known biological model that is already use in radiobiology research.

**Methods:** In order to investigate the beam structure which will trigger a FLASH effect with protons, we developed a chopper system allowing us to mimic the beam structure of clinical accelerator such as MEVION HYPERSCAN® and IBA Proteus®ONE (20 µs pulses, 1.5 ms pauses between pulses), using our continuous beam particle accelerator, ALTAÏS, at LARN laboratory. To ensure that we are in UHDR range, we developed a homemade Faraday Cup for the dosimetry. C. Elegans have been irradiated with XR and proton to find a biological readout that could be impacted by the FLASH effect.

**Results**: The irradiation system has been validated and the irradiation protocol of C. Elegans has been tested and validated as well. Primary irradiation of C. Elegans in XR and conventional proton shows a statistically significant delay in the growth of the worms ($p<0.001$).

**Conclusion:** We have developed an experimental device allowing to modify many parameters (pulse width, time between pulses, number of pulses and frequency) in the beam structure for the FLASH study. The device has been tested and is operational for the irradiation of C. Elegans. The first results are encouraging, and FLASH irradiations are in progress to find a smaller delay in worm growth.

**A state-feedback vaccination law for an age-structured SIRD model**

Candy Sonveaux, Joseph Winkin

In this work, an SIRD model is used to describe the evolution of a population suffering from a mortal illness (SIRD denoting Susceptible, Infected, Recovered and Death individuals, respectively). This model is an extension of the well-known SIR model of Kermack and McKendrick with the particularity of taking the age into consideration. The purpose of the work is to design an age-dependent vaccination-law, based on the state of the model, to imply disease eradication. In addition, since the whole state of the model (S, I, R and D) is not known at each time, an observer is designed in order to reconstruct the state on the basis of the measurements (D).

# Quantum chemistry study of the second harmonic generation $\chi^{(2)}$ tensor in chloranilic acid-based crystals.

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This research concentrates on the study of a series of charge-transfer crystals between chloranilic acid ($C_6H_2O_4Cl_2$) and organic bases (amines and pyridine). The target property of this work is the second harmonic generation (SHG) second-order nonlinear optical (NLO) response described by the $\chi^{(2)}$ tensor and the main objective is to investigate the relationships between the NLO responses of the crystals, the atomic charge distributions, and the supramolecular structural features of these systems.

All computations were carried out at the density functional theory (DFT) level with periodic boundary conditions (PBC), employing the CRYSTAL17 [1] suit of software. The work steps were the following. **I)** A full geometry optimization (atomic fractional coordinates as well as cell parameters) of the systems structures (starting from the single crystal X-ray diffraction structures), employing the ωB97X exchange-correlation functional (XCF). **II)** The calculation of the $\chi^{(1)}$ and $\chi^{(2)}$ tensors at the Coupled Perturbed Hartree–Fock/Kohn–Sham level (CPHF/KS) with the ωB97X (XC) functional. For dynamic field, a damping factor was employed in order to check and screen the electronic transitions. **III)** Topological analysis of the wavefunctions were performed in the framework of Bader's quantum theory of atoms in molecules (QTAIM) [2] using the TOPOND14 [3] software: Bader charge analyses were carried out, as they are a valuable tool to evaluate the charge transfer between the closely packed acid and base molecules. The topology of the electron density was also scrutinized in order to understand the nature of the multiple intermolecular interactions as well as to estimate their strength and directionality.

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# Designing organic emitters for next-generation Organic Light Emitting Diodes (OLEDs): a matter of symmetry and correlation

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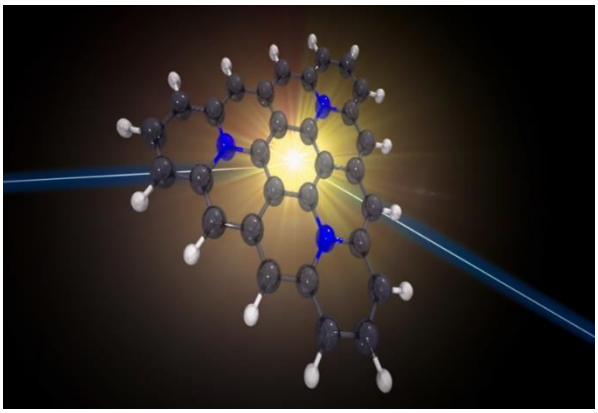
Nowadays Organic Light Emitting Diodes (OLEDs) represent an established technology in modern electronic devices, from flat screen TVs to bright lighting applications. Right now, while I am writing these words on my laptop and you are reading these sentences on your smartphone, millions of tiny molecules are electrically stimulated to emit the colourful light that reaches our eyes. Several factors affect the performance of an OLED, and one of them depends on how efficiently our molecules can convert electrical energy into light. More specifically, in an OLED made up of pure organic molecules, an effect called "spin-statistics limit" reduces this conversion efficiency to 25%. Throughout the years, different design strategies have been conceived to overcome this limit, the most efficient represented by the so-called Thermally Activated Delayed Fluorescence (TADF) emitters.

In this contribution, I will present a new family of triangular-shaped organic compounds bearing intriguing electronic properties able to increase the light-emission efficiency to 100%. In our work, we defined the computational protocol to describe these systems[1-3], and combining quantum chemistry and group theory, we related the optical properties of these molecules to their symmetry[4]. With this information in our hands, we established a series of design rules aimed at helping the identification of new emitters for next-generation OLEDs.



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# LIFTS: Learning Featured Transition Systems

Sophie Fortz

LIFTS stands for ``LearnIng Featured Transition Systems''. It aims at automatically learning transition systems that capture the behaviour of a whole family of software-based systems. Reasoning at the family level has been shown to yield important economies of scale and quality improvements for a broad range of systems such as software product lines, adaptive and configurable systems. Yet, to fully benefit from the above advantages, a model of the system family's behaviour is necessary. Such a model is often prohibitively expensive to create manually due to the combinatorial explosion of system variants (that is, all the configurations corresponding to the different members of the system family). For large long-lived systems with outdated specifications or for systems that continuously adapt, the modeling cost is even higher. Therefore, this thesis proposes to automate the learning of such models from existing artifacts. To advance research at a fundamental level, our learning target are Featured Transition Systems (FTS), an abstract formalism that can be used to provide a pivot semantics to a range of state-based modeling languages such as UML state diagrams (adapted to software families).

# Posters

# Development of an AlZnSnMg anode for the cathodic protection of steel in sea water

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## Abstract :

In this work, two aluminum alloys, Al-5Zn-0.5Sn and Al-5Zn-0.5Sn-2.6Mg, were prepared by melting in an induction furnace to be used as sacrificial anodes for cathodic protection of marine structures. The alloys are characterized by scanning electron microscopy mapping coupled to energy dispersive X-ray analysis, X-ray photoelectron spectroscopy and X-ray diffraction. Afterwards, the corrosion behavior was studied in 3 wt.% NaCl solution through immersion tests, potentiodynamic polarization, electrochemical impedance spectroscopy and weight-loss measurements. Results display that active dissolution of Al-5%Zn-0.5%Sn-2.6%Mg alloy and its quasi-uniform corrosion is associated with the major precipitates $MgZn_2$ and $Mg_2Sn$ particles formed during the melting process. Galvanic coupling measurements over 45 d were carried out on both alloys. The sacrificial cathodic protection of both anodes was successful but the couple efficiency was greater for Al-Zn-Sn-Mg owing to its more negative corrosion potential and uniform dissolution.

## Key words:

Cathodic protection, AlZnSnMg, particles

## References:

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# Study of the impact of UVB-induced senescent keratinocytes on skin cancer cells

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The global ageing of the population reinforces the necessity to better understand the biology of normal and pathological ageing. Ageing is notably associated with the accumulation of senescent cells in tissues but also with an increased risk of developing cancer. Cellular senescence, first defined as a stable growth arrest, is now associated to various age-related diseases. Indeed, the senescent cells secretome is notably known to be involved in the proliferation, migration and invasion of cancer cells. To study ageing and cancer development, skin is a tissue of choice since it is highly exposed to environmental stresses such as solar radiation, which promotes both the development of skin cancers and accelerated skin ageing (also called photoageing). This project is focused on the understanding of the impact of senescent epidermal keratinocytes on their cellular microenvironment. To do so, human normal epidermal keratinocytes (NHEKs) are exposed repeatedly to UVB in order to induce their senescence. The conditioned medium of these senescent keratinocytes, containing their secretome, is harvested to test its effect on the migration of melanoma and carcinoma cell lines. We detected a pro-migratory effect of senescent keratinocytes secretome on different cancer cell lines. In order to determine which factor(s) of this secretome could be involved in this pro-migratory effect, we are investigating the composition of the secretome of senescent keratinocytes by mass spectrometry.

**Advancing esophageal adenocarcinoma treatments by resistant gene signature identification and venom testing**

**Chloé Matthys**

Esophageal cancer is the six most deadly cancer worldwide and ranks seventh in terms of incidence. Moreover, the 5-year survival is relatively poor, not exceeding 15%. Esophageal cancer comprises two main histological subtypes namely esophageal adenocarcinoma (EAC) and esophageal squamous cell carcinoma (ESCC). The incidence of EAC is increasing and has exceeded ESCC in some countries of North America and Europe. Different studies have highlighted some driver mutations present in EAC. This leads to the development of targeted therapies. However, surgery and/or chemo(radio)therapy remain the treatment of choice. Response rate of the chemotherapeutic treatment is limited. That is why development of new treatments is needed. We hypothesize that the complete molecular characterization of samples obtained at diagnosis and relapse will unravel the mechanisms underlying multidrug resistance in EAC. We aim to identify a gene signature that could predict the patient response to treatments through transcriptomic analysis. Since we know the overall survival of each patients, we may also search for a prognosis signature that might be used in a decision tree. This gene signature will lead further to the identification of new potential targets for the development of new therapies. Venomics is a promising field for the discovery of new treatments. We hypothesize that we could find a venom peptide that display a cytotoxic activity against resistant EAC cells. We aim to assess therapies (venom peptides) using preclinical models including esophageal cancer cell lines and patient-derived organoids. Moreover, in order to follow cell subpopulations that could trigger treatment resistance, we will use a functional lineage-tracing system, ClonMapper. This system integrates DNA barcoding with single-cell RNA sequencing and clonal isolation to characterize clones within an heterogenous population such as the tumoral environment.

# Quantum chemistry study of the second harmonic generation $\chi^{(2)}$ tensor in chloranilic acid-based crystals.

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This research concentrates on the study of a series of charge-transfer crystals between chloranilic acid ($C_6H_2O_4Cl_2$) and organic bases (amines and pyridine). The target property of this work is the second harmonic generation (SHG) second-order nonlinear optical (NLO) response described by the $\chi^{(2)}$ tensor and the main objective is to investigate the relationships between the NLO responses of the crystals, the atomic charge distributions, and the supramolecular structural features of these systems.

All computations were carried out at the density functional theory (DFT) level with periodic boundary conditions (PBC), employing the CRYSTAL17 [1] suit of software. The work steps were the following. **I)** A full geometry optimization (atomic fractional coordinates as well as cell parameters) of the systems structures (starting from the single crystal X-ray diffraction structures), employing the ωB97X exchange-correlation functional (XCF). **II)** The calculation of the $\chi^{(1)}$ and $\chi^{(2)}$ tensors at the Coupled Perturbed Hartree–Fock/Kohn–Sham level (CPHF/KS) with the ωB97X (XC) functional. For dynamic field, a damping factor was employed in order to check and screen the electronic transitions. **III)** Topological analysis of the wavefunctions were performed in the framework of Bader's quantum theory of atoms in molecules (QTAIM) [2] using the TOPOND14 [3] software: Bader charge analyses were carried out, as they are a valuable tool to evaluate the charge transfer between the closely packed acid and base molecules. The topology of the electron density was also scrutinized in order to understand the nature of the multiple intermolecular interactions as well as to estimate their strength and directionality.

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# Simulation of surface enhanced vibrational spectroscopy: A journey to a unified method

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Surface Enhance Infrared Absorption (SEIRA) is an experimental method where trace amounts of a compound are detected by enhancing their absorption in the infrared spectrum[1]. This enhancement is a result of the interaction of the molecules with a localized plasmon, usually from a metallic nano-particle. A common hypothesis is that the molecule is mainly affected by the high electric-field resulting from the plasmonic resonance, with some sources even stating that the enhancement is proportional to the square of the electric-field intensity[2,3]. However, the exact nature of this interaction has not been proven yet.

Here we simulate this interaction with Discrete Dipole Approximation. Those simulations yield similar results to what can be found in experimental studies with an apparent decrease of the overall cross-section absorption at the molecule resonance. This decrease is tied to the effect of molecule on the polarization inside the nano-particle according to our results. This is unexpected as the molecule was thought too small in comparison to affect a metallic nano-particle. This work sheds a brighter light on the mechanism of SEIRA and allows access to original data that are unpublished yet.

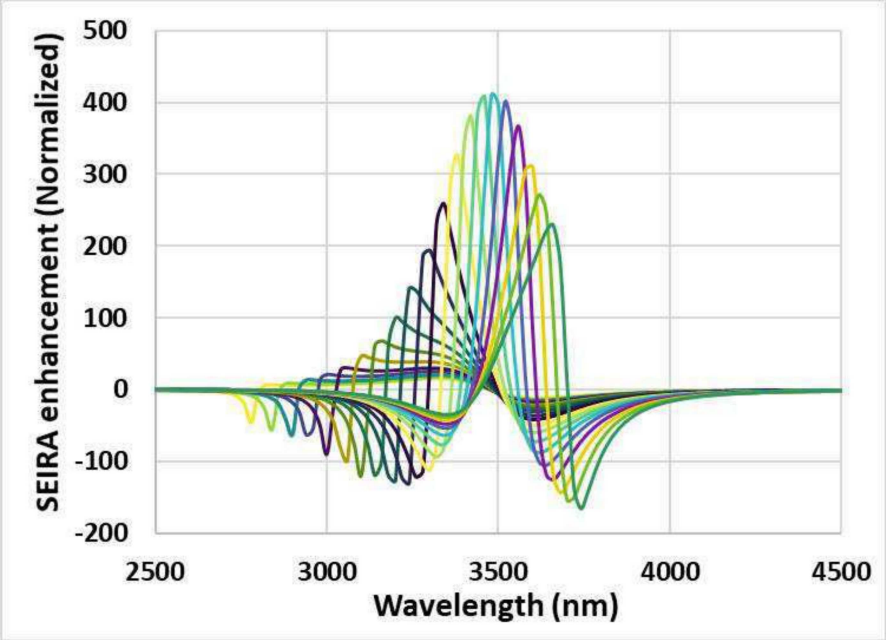


*Figure: SEIRA enhancement of several model molecules with a different wavelength for its vibrational mode*

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**Intracellular localization of ABCB5, a transmembrane protein expressed in melanoma**

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ABCB5 is a member of the ATP-binding cassette transporter superfamily predominantly expressed in pigmented-producing cells. It is a close homolog to the multidrug transporter ABCB1. Eleven ABCB5 transcripts have been identified. Among those, four isoforms are known to be transcribed: full-length (ABCB5FL; NM_001163941.1); alpha (ABCB5α; NM_001163942.1); beta (ABCB5β; NM_178559.5); and gamma (ABCB5γ; NM_001163993.2). ABCB5FL is a typical full transporter and ABCB5β is an atypical half transporter, while the other isoforms are soluble proteins. ABCB5β has been repeatedly in the spotlight for its roles as a marker of skin progenitor cells, melanoma stem cells and as a marker of limbal stem cells. It was also reported to be a mediator of multidrug resistance in melanoma, colorectal cancer, hepatocellular carcinoma and in several haematological malignancies. However, despite these reports, these two transporters remain little characterized. The elucidation of the respective localization of both isoforms ABCB5β and ABCB5FL and their subcellular trafficking, will help us to formulate hypotheses regarding their respective functions.

To assess the subcellular localization of ABCB5β, we did subcellular fractionation using an isopycnic centrifugation method and immunofluorescence analysis. MelJuSo and HEK293T cells were fractionated by differential centrifugation described by de Duve et al. Fractions were collected to conduct enzymatic assays to measure the activity of different organelles markers. We observed that the distribution of the tagged protein ABCB5β–mCherry, co-distributes to a large extent with alkaline alpha-glucosidase profile, used as a marker of the endoplasmic reticulum. Then, for immunofluorescence analyses, we engineered different constructs with a tag either at the N- or C-terminal region of the ABCB5β protein. Only the ABCB5β proteins tagged at the N-terminal region could be detected. Interestingly, co-labelling of the ABCB5β-N-ter tagged proteins and of selected organelle markers further supported an ER localization for this protein. Lastly, the N-terminal tagged ABCB5β whose expression is driven by a weak PGK promoter led to the same distribution in MelJuSo melanoma cells. We are currently working on the production of a monoclonal antibody to address the localization of the native ABCB5β protein to corroborate our overexpression data. Overall, this study is a significant step toward the elucidation of the function of the ABCB5 protein in normal melanocytes and in melanoma.

# Growth mechanisms and properties of magnetron sputtered TiO2 thin films on complex 3D foam substrates

The synthesis of functional material (e.g. TiO2) on foams is a becoming an important research area, particularly in photocatalysis [1,2]. However, coatings on foams are most of the time synthesised using the sol-gel and soft template methods, or even the hydrothermal and calcination routes. PVD methods are rarely used to coat such substrates and when it is, the growth mechanisms are never mentioned. However, PVD deposition can bring significant interest on those complex 3D foam substrates, such as accurate control and tuning of film morphology, composition, and/or synthesis of metastable phases.

The scope of this work is to study the growth and properties of TiO2 films deposited on Ni and C foams by the means of DC magnetron sputtering and HiPIMS, and to get insights on how the film grows on such complex 3D substrates, especially regarding the crystal structure and the morphology of the coating inside the foam. The physico-chemical properties of the deposited films are investigated using XPS, SEM and XRD. Thanks to high resolution XPS spectra, the chemical environment as well as the stoichiometry is studied. SEM cross-sections of the TiO2@C foam assemblies allow to observe the change in coating morphology with increasing depth inside the foam. XRD confirms the synthesis of crystalline TiO2, whose structure is either anatase, rutile or a mix of both depending on the deposition technique. In addition, XRD also confirms the synthesis of anatase {001} facets, which display the highest photocatalytic activity [3].

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# Structural and functional characterization of a copper efflux membrane protein: PcoB from *Caulobacter crescentus*

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**Abstract**

Copper has been used for decades as an antibacterial agent. As a response, many bacteria have an increased resistance by various mechanisms mainly operating by efflux. Therefore, selectively targeting the prokaryotic copper regulation system is essential for developing new antibiotics.[1] In the *C. crescentus* aquatic α-proteobacteria, the copper efflux is predominantly regulated by a two-component PcoA and PcoB system.[2] Whilst data are available for PcoA systems, only limited information is reported for PcoB. The general objective of this project is to characterize the structure and function of the *Caulobacter crescentus* membrane protein PcoB, which is hypothesized to be a copper-efflux protein.

First, we deal with the purification and reconstitution of PcoB in artificial membranes. This protein is overexpressed in inclusion bodies with high yield in *E. coli*, purified using $Ni^{2+}$ affinity, and refolded by the SDS-cosolvent method.[3] To allow the characterization of its transport function, the detergent-solubilized protein is also reconstituted in liposomes. Circular dichroism (CD) spectroscopy is used to compare the secondary structure content of proteins solubilized in detergent micelles to those reconstituted in liposomes.

Second, a three-dimensional model of PcoB tertiary structure, supported by a CD fingerprint, is built and shows a $\beta$-barrel with a N-terminal disordered chain. This peculiar intrinsic disorder property is also confirmed by various bioinformatic tools.

Finally, we consider the *in vitro* PcoB functional properties with tailored techniques: copper binding, pore-forming activity, and copper-release action. The selectivity towards $Cu^{2+}$ will also be confirmed.

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# Characterization of the molecular role of PcoB in copper efflux in Caulobacter crescentus

*Amira Khochtali[1*], Jean Yves Matroule[2]*

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In most living organisms, Copper (Cu) is a cofactor of key metalloenzymes, yet it becomes toxic at high concentrations, therefore implying a tight regulation of its intracellular homeostasis. The dimorphic α proteobacterium *Caulobacter crescentus* ensures a bimodal response to Cu stress. The motile swarmer (SW) cell favors a flight response, whereas the sessile stalked (ST) cell engages an operon-encoded detoxification system involving the periplasmic Cu oxidase (PcoA) and an outer membrane protein (PcoB) most likely acting as an efflux pump for Cu[1]. However, the molecular mechanisms sustaining Cu efflux by PcoB are still unknown.

A pulldown-MS analysis was unable to identify any partner that could assemble with PcoB into an energized complex spanning the bacterial envelop, suggesting that Cu efflux by PcoB only relies on PcoB itself. Consistent with its role as an outer membrane efflux pump, PcoB 3D structure prediction shows a C terminal (C-term) domain forming a β barrel and an intrinsically- disordered N terminal (N-term)[2] domain rich in histidines (9 His) and methionines (4 Met), suggesting that this N-term domain may bind Cu and be important for Cu efflux. Accordingly, the deletion of the PcoB N-term domain significantly reduces Cu efflux and sensitizes *Caulobacter* to Cu. Surprisingly, point mutations of these His and Met residues had no effect on cell growth and Cu accumulation under Cu stress, raising the question of the precise role of PcoB N-term domain in Cu efflux. Preliminary data reveal that PcoB and more surprisingly PcoA protein levels are reduced in the PcoB N-term mutant, suggesting that PcoB N-term region plays a role in the expression and/or stability of PcoA and PcoB.

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# Neuroinvasion of SARS-CoV-2 in SH-SY5Y cells can be partially blocked by using entry inhibitors

Margaux Mignolet[1], Matthieu Gueibe[1] , Valéry Bielarz[1], Kévin Willemart[2], Kathleen De Swert[1], Jacques Gilloteaux[1,3], Nicolas Gillet[2], Charles Nicaise[1]

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During the first pandemic wave of Covid-19, SARS-CoV-2 pre-alpha strain was responsible for neurologic complications in severely-affected patients. Part of this effect is mediated by a direct invasion of the brain cells via different entry routes, including axonal transport or hematogenous route and receptors (ACE2, TMPRSS2, NRP1, …). In this study, we modeled the neuro-invasion on SH-SY5Y cell line to study SARS-CoV-2 intracellular lifecycle and to assess its potential cytopathic effects. The internalization of the virus was visualized using gene S RNA *in-situ* hybridization, and confocal microscopy. SARS-CoV-2 could not efficiently replicate as negative-sense RNA was not detected and new viral particles were not massively released in the culture medium. Finally, a mild cytopathic effect was observed by shortened neuritic processes as well as a decrease in neuropeptide Y release within 24 hours post-infection. Preliminary data suggest that this mild cytopathic effect can be significantly prevented by interfering with host cell surface receptors using camostat mesylate or human recombinant soluble ACE2. Such results hold promise for preventing SARS-CoV-2 neuroinvasion.

# Deciphering spatiotemporal regulation of antibiotic and copper coresistance in *C. crescentus*

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Bacteria are frequently exposed to antibiotics (AB) and copper (Cu) due to their ever-increasing use in agriculture, industry, and medicine. This has led to the co-selection of mechanisms increasing AB/Cu coresistance. Yet, little is known about the transcriptional regulation underlying this double resistance. Metals like copper (Cu) are essential at low amount but toxic at higher concentrations, therefore requiring an efficient Cu homeostasis.

In order to identify novel Cu homeostasis strategies in the aquatic alpha-proteobacterium *Caulobacter crescentus*, a genetic screen was undergone a few years ago by the team from a mini-Tn5 mutant library seeking for Cu-sensitive mutants. Thereby, a mutation was identified in the *tipR* (CCNA_00852) gene. TipR is a homolog of the AcrR regulator in *E. coli*, which regulates the antibiotic efflux pump AcrABTolC. Interestingly, we were able to identify a hypothetical Cu binding site via in silico structural analysis. In accordance with the genetic screen, the *ΔtipR* mutant showed sensitivity to Cu in liquid culture, suggesting that TipR plays a role in Cu tolerance. A ChIP-Seq analysis together with a bioinformatic regulon prediction allowed us to identify potential TipR target genes such as the operon coding for *acrABnodT* (CCNA_00849: CCNA_00851), an efflux pump neighbouring the *tipR* gene. AcrABNodT was homologous to the AcrAB and CusC proteins from the AcrABTolC pump and CusCBA pump in *E. coli*, respectively. The homology analysis led to the hypothesis that AcrABNodT could have dual resistance to antibiotics and Cu. Surprisingly, no Cu sensitivity was observed upon deletion of this operon, suggesting (1) a potential redundancy with another Cu efflux pump or (2) that AcrABNodT has no role in Cu efflux.

The CCNA_03857 gene predicted to encode a transporter was another promising TipR target candidate, which was also revealed by the genetic screen. Preliminary data seems to indicate that CCNA_03857 is not involved in Cu homeostasis, although a role in Cu redistribution or in the transport of another substrate cannot be ruled out. Furthermore, recent data suggests that TipR also plays a role in cefuroxime (cephalosporin) and ciprofloxacin (fluoroquinolone) resistance in *C. crescentus*, highlighting for the first time the regulation of AB/Cu coresistance by a one-component regulator.

# A Data Recommender System for Decision-Makers

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**Abstract.** Companies nowadays are increasingly dependent on data. In an environment that is more dynamic than ever, they are looking for tools to leverage those data and obtain valuable information in a rapid and flexible way. One way to achieve this is by using Data-Driven Decision Support Systems (Data-Driven DSS). In this project, I focus on one such type of DSS, namely the Self-Service Business Intelligence (SSBI) Systems. These systems are designed specifically to avoid the involvement of the IT department when creating business reports by empowering businesspeople in the production of their own reports, thereby reducing the time-to-release of a given report and improving the responsiveness of companies. Business decision-makers, when developing their own reports, however face barriers. These challenges are related to the current self-service features that are not sufficiently adapted to their business needs and their lack of IT knowledge. In my research project, I focus on one of their most important challenges, namely: the data picking within technical and large databases. Today's databases are indeed more and more complex to deal with for non-IT experts due to their continuously increasing volume and technical jargon. The objective of my project is to help decision makers to deal with these data by mobilizing different Artificial Intelligence (AI) techniques such as Natural Language Processing techniques, Semantic and Recommender Systems. Concretely, these techniques will be mobilized to develop a data recommendation system based on a user's query expressed with his own jargon. This system will be fully adapted to the user (i.e. his needs and preferences) and will be tested in several real companies.

# Data-Driven Strategy Maps: A Hybrid Approach to Strategic and Performance Management Combining Hard Data and Experts

Lhorie Pirnay

This research project aims to explore the potential of using hard data in the development of Strategy Maps, which are decision support tools that depict the interrelationships between key performance indicators (KPIs) of a company. The current state of practice for Strategy Maps relies heavily on the knowledge and intuition of experts, which can lead to inaccuracies, incompleteness, and a lack of longitudinal perspective. With the advent of technological innovations, it is now possible to collect, store, and analyze large amounts of data, which can be used to enhance strategic decision-making. The first chapter of the research project reviews the current literature on the practical development of Strategy Maps and finds that the methodologies used to estimate causalities between KPIs are mainly qualitative and based on soft data (human expertise). The second chapter presents a new data-driven framework to validate causalities based on data analytics. The last chapter develops a hybrid methodology that combines both human and data inputs in order to build a robust and adoptable tool for managers. Overall, this research project aims to demonstrate the value of integrating hard data into the development process of Strategy Maps in order to increase their reliability and effectiveness as decision support tools. The proposed hybrid methodology may provide managers with a valuable tool that leverages both human expertise and data analytics to make more informed strategic decisions.

**High-throughput screening for inhibitors of Elongator**

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The six-subunits Elongator complex participates in the addition of a modification on $tRNA^{Lys}_{UUU}$, $tRNA^{Glu}_{UUC}$ and $tRNA^{Gln}_{UUG}$. The modification of uridine 34 ($mcm^5s^2U_{34}$) is required to offset the translational inefficiency resulting from low effective stacking interactions of the A-U base interaction. It was shown to be relevant for human health. The anti-tumor activity of RAF inhibitors in melanoma patients (BRAF-V600E mutation) is often rapidly lost but cells are re-sensitized by the inactivation of Elongator.

We use the power of yeast genetics to identify inhibitors of Elongator to probe its biological function in detail. These molecules may later have bio-medical interest.

The screening for chemical compounds inhibiting Elongator relies on the inducible expression of an endonuclease that cleaves the target tRNAs in a $mcm^5$ dependent manner, which results in lethality. In presence of a chemical inhibitor, the absence of modification prevents the cleavage and allows yeast cells to survive and proliferate. A library of 30000 compounds was screened and the candidate compounds were retested in a completely independent set up relying on a genetic anti-suppressor system.

We are currently analyzing the mode of action of promising candidates to determine which step of the synthesis of the modification they target. We will next use them to study the effect of fast inhibition of Elongator on both the proteome and cellular fitness.

# Identification of the O-chain ligase in *Brucella abortus*

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Gram-negative bacteria are known to present on their surface a major component called lipopolysaccharide (LPS), formed of a lipid A, a sugar core and a long polysaccharide, called O-chain. *Brucella* spp*.,* which are facultative intracellular pathogens, show two types of LPS, rough and smooth, the first one lacking this O-chain polysaccharide. Both forms are present on single cells (Vassen *et al.,* 2019). While the O-chain ligase necessary to add this O-chain has been identified in many bacterial species, this enzyme has not yet been described in *Brucella* spp.

In this work, we aimed to characterize two putative candidate genes for the O-chain ligase. The first candidate is BAB2_0106 (*waaL*), a homolog of *Escherichia coli* WaaL. Deletion of *waaL* does not impact the presence of O-chain, suggesting that WaaL might not be the O-chain ligase in *Brucella* spp.. Our second candidate BAB1_0639 (*wadA*) revealed to be interesting. Surpisingly, *wadA* is essential in *B. abortus*, while it is not in its close relative *B. melitensis*, despite the fact that these *wadA* orthologs are strictly identical. However, deletion of *wadA* in *B. abortus* is possible in a strain unable to synthesize the O-chain (Δ*gmd*), which suggests a potential toxicity due to O-chain accumulation on its lipid carrier bactoprenol. Indeed, bactoprenol is also a carrier for peptidoglycan precursors, and thus saturation of this carrier could lead to a shortage of peptidoglycan synthesis.

Previous reports identified WadA as the glycosyltransferase necessary to add the last core sugar (glucose) during the synthesis of the LPS core (González *et al*., 2008). Our results reveal that the absence of this last glucose correlates with a growth defect in liquid culture possibly occurring through an alteration of LPS interactions with essential components of the outer membrane, such as the Omp2b porin, LptD or BamA. Additionally, we identified a second putative activity for WadA with a C-terminal domain acting as the O-chain ligase. The O-chain ligase activity was suggested accurate through results found by Western Blot and immunofluorescence microscopy that indicate absence of the polysaccharide when deleting this O-chain ligase domain. Complementation of a mutant deleted for the O-chain ligase domain with the coding sequence for the O-chain ligase domain only results in a smooth strain with normal growth, suggesting that the ligase activity is carried out by this domain, and that glucose is present on the core of the LPS, since the O-chain is attached to the glucose of the core. O-chain ligases of the WaaL family carry several positively charged amino acids proposed to be involved in the ligase activity. Using site-directed mutagenesis, we demonstrate the importance of one positively charged amino acid, Arg-614, in the O-chain ligase domain for its activity.

Overall, our data gives new insights on the LPS synthesis, identifying WadA as the main O-chain ligase in *Brucella* spp. but also describing for the first time a bifunctional enzyme in this pathway, adding a glucose to the LPS core at the cytoplasmic side of the inner membrane, and linking the O-chain to this added glucose at the periplasmic side of the inner membrane.

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# Non-covalently synthesis of porous organic salts

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***Keywords: hydrogen bonding; ionic bonding; high polarity; permanent porosity;***

The preceding years have experienced the booming development of porous materials in a wide range of fields, from the inorganic skeleton of zeolites, activated carbon, silica, to hybrid metal–organic frameworks (MOFs), covalent organic frameworks (COFs), conjugated microporous polymers (CMPs), covalent triazine frameworks (CTFs), and porous aromatic frameworks (PAFs). Although these porous materials exhibit advantages in scientific fields, porous materials with rigid structure and permanent porosity have been rarely reported. Porous organic salts (POSs) are a new member of porous materials and constructed by ionic bonding and hydrogen bonding between organic acid and base. Because of the special ionic bond, POSs provide the confined channels for transportation of high polar molecules which makes them distinct from other porous organic materials (POMs). Aside from that, POSs possess permanent porosity that means voids show long-term stability and reversibly accessibility after removing guest molecules. Generally, permanent porosity correlated closely with the strength of ionic bonding and rigidity of framework. However, it is worth to notice that ionic bond is non-directional, which makes the joint of framework too flexible to sustain high intermolecular free volume. Hydrogen bond is a powerful intermolecular force and more importantly, it is directional which can deteriorate flexibility resulting from non-directional ionic bond. The POSs with high polarity channel and new promising applications have become a new family of porous organic frameworks[1].

In this work, POS-1 was successfully synthesized using 1,4-benzenedisulfonic acid and 2,7,15-triaminotriptycene. The single crystals were crystallized in methanol solution. The single crystal X-ray diffraction results revealed that POS-1 exhibit monoclinic crystal system with space group of *C*2/*c*. The lattice parameters of a = 13.31 Å, b = 18.62 Å, c = 29.72 Å and $\alpha = \gamma = 90°$, $\beta = 96.73°$. There is 1D pore channel along a axis. The volume of the void space is 14% with the space of 10.5 ×10.5 Å. The asymmetric unit is composed of one 2,7,15-triaminotriptycene and 3/2 1,4-benzenedisulfonic acid and 7/2 water molecules. Because of the asymmetric position of amino group in triptycene, there are torsion in the unit cell. The 1,4-benzenedisulfonic acid and 2,7,15-triaminotriptycene extend along a, b and c axis with an angle. The molecules connect to three-dimensional network through hydrogen bonds. The CH-$\pi$ interaction exist when densely packing. There is no defined supramolecular cluster because the length of benzene and triptycene is not well matched. And also, aside from the charge-assisted hydrogen bond between sulfonate group and amino group, there is neutral hydrogen bond between water molecule, sulfonate group and amino group.

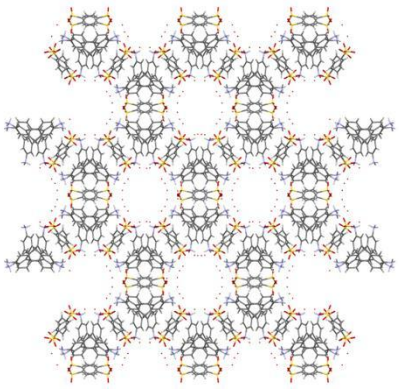

Figure 1. The packing diagram of POS-1. (C: gray; N: blue; O: red; S: yellow; H: white).

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# Effects of disorder on properties of two-dimensional $MoS_2$

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Comprehensive research on electronic and spintronic properties of graphene and $MoS_2$ has been the focus of scientific attention for several years and still is [1,2]. An important issue, however, is the presence of defects that can influence these properties [3,4]. In the case of $MoS_2$, experiments have demonstrated that edges (1D defect) can host local magnetic moments [5]. However the computational cost of the ab-initio DFT calculations for experimentally relevant system size is a downside.

In this work, we first show that sulfur vacancies in monolayer $MoS_2$ induce gap states in the electronic band structures. As a second contribution, we have investigated theoretically the magnetic properties for several nanometers long $MoS_2$ nanoribbons with zigzag edges using fine-tuned parameters in a tight-binding (TB)-Hubbard Hamiltonian. We could successfully reproduce the metallic state induced by the edges, compute large-scale nanoribbons and predict the spin domain-wall energy as well as study the effect of edge disorders on the magnetic properties [6]. Besides the full TB parametrization of the nanoribbon, we also described the bands crossing the Fermi level with a one-dimensional linear chain model, allowing us to easily compare ferromagnetic and anti-ferromagnetic configurations and giving us an useful tool to study the energy cost for switching spins on various spots and scales. This model can be useful to study the stability and the properties of real size nanoribbons presenting spin defects and their applications.

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Titre: Identification of Cyber Physical System (CPS) & Orchestration of fuzzing testing

Guillaume Nguyen

Abstract:

Cyber-security has been a hot topic since quite some years now. With the increasing number of devices (connected or not), the need for a clean environment allowing effective and efficient testing is increasing as well. Furthermore, some devices are connected to the physical world with the ability to have an effect on it. Those specific devices are called Cyber Physical Systems (CPS). With such power in the hands of machines, it is imperative that they behave as expected and that they resist to disruptive environments (whether from cyber attacks or unwanted noise). Indeed, the impacts of unexpected behavior could lead to great damage (disruption of the production line, overheat of a nuclear reactor, false fire alarm, etc.). To test such systems, there are multiple techniques. Fuzzing Testing works particularly well with any type of system by sending pseudo-random inputs. Currently, there are no frameworks that allow for the classification of CPS and enable the automatization of the generation of tests. That is why this thesis will focus on finding the most suitable definition of CPS, a way to classify them and comparing the various fuzzing techniques to find the most effective ones based on relevant features and requirements.

# Investigation of the Antibacterial Properties of Silver-Doped Amorphous Carbon Coatings Produced by Low Pressure Magnetron Assisted Acetylene Discharges

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**Abstract:**

The surfaces are transmission vectors of pathogens such as bacteria and viruses. By indirect contact mode between our hands and fomites, these microbes spread in our environment and contaminate us. That is all the more true in the hospitals where the immunosuppressed patients are most likely to contract infections. These latter are responsible for a significant part of morbidity and mortality worldwide, not only but also, a financier burden on our society.

The released-based plasma coatings are promising solution to this major problematic. The advantage of the release approach is to provide the anti-infectious agent locally, while avoiding any adverse toxic impact for human beings. Whatever the state it is in (ion, nanoparticles or colloids), silver (Ag) have known effects and it is used since the ancient times. Developed within the framework of nanomedicine, materials based on silver ion release have been among the most studied candidates for antimicrobial purposes.

In this work, we evaluate the possibility to produce antimicrobial, antibacterial and antiviral coating to be applied on any surfaces. Amorphous hydrogenated carbon matrix doped with silver (a-C:H:Ag) were produced by low pressure magnetron assisted acetylene discharges and deposited on stainless steel substrates. The colony-forming unit (CFU) method, LIVE/DEAD bacterial viability and modified Kirby-Bauer diffusion assays were used to assess the toxicity of this coating against *Escherichia coli* (Gram-negative) and *Staphylococcus aureus* (Gram-positive) bacteria. The antiviral properties were evaluated by infectivity assays, Tissue Culture Infectious Dose 50% (TCID50) calculated by Reed-Muench Method and a quantitative colorimetric MTS assay based on the cytopathic effect (CPE). We used a Porcin Respiratory Coronavirus (PRCV), a virus of the *Coronaviridae* family that shares the same common features with SARS-Cov-2. The achieved results during this work show very promising antibacterial and antiviral activities. The mechanism of action of the silver-based coatings with a carbon matrix were investigated by X-Ray Photoelectron Spectrometry (XPS) and Scanning Electron Microscopy (SEM). The results obtained suggest a crucial role of silver segregation towards the surface and formation, of nanoparticle to explain the antimicrobial effect against bacteria and viruses. The data have been published [1].

**Keywords**: antibacterial coating, antiviral coating, silver, a-C:H, bacteria, virus, silver segregation

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# Consequences of the inactivation of the mannose-6-phosphate pathway on the growth, migration and drug sensitivity of HeLa cells.

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Lawrence *et al.* reported that the frequency of mutations in *GNPTAB* is significantly increased in breast and uterine cancers. *GNPTAB* encodes α and β subunits of GlcNAc-1-Phosphotransferase, an enzyme involved in the synthesis of Mannose 6-Phosphate (M6P) moieties on glycans carried by lysosomal enzymes. These M6P residues serve as sorting signals to the lysosomes. A deficiency in GlcNAc-1-Phosphotransferase is known to cause Mucolipidosis II/III, i.e. lysosomal storage diseases characterized by acid hydrolases hypersecretion and abnormal macromolecule storage in enlarged lysosomes. Since lysosomes and lysosomal enzymes play several roles in cancer development, progression and drug resistance, we wonder whether GlcNAc-1-phosphotransferase inactivation could have pro-cancerous consequences. In support of this view, we found that the knockout of *GNPTAB* in HeLa cells promotes their anchorage-independent growth. Moreover, a wound healing assay on a polystyrene surface revealed an increased migration of *GNPTAB*-KO cells compared to controls cells after supplementation of the culture medium with IGFII. Lastly, we identified that the KO of *GNPTAB* causes resistance to cell death induced by different drugs, including doxorubicin. Taken together, these findings raise the possibility that GlcNAc-1-Phosphotransferase inactivation may promote cancer cell proliferation, metastasis and resistance to chemotherapy. The underlying mechanism(s) linking lysosomal acid hydrolases missorting, due to a GlcNAc-1-Phosphotransferase deficiency, and cancer cell behaviour is currently under investigation.

# Pattern reconstruction through generalised eigenvectors

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One of the most widespread theories to explain the emergence of patterns is due to Alan Turing. His theory consists of a reaction-diffusion system of two species, whose stable spatially homogeneous equilibrium is disturbed in order to obtain a new inhomogeneous state, called a Turing pattern [1]. We consider its extension on a network, therefore the two species interact on the nodes and diffuse through the links [2]. In the latter paper, authors have proved that the emergence of the instability can be related to the spectrum of the Laplace matrix associated to the underlying network; in particular it should exist an eigenvalue that returns a positive Lyapunov exponent, named for simplicity "unstable" eigenvalue. Then one can show that in the short time regime, the pattern can be described by a linear combination of the eigenvectors associated with the unstable eigenvalues of the Laplacian. Interestingly enough the same result holds true for the asymptotic regime. The above claim relies on the existence of a basis of eigenvectors. We hereby introduce and study the case of defective networks, i.e., networks whose Laplacian matrix is not diagonalisable and thus does not have a linearly independent set of eigenvectors. Our aim is to show the effect of generalised eigenvectors on the Turing pattern. First we prove that one can extend the theory developed so far [2] to this new setting providing sufficient conditions for the emergence of Turing patterns, then by using the Brusselator model as a generic nonlinear system, defined on a non-normal network [3] we illustrate the impact of generalised eigenvectors in the pattern reconstruction. As shown in Fig.1, when only the eigenvectors are used (panel a)), the pattern is not fully recovered, whereas the pattern is reconstructed almost perfectly when also the generalised eigenvectors are considered (panel b)). Therefore, our results reveal the importance of the generalised eigenvectors: conditions for the Turing instability can be found and the pattern can now be reconstructed.

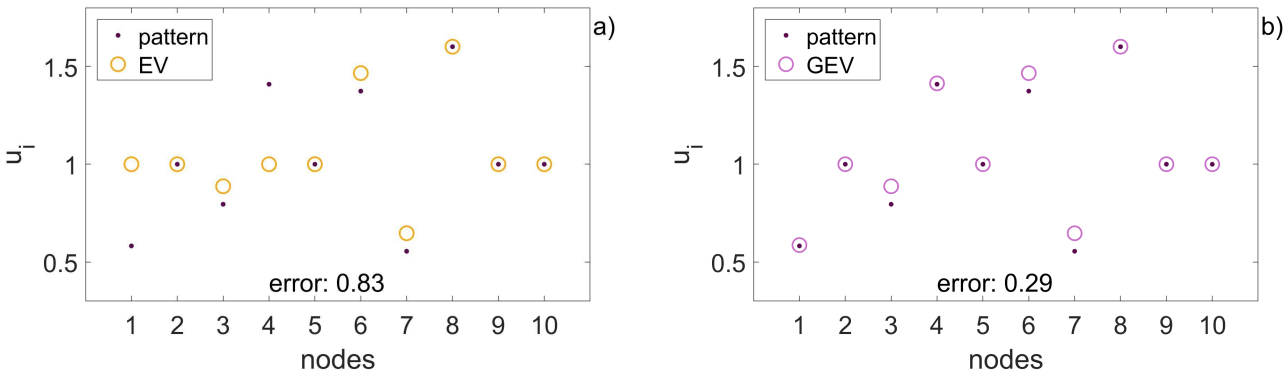


Figure 1: Brusselator model, with parameters $b = 3.92$, $c = 3$, $D_u = 0.2$ and $D_v = 0.8$, on a random non-normal network of 10 nodes. Pattern vs. reconstructed pattern; a) only eigenvectors (EV), b) with generalised eigenvectors (GEV). The three eigenvectors used are each associated with an unstable eigenvalue, one of multiplicity 2 and two of multiplicity 1, and the generalised eigenvector used is associated with the unstable eigenvalue of multiplicity 2. The error used is the absolute error, weighted by the number of unstable eigenvectors used, divided by the total number of unstable eigenvectors and generalised eigenvectors.

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# *Targeting the splicing factor TFIP11 in cancer by an intrinsically disordered protein-based drug design strategy*

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The spliceosome is the main cellular machinery guiding the splicing reactions of pre-mRNA. Recent studies have revealed that cancer cells survival is highly dependent on that splicing function. These findings have resulted in a growing interest in targeting splicing regulatory proteins in the treatment of cancer.[1,2] In this project, we consider the human splicing factor TFIP11 (Tuftelin Interacting Protein 11). Its depletion was recently shown to alter cell cycle progression and to induce apoptosis in cancer cells, pointing up TFIP11 as a potential target for cancer therapy.[3]

TFIP11 belongs to a particular class of proteins called intrinsically disordered proteins (IDPs). Unlike globular proteins, IDPs lack a well-defined tertiary structure and exist as conformational ensembles. Their various context-dependent conformations allow them to interact with multiple partners. About 30% of the TFIP11 sequence is predicted disordered, especially two regions within the N-terminal extremity. They were shown to be crucial for TFIP11 protein-protein interactions (PPIs) and for spliceosome correct assembly.[3]

The aim of this research is to decipher TFIP11's behavior and to identify hit molecules able to block TFIP11's disorder (closely linked to its multi-functionality) or its PPIs. A rational drug design approach, challenging in the context of IDP, will be applied.[4,5] For that purpose, we combine *in vitro* and *in silico* approaches using spectroscopic (intrinsic fluorescence, circular dichroism, dynamic light scattering, …) and computational (molecular dynamics and virtual screening) methods. Further developments including lead molecules optimization, *in vivo* assays,... will then be required to achieve safe and effective anti-cancer drugs.

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# **Abstract entitled :** A Consensus-based Framework for Federated Learning using Inductive Logic Programming

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Nowadays, the data used by artificial intelligence systems are often dispersed across the world on various heterogeneous, and non-secure platforms. It can also reside on static machines as well as mobile devices. Federated learning is an emerging machine learning paradigm involving multiple clients, e.g., mobile phone devices, with an incentive to collaborate in solving a machine learning problem coordinated by a central server. The traditional Federated Learning framework is recognized as poorly resilient to attacks that can de-anonymize sensitive data when exchanging the model updates between clients and central servers. As an alternative approach to that end, we investigate the use of inductive logic programming. It uses both techniques from machine learning and logic programming with the objective of inducing theories, as sets of logical rules, that generalize the given training examples. Theories will therefore be exchanged between nodes, which solves many security concerns. However, learning in that way on different nodes requires to unify different theories, which we plan to obtain through the development of consensus techniques.

**Keywords:** Federated learning , Inductive logic programming, machine learning, logic programming.

# Investigating the Diels-Alder Reactions Combining Density Functional Theory with Bonding Evolution Theory (BET)

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## abstract

The Diels-Alder reaction is one of the key organic chemistry reactions, leading to a broad range of products. In our work, we have studied four types of Diels-Alder reactions, between a single diene, (buta-1,3-diene) and different dienophiles, [ethylene, acrylaldehyde, acrylonitrile, (4aS,8aR)-3,4,4a,5,8,8a-hexahydronapthalen-1(2H)-one], in order to unravel the role of the substituent beared by the dienophile on the reaction mechanism, *i.e.* how the bond formation/breaking processes occur along the reaction path.

So, we have analyzed the reorganization of electron pairing by means of the Bonding Evolution Theory (BET)[1], by combining the topological analysis of the electron localization functions (ELFs)[2] and Thom's catastrophe theory (CT)[3]. The study has been performed at the Density Functional Theory (DFT) level, with the M06-2X exchange-correlation functional and the 6-311++G** basis set. In addition to the calculation of the ELFs, DFT was used to evaluate the thermodynamical state functions for reactants, transition states, and products.

We observed that all reactions have low activation enthalpies, are exothermic, exergonic, and spontaneous. The study of the synchronicity and the concertedness revealed that, only the reaction between 1,3-butadiene and ethylene takes place according to a synchronous and concerted mechanism (the process leading to the formation of the two bonds occurs at the same time). The others take place according to an asynchronous but still concerted mechanism (the process leading to the formation of the bonds occurs at different times).

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# Linear and nonlinear optical response from the fluorescent photonic structures occurring in beetle integuments

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Fluorescence emission occurs in the integuments of many natural species including but not limited to insects, arachnids, mammals, anthozoans (e.g., sea anemones and corals), birds, and scyphozoans (i.e., true jellyfish) [1-3]. In insects, fluorophores, such as papiliochrom II and biopterin, are at the origin of such light emission. In some cases, they are naturally embedded in photonic nanostructures, which influence the emission in terms of spectral intensity, decay time and spatial distribution [4,5]. Using linear and non-linear optical and fluorescence techniques, the case of the *Hoplia coerulea* male beetle was investigated. The photonic structures found in the scales covering its body comprise fluorophores. These structures control both the insect's colouration and the emission from the embedded fluorophores [5,6]. Contact with liquids gives rise to variations of the emission properties. The combination of these observations and optical modelling allows the study of the photonic confinement within the beetle's nanostructures. Additionally, Third-Harmonic Generation and two-photon fluorescence analyses unveiled the multi-excited states character of the fluorophores and, through light polarisation effects, the role of the photonic structures' anisotropy in the fluorescent behaviour [7]. In addition to the elaboration of new concepts and the development of technological applications through a bioinspiration approach, such investigations help the understanding of the biological functionalities behind the observed fluorescence response.

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# Investigation of the bidirectional copper transport across the inner membrane of the free-living *Caulobacter crescentus*

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Copper (Cu) is essential for most living organisms at low concentrations and turns toxic at higher concentrations. This duality implies a tight regulation of cellular Cu content by coordinating Cu influx and efflux. In bacteria, most studies have characterized Cu efflux machinery in pathogens, leaving the mechanisms of Cu entry largely unknown.

In this research project, we aim to uncover the bidirectional Cu transport across the inner membrane of the free-living model *Caulobacter crescentus*. In an attempt to identify transporters involved in Cu export, three homologs of CopA, a widely distributed Cu exporter in bacteria, were found in *C. crescentus* genome. Surprinsingly, single knock-outs of the three CopAs paralogs did not show any increased Cu sensitivity. To address a potential redundancy between the three CopA homologs, double and triple CopA mutants were generated and none of these strains led to a Cu-sensitive phenotype, suggesting a alternative mechanism involved in cytoplasmic Cu export. In order to identify a new Cu exporter, we plan to implement a forward genetic approach by generating a mutant library that will aim to identify synthetic lethal mutations in the triple *copAs* mutants.

Besides the exporters, we aim to identify novel inner membrane Cu importers and to determine whether their role can be extrapolated to other bacterial species since Cu entry into the cytosol is still a matter of debate.

# Tackling quantum algorithms using modular values
# 2022 Annual Meeting of the Belgian Physical Society

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Quantum algorithms can solve problems more efficiently than classical ones. Among the first and most representative examples of this superiority are the Deutsch algorithm and its generalization, the Deutsch-Jozsa algorithm. The latter verifies if a function, $f : \{0,1\}^N \to \{0,1\}$, is balanced or constant. The quantum procedure only needs one step to solve the problem while the classical one requires $2^N - 1$ repetitions in the worst case.

Usually, measurements are considered ideal, non-reversable projective operations. To perform one, the system should interact with a measuring device, or ancilla. For some measurements, the system and the ancilla interact through a unitary operator. In that case, when the interaction strength between the system and the measuring device is weak enough, the unitary operator can be expanded in a Taylor series to first order. This constitutes a weak measurement. When describing the observations of quantum weak measurement with pre-selection (which consists of choosing the initial state) and post-selection (which requires a projective measurement after the weak measurement and corresponds to choosing the final state), quantities called weak values appear. In that case, the ancilla's wavefunction is shifted in position by an amount that is proportional to the real part of the weak value. Its wavefunction is also shifted in momentum by an amount that is proportional to the imaginary part of the weak value. As the weak value is an unbounded and complex number, it has found several applications in metrology, sensing, as well as in quantum foundations and probing quantum paradoxes.

When considering observables that are unitary, the modular value, $A_m = \dfrac{\langle \psi_f | e^{-ikA} | \psi_f \rangle}{\langle \psi_f | \psi_i \rangle}$, arises. It is linked to the weak value in very specific cases, in between others, when $k$ is small and the exponential can be expanded in Taylor. Nonetheless, modular values are associated to an interaction of any strength, a weak coupling between the system and the ancilla is not needed.

In this work, we present a new approach to quantum algorithms using modular values. The procedure exploits the degrees of freedom and complex properties of modular values. It could reduce the involved number of gates and hence the error in the execution of the algorithm. Nonetheless, the method always requires one extra qubit to readout the result of the quantum modular value.

We applied this procedure to the Jozsa and Deutsch-Jozsa algorithms both theoretically and experimentally, in the IBM Quantum Computer.

# Plasmons in nanostructured and corrugated 2D materials

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Graphene has been focusing attention as a support for plasmon for over a decade. In order to obtain plasmon resonance in the visible range, graphene nanoparticles or nanoribbons have been largely investigated. However, the intervalley scattering due to the edges is a critical source of damping of plasmon resonances in nanostructured graphene. In edge-free highly corrugated graphene, nanoscale confinement of charge carriers without intervalley scattering is possible. We theoretically evidence the appearance of plasmon excitations in the IR/Visible related to such corrugation (figure 1). These results are supported by SERS measurements on corrugated graphene suggesting the existence of plasmon in corrugated graphene[1].

We also investigate 1D plasmon in other 2D materials. Due to the reduced dimensionality of such plasmons, one can expect even larger confinements of light. Some 1D plasmons are associated with atomic reconstructions at the edge of nanoribbon or grain boundaries that can be at the origin of a 1D metallic channel in 2D materials. In this work, we theoretically examine the metallic behavior of experimentally observed mirror twin boundaries in transition metal dichalcogenide (TMDs) and show that 1D plasmon can be sustained in such nanostructures.

The plasmonic excitations are analyzed using an eigenmode decomposition of the microscopic dielectric function obtained by DFT simulations available in the GPAW code.

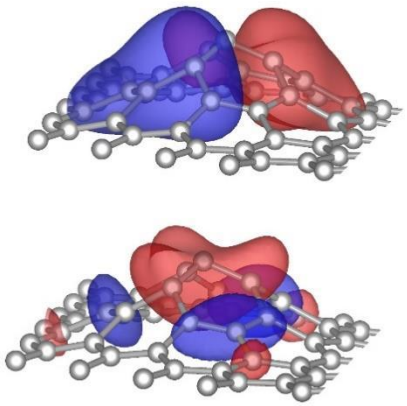

**Figure 1**: Charge distributions of optical excitations corresponding to loss peak near 1.9 eV and 2.9 eV from our calculated EELS spectrum of a model graphene nanocorrugation.

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