For Women in Science

FONDATION L'ORÉAL

2020

L'ORÉAL-UNESCO
For Women in Science

International Rising Talents

L'ORÉAL UNESCO

INTERNATIONAL RISING TALENTS

RESEARCH PROJECTS

SUMMARY

THE FUTURE OF SCIENCE

THE FUTURE OF SCIENCE

Since 2000, the L'Oréal-UNESCO *For Women in Science* programme has highlighted the achievements of younger women who are in the early stages of their scientific careers.

Each year, the International Rising Talents programme selects the 15 most promising women scientists among the almost 260 doctoral and post-doctoral researchers of the L'Oréal-UNESCO *For Women in Science* programme. These young women are the very future of science and recognising their excellence will help ensure that they reach their full potential.

MEDICINE

Group 1

MEDICINE

Dr Laura-Joy Boulos

NEUROSCIENCE

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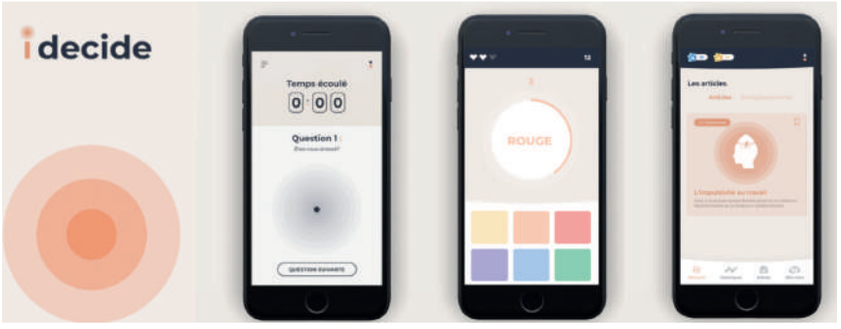
THE BRAIN IN A POST-WAR CONTEXT: FROM NEUROSCIENCE TO ARTIFICIAL INTELLIGENCE

INTRODUCTION

The brain is one of the greatest machines. It perceives, it memorizes, it anticipates, and **it decides.** However, some memories are not easily erased, and **some decisions are too risky thus hard to make**, often leading to treatment-resistant mental illnesses. Our research focuses on **brain mechanisms under uncertainty**. We take profit of the unfortunate post-war context in the Levant to study the impact of violent memories and prolonged uncertainty on decision-making and its neurobiological correlates. To do so, we collect data through a mobile application that we have developed in collaboration with the digital industry. We further administer scientifically validated neurocognitive tests focusing on executive functions and decision-making to calibrate the data obtained through our app with the data obtained through the tests. Our aim is to detect behavioral patterns and transform them into **artificial intelligence-based solutions** that facilitate decision-making in situations where the stress is high and the outcome uncertain.

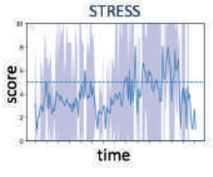
MATERIALS AND METHODS

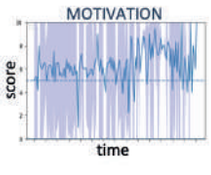
We collect data through a mobile application called ï-decide that we have developed in collaboration with the digital industry. The app provides us with information regarding daily decisions, like whether they are affected by stress, motivation or any other contingencies. We further calibrate the data obtained through our app with data obtained through scientifically validated tests as well as by exploring brain imaging and physiological biomarkers.

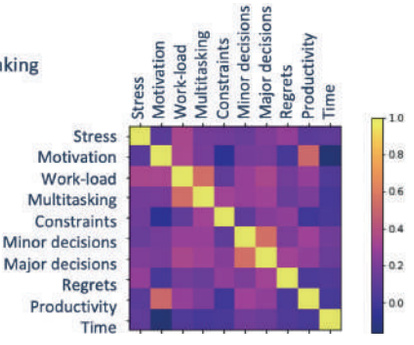


RESULTS

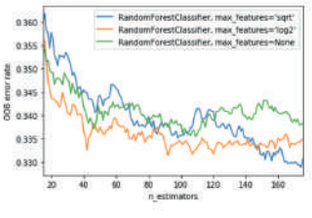
MONITORING & CORRELATION
of different factors that can affect decision-making







PREDICTION
of behavior and cognition (Random Forsest)



CONCLUSION

Our goal is to gather big longitudinal data (as opposed to the punctual data of classical neuropsychological testing) in order to detect behavioral patterns, translate them into algorithms and propose artificial intelligence-based solutions that facilitate decision-making in situations where the stress is high and the outcome uncertain, in healthy individuals as well as in populations at risk. We thus propose a new approach of research **at the intersection between humanities & technology**, academic neuroscience & industrial AI with the ultimate ambition to accelerate the creation of novel solutions to real-life problems.

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MOLECULAR BIOLOGY, MEDICAL MICROBIOLOGY

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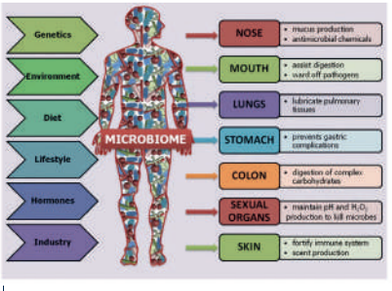
THE MICROBIOME, TRANSCRIPTOME, AND INFERRED FUNCTIONAL METAGENOME IN TUBERCULOSIS

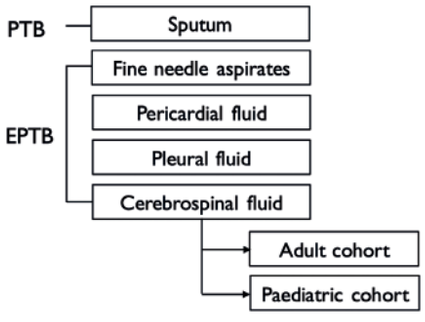
INTRODUCTION

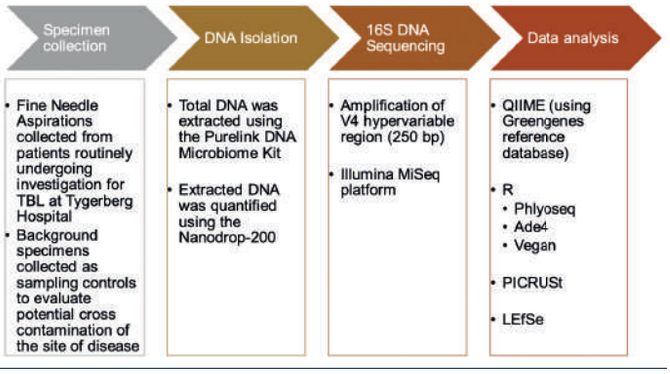
Tuberculosis (TB) continues to be the single biggest infectious cause of death. Extrapulmonary tuberculosis (EPTB), common in immunocompromised individuals, represented 15% of all diagnosed cases of TB in 2018. EPTB is associated with high mortality, especially in HIV-positive populations. In Sub Saharan Africa, there is an association between the prevalence of TB and HIV infection, hence approximately a third of the HIV-positive population has TB co-infection.



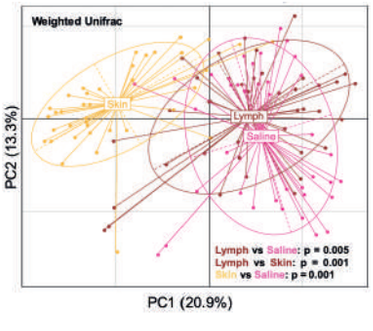
The microbiome has been recognized to play an important role in both health and in disease. However, there is little known about the microbiome in PTB, and the EPTB microbiome is currently undefined.
We thus aim to examine the microbial composition as well as its predicted functional capacity associated with pulmonary and extrapulmonary TB.
This may improve our understanding of host-pathogen interactions and show new diagnostic or therapeutic targets.

MATERIALS AND METHODS

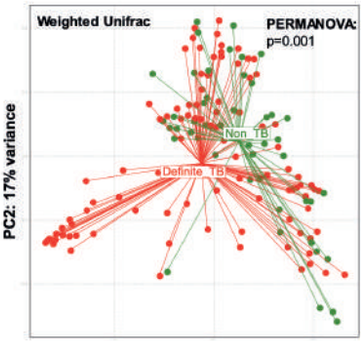




RESULTS



Lymph microbiome is distinctly different from skin and environmental controls.
Beta diversity analysis revealed differences in the microbial community composition of Definite TB cases compared to Non TB controls.
Mycobacteria made up ~30% of taxa in cases vs. 2% of taxa in controls. Conversely, Nelumbo was less common in cases (0.001%) than controls (0.2%).



CONCLUSION

The presence/absence on M.tb drives a major difference resulting in differences in microbial communities between active extrapulmonary TB cases and controls. These findings show for the first time that patients with EPTB have a distinct microbiome (including many non-Mycobacteria taxa) and a shifted functionality compared to controls. Other non-Mycobacteria genera e.g. Nelumbo have been identified as discriminating for active TB. Overall, these observations suggest that the context of the microbial community as a whole may be important in order to understand TB pathogenesis.

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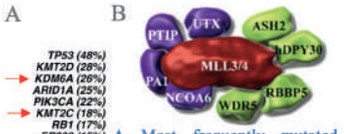
UNCOVERING THE GENOMIC TARGETS OF THE EPIGENETIC FACTORS FREQUENTLY MUTATED IN BLADDER CANCER

INTRODUCTION

80% of all bladder cancer patients is mutant for at least one gene involved in chromatin regulation. This situation makes the bladder cancer as a disease of chromatin, and a perfect model for studying cancer epigenetics. Almost all the chromatin modifier genes mutated in bladder cancer have roles in active chromatin organization. These chromatin genes belong to Trithorax group and oppose the repression mediated by Polycomb group of proteins (Schuettengruber et al.,2017).



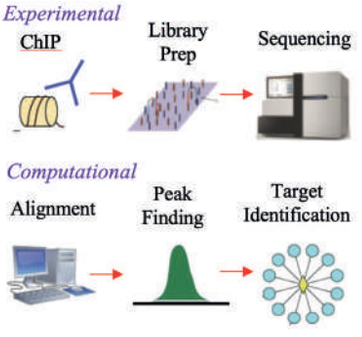
A Most frequently mutated genes in bladder cancer (adapted from Robertson *et al.* 2017). KDM6A and KMT2C are shown with red arrow. **B** Schematic showing the MLL3/4 complex (adapted from Smith *et al.* 2011). MLL3 stands for KMT2C and UTX stands for KDM6A, respectively.

At this point, high rate of mutations identified for KDM6A, a histone H3 lysine 27 demethylase, and KMT2C, functioning in the same complex together with KDM6A and involved in methylation of lysine 4 on histone H3, especially stands out (Robertson et al., 2017). In this project, my aim is to identify the targets of KDM6A and KMT2C in the genome in both normal bladder cells and bladder cancer cells, and uncover the regulatory mechanisms related with the functions of these two chromatin proteins.

MATERIALS AND METHODS

First, the normal bladder epithelium cells will be obtained and grown in proper media containing corneal epithelium growth factors. The cells will be collected in enough numbers for chromatin immunoprecipitation experiments. Using suitable antibodies for KDM6A and KMT2C, ChIP experiments will be performed. To identify the binding profiles of the immunoprecipitated DNA, sequencing libraries will be prepared and the resulting libraries will be sequenced on Illumina Hiseq 2500 platform.

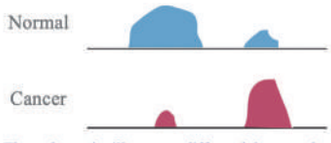
The resulting data will be analyzed using the Bioconductor package 'QuasR' (Gaidatzis et al., 2015). ChIP-seq peaks will be identified using the algorithm called 'MACS' (Zhang et al., 2008). Identified peaks will be intersected with the promoter regions of the genes to identify the target genes occupied by KDM6A and KMT2C. The molecular mechanisms the target genes are involved will be determined using Gene ontology and pathway analysis.



The schematic showing the workflow of the project

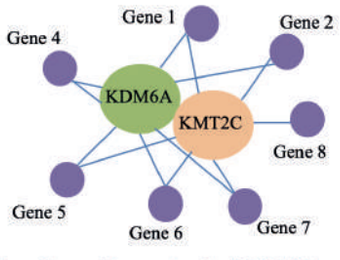
EXPECTED RESULTS

Using the scientific approach described above, I will be able to infer genomic binding sites of KDM6A and KMT2C both in normal and tumorigenic bladder cancer cells. Integrative analysis of this data with the other genomics data we generate in the lab will enable the identification of the disrupted chromatin states in the case of mutation in KDM6A or KMT2C in bladder cancer.



The schematic illustrates differential genomic occupancy profiles of KDM6A/KMT2C in normal bladder cells and bladder cancer cell lines

Identification of the genes whose promoter regions occupied by KDM6A and KMT2C will show the pathways which are dependent on KDM6A and KMT2C regulation.



Example regulatory network of KDM6A and KMT2C

CONCLUSION

The results we are going to obtain will clearly give insights about the chromatin-level misregulation arising in bladder cancer and will guide the design of functional experiments. The epigenetic signatures we will identify might be potentially used to both stratify bladder cancer patients and to develop specific treatment strategies.

Stratification and treatment of patients according to epigenetic profiles

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Dr Rui Bai

BIOLOGICAL SCIENCES

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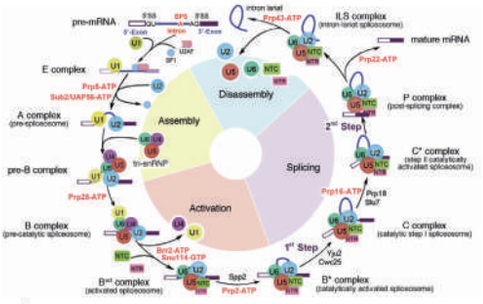
STRUCTURAL INSIGHTS INTO THE SPLICEOSOME AND MECHANISTIC INVESTIGATIONS OF RNA SPLICING

INTRODUCTION

Splicing of messenger RNA, involving non-coding intron removal and exon ligation, is an important step during gene expression in eukaryotes. RNA splicing is accomplished by spliceosome through two S_N2-type transesterification steps, branching and exon ligation. Spliceosome is a multi-megadalton machinery composed of more than 300 components. Each cycle of RNA splicing is precisely regulated by snRNAs and different splicing factors, and executed by the spliceosome

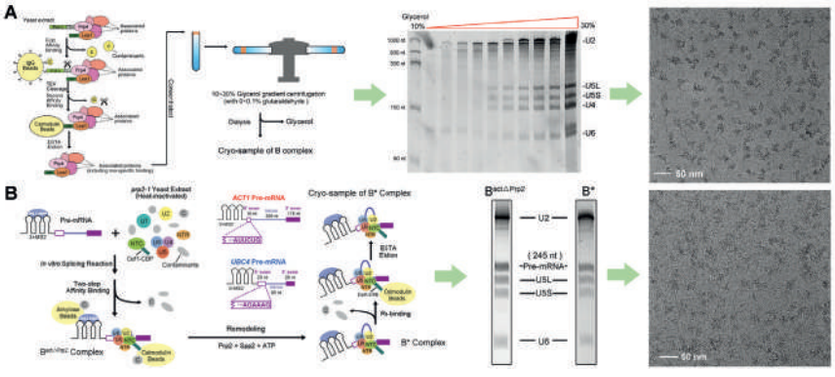


in a highly dynamic but ordered fashion, which can be divided into four phases: assembly, activation catalysis and disassembly.

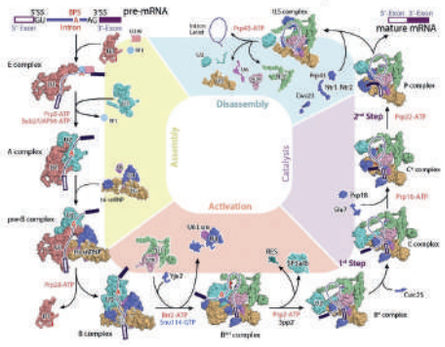
Based on its composition, spliceosome has been identified to have at least eight fully assembled functional states: pre-B, B, Bact, B*, C, C*, P and ILS complexes. Structural elucidation of different functional spliceosomes will definitely help us to understand the molecular basis of RNA splicing, establishing the foundation to pathogenesis of RNA splicing related diseases and providing insights into drug development.

MATERIALS AND METHODS

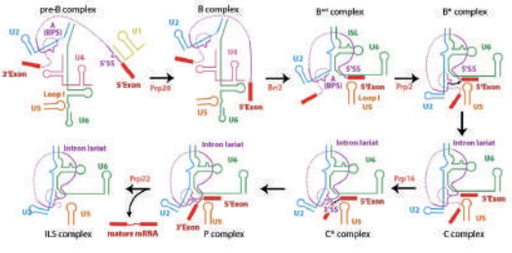
We focused on different functional states of spliceosome from Saccharomyces cerevisiae, used endogenous mutant and in vitro assembly to stall specific states of the spliceosome, and purified the homogeneous protein samples by tandem affinity purification. Using Cef1 as the affinity tag, we isolated endogenous yeast spliceosomes directly from cell nuclei. The pre-B, B, tri-snRNP, B^{act}, C, C*, P, and ILS complexes are all present with difference abundances. The most transient state B* complex was reconstituted by in vitro assembly approach.



RESULTS



We finally reconstructed near-atomic resolution structures of eight different functional spliceosomes by single-particle cryo-electron microscopy, namely pre-B complex at 3.3 ~ 4.6 Å, B complex at 3.9 Å, B^{act} complex at 3.5 Å, B* complex at 2.7 ~ 3.8 Å, C complex at 3.4 Å, C* complex at 4.0 Å, P complex at 3.6 Å and ILS complex at 3.5 Å. The eight structures of different states of the spliceosome gave rise to a complete structural view of pre-mRNA splicing for the first time in the world, which shed lights on molecular basis for the spliceosome assembly and activation, branching and exon ligation reactions, and spliceosome disassembly.



CONCLUSION

These structures revealed the recognition of splice sites, the structural organization of the spliceosome, the rearrangement of RNA catalytic center, the catalytic mechanism of the active site and Mg^{2+}, and the important roles of splicing factors. The spliceosome is proven to be a protein-orchestrated metalloribozyme. Conserved snRNA constitute the splicing active site with two catalytic metal, which are delivered into the splicing active site for branching and exon ligation. The protein components of the spliceosome stabilize the conformation of the snRNAs, drive spliceosome remodeling, orchestrate the movement of the RNA elements, and facilitate the splicing reaction.

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BIOMATERIALS

Group 2

BIOMATERIALS

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BIOMEDICINE

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Mauritius

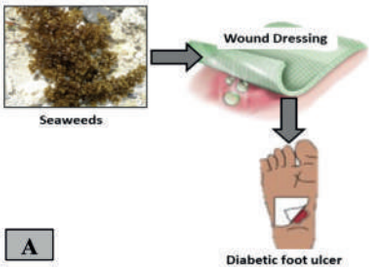
EXPLOITING THE POTENTIAL OF FUCOIDAN FROM LOCAL SEAWEEDS FOR THE TREATMENT OF DIABETIC FOOT ULCERS

INTRODUCTION

In Mauritius, diabetes is one of the most common chronic medical problems with an alarming 20.5% of the adult population diagnosed with type 2 diabetes. Diabetic foot ulcers (DFUs) add significantly to the economic burden of a country mainly due to ulcer management, and slow healing. As a result, there is an urgent need to reduce the healing time of DFUs.

The challenge in repairing wounds related to DFUs are mainly due to wound infection, lack of extracellular matrix (ECM), and poor angiogenesis.

My research aims at developing high value-added products which could be used to treat diabetic wounds using cheap locally available resources such as seaweeds (A).

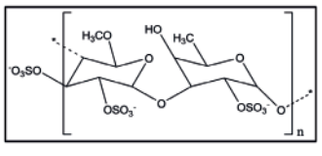


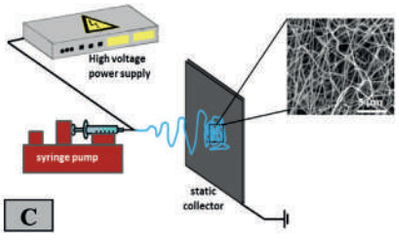
A

MATERIALS AND METHODS

The polysaccharide Fucoidan was blended with a biodegradable polyester in varying weight ratios and fabricated into nano-wound dressings using the electrospinning process (C).

B





C

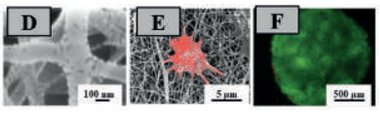
The biocompatibility of the resulting nanofibrous mats was then tested in vitro using a range of cell lines including fibroblasts, keratinocytes, endothelial cells, macrophages and induced pluripotent stem cells.

The in vivo wound regeneration potential of the Fucoidan-containing nanofibrous mats were investigated using Wistar rats over a period of up to 4 weeks.

RESULTS

The detailed analysis of the blend nanofiber properties revealed surface enrichment of FUC on the blend nanofibers (D). In addition, the latter were observed to be stable in phosphate buffer solution (PBS) for upto 5 weeks.

Addition of FUC enhanced fibroblast and pre-osteoblasts cell viability significantly.



PDX/FUC mats promoted early fibroblast cell attachment and proliferation. The presence of FUC within the blend fibers favored the differentiation of pre-osteoblasts into mature osteoblasts with the formation of Ca deposits (E).

Interestingly, induced pluripotent stem cells maintained high viability on the blend fibers (F). Compared to pure PDX, PDX/FUC led to reduced in vivo inflammatory response.

In vivo diabetic wound healing studies is scheduled in April 2020. FUC is expected to accelerate the healing process by reducing inflammation and promoting the proliferation of fibroblasts and keratinocytes.

CONCLUSION

FUC blended with PDX in varying weight ratios and fabricated into nanofibers using the electrospinning technique. The resulting blend fibers were found to possess excellent surface and biological properties for skin tissue regeneration. In particular, the scaffolds enhanced fibroblasts proliferation, pre-osteoblasts differentiation and reduced in vivo inflammatory responses.

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HEALTH SCIENCES

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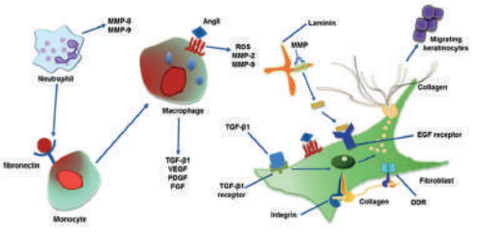
NOVEL NANO-DRESSING MATERIAL FOR WOUND HEALING: A GOLDEN HOPE FOR DIABETIC PATIENTS

INTRODUCTION

Poor wound healing is one of the most severe complications of uncontrolled diabetes. It is estimated that every 30 seconds, a lower limb or part of it, is lost in the world as a result of diabetes (IDF Atlas, 8th edition 2017). Hyperglycemia is usually associated with bacterial infection and inflammation, which result in impairment in cell migration and wound healing.

Integrins receptors are activated by binding to extracellular matrix (ECM) proteins and mediate wound healing. In diabetes, ECM proteins are glycated which results in poor wound healing.

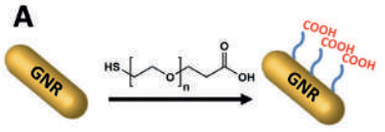
In this project, an ECM protein will be coupled to gold nanorods and loaded into polymeric fibers.

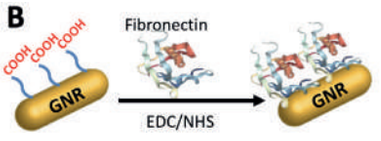


Fibronectin-gold nanofibers will exert anti-inflammation and antibacterial activities and enhance the diabetic wound healing.

MATERIALS AND METHODS

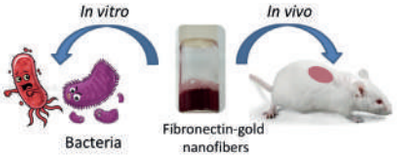
An ECM protein (Fibronectin) will be immobilized onto the surface of carboxylated gold nanorods using carbodiimide and N-hydroxysuccinimide chemistry, then loaded into polymeric nanofibers.





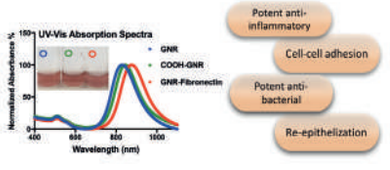
The cytotoxicity of the fibronectin-gold nanofibers will be examined against human dermal fibroblasts. The healing activity of the nanofibers will be investigated in diabetic rats by evaluating the size of the wound over 21 days after dorsal skin excision.

The inflammatory activity of the fibronectin-gold nanofibers will be evaluated by estimating the gene expression levels and production of inflammatory cytokines in the wound tissues. The antibacterial activity of the nanofibers will be investigated in vitro.



EXPECTED RESULTS

Fibronectin conjugated into the nanorods is more stable upon delivery into the wound site compared to the free protein and will compensate for the deficient or degraded fibronectin in the ECM due to hyperglycemia. Fibronectin delivered by gold nanorods will bind to other ECM proteins and to integrin receptors in order to activate cell adhesion, migration and keratinocytes re-epithelization.



Fibronectin-gold nanofibers is supposed to provide the diabetic wound with adequate hydration, adhesion and mechanical strength to support cells migration and healing.

Fibronectin-conjugated gold nanofibers are supposed to enhance the collagen deposition at the site of wound. The conjugated gold nanorods are supposed to demonstrate potent anti-inflammatory activity by modulating the gene expression levels of several pro-inflammatory and anti-inflammatory cytokines, in addition to prevent the bacterial infection of the wound.

CONCLUSION

Gold nanorods have several biomedical applications such as imaging, diagnosis and therapy due to their unique optical and chemical properties. Conjugating the gold nanorods with one of the ECM proteins will drastically enhance the stability, delivery and healing activity of the protein at the wounded tissue. Fibronectin-gold nanofibers would provide a hope for diabetic patients to save their limbs from amputation and to improve their quality of life.

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For Women in Science

FONDATION L'ORÉAL

Dr Mikyung Shin

BIOMATERIALS

SUNG KYUN KWAN UNIVERSITY(SKKU)

Nature-inspired Biomaterials Engineering Laboratory
NBEL
Prof. Mikyung Shin
SINCE 2019

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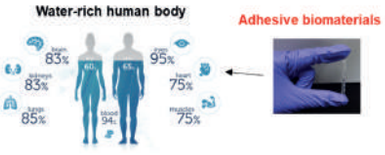
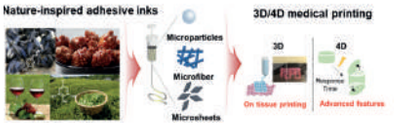
Suwon, South Korea

NATURE-INSPIRED ADHESIVE MICRO-FORMULATIONS FOR 3D/4D MEDICAL PRINTING

INTRODUCTION

In clinical settings, all body fluids, such as blood, gastric juice, and cerebrospinal fluids, are managed with precautions. During surgery, excessive bleeding often causes increase of operation time and inhibition in correct vision of surgical window. Thus, the resistance of biomaterials against all body fluids is considered as an essential feature for enhancement of their desirable properties (e.g., therapeutic efficacy). For this reason, tissue adhesive biomaterials have been attracted for a variety of biomedical applications, hemostatic agents, wound closure, and other applications towards medical devices, drug delivery platform and artificial organs.

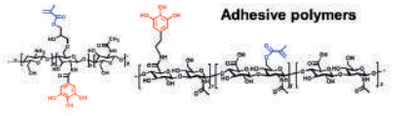


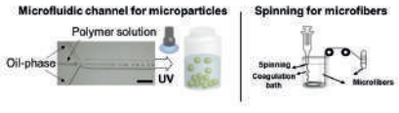


Since 2007, marine mussels' byssal thread or plant astringency has been a target system to implement tissue adhesive materials due to their wet-resistant, robust adhesion. Herein, nature-inspired adhesive inks are newly designed for 3D/4D printing.

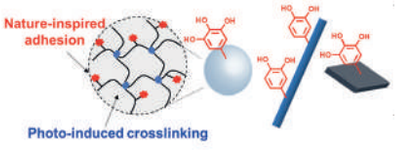
MATERIALS AND METHODS

To design wet-resistant, adhesive inks, we would develop a new type of adhesive polymers with both photo-crosslinkable groups and polyphenols.



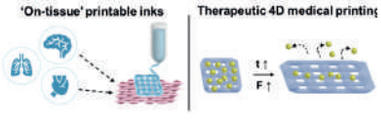


The photo-crosslinkable crosslinking (e.g., thiol-en reaction, methacrylate) can generate stable formulations in microscale for easy extrusion without high pressure in printing. In addition, polyphenols moieties (e.g., catechol, gallol depending on the number of hydroxyl groups on their chemical structure) can provide excellent adhesiveness of those micro-formulations in dynamic environments. The use of micro-formulation is effective for shape fidelity of final objects.



RESULTS

The adhesive materials would have benefits of direct 'on-tissue' printability because of their robust adhesion even onto biological tissues with high water contents and low frictional forces. To date, none of research has reported tissue adhesive micro-formulations (e.g., not bulk materials) as well as their printability as a bioink. In addition, '4D medical printing' has not been implemented due to functional limitation of bioink materials.



This is an emerging concept in that i) adhesiveness of 'micro-building blocks' to show injectability in bulk scale can have interfacial stability in-between the blocks, allowing on-tissue 3D printing and ii) additional features from polyphenols, such as anti-oxidant and anti-bacterial properties, provide an advanced bioink for 4D medical printing which manufactures 'therapeutic objects' with responsiveness against external stimuli.

CONCLUSION

In conclusion, we have developed nature-inspired adhesive polymers for drug delivery, hemostatic agents and coating of medical devices. For further biomedical applications, we would implement adhesive micro-formulations for 3D/4D printing. With these achievements, a nature-inspired bioink system would be promising for next generation of personalized tissue repair and fabrication.

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MATHEMATICS & APPLIED PHYSICS

Group 3

MATHEMATICS & APPLIED PHYSICS

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MATHEMATICS

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SYMMETRY METHODS IN THE STUDY OF NONLINEAR MODELS OF PHYSICAL AND BIOLOGICAL PROCESSES

INTRODUCTION

In a wide range of application areas, from the fate of the world's climate to the state of local rush hour traffic, mathematical models provide us with practical perspectives on complex phenomena. Especially important are partial differential equations (PDEs) which model various processes in fields as diverse as classical and quantum mechanics, electromagnetism, general relativity, wildlife biology, genetics, medicine and investment finance.

Lie symmetries (named after Sophus Lie) present a powerful and the only algorithmic technique for construction of exact solutions of nonlinear PDE models. Moreover, high symmetry properties distinguish the equations describing natural phenomena from other PDEs. The problem of singling out from a class of PDEs those admitting Lie symmetry algebra of the maximally possible dimension is called group classification problem.

The main goal of the project is to enhance existing approaches of solving group classification problems and to apply these techniques to important classes of nonlinear PDEs arising as models in mathematical physics and mathematical biology.

METHODS

There are two classical approaches of solving Lie symmetry classification problems. The algebraic one is based on subgroup analysis of the equivalence group of a given class of PDEs. The second one involves integration of determining equations which constitute an overdetermined systems of first-order linear PDEs. Both of these methods have their limitations and cannot be applied to all classes that are important for applications.

To solve more complicated group classification problems new techniques are needed. Some of such novel methods were developed in [1,2]. These are the method of mapping between classes and the method of contractions. Both of them will be used in the course of the project.
Moreover, we intend to simplify the algebraic approach by means of using Élie Cartan's method of moving frames in the Fels–Olver version [3,4].

For finding exact solutions we will apply developed in [1] techniques which include combination of the reduction and the equivalence methods as well as the method of mappings between classes.


Sophus Lie


Emmy Noether


Élie Cartan

EXPECTED RESULTS

New algebraic method of group classification which involves moving frames concept will be developed. The approach suggested is expected to be simpler then the method which is based on direct integration of overdetermined systems of first-order linear PDEs. This will give the opportunity to solve more complicated group classification problems for classes of PDEs arising as models in real-world applications.

Lie symmetry classifications will be carried out for classes of variable coefficient nonlinear PDEs modelling phenomena in physics and biology, e.g., generalized Kawahara, Fisher and reaction-diffusion equations.

In particular, the generalized Kawahara equations model long waves in a sea under ice cover [5] and Fisher equations describe the propagation of a mutant gene in a population.
The exact solutions of the derived nonlinear PDEs with high-symmetry properties will be constructed. Such solutions will help to get information about the described real phenomena, and to check the validity of models themselves against experimental data.

CONCLUSION

The main output of the project:

1.Development and optimization of group classification methods for classes of nonlinear PDEs.

2. Application of advanced symmetry classification procedures to analysis of nonlinear mathematical models. Finding models with high symmetry properties and their conservation laws.

3. Construction of exact solutions describing physical and biological phenomena.

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[5] O. Kuriksha, S. Pošta and O. Vaneeva, J. Phys. A: Math. Theor. 47 (2014) 045201.

Dr Paula Giraldo-Gallo

PHYSICS

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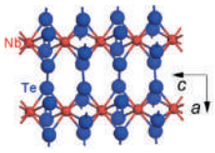
OPTIMIZATION OF ELECTRONIC PROPERTIES OF QUASI-1D TRANSITION METAL CHALCOGENIDE MATERIALS

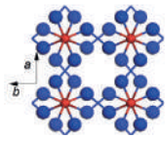
INTRODUCTION

Material scientists aim at finding ways of leading materials toward behaving in a way that optimizes specific applications. Research Question: Can the novel electronic states of quasi-1D transition metal chalcogenides (q-1D TMC's), such as superconductivity and topological states, be tuned, through chemical composition variation, to exist much closer to ambient conditions?
How close?

The q-1D TMC's form one dimensional zig-zag chains of transition metal atoms and chalcogen atoms that couple weakly with other chains through van der-Waals forces; e.g. $NbSe_3$, $HfTe_3$, $NbTe_4$, $TaTe_4$, $HfTe_5$, among others.



Among this family we find semiconductors, semimetals, metals or topological insulators, and they can show charge ordering and superconductivity. Their electronic properties can be easily tuned, allowing the variation of critical temperatures of phase transitions to novel ground states.



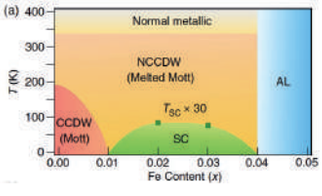
MATERIALS AND METHODS

1. Single crystal synthesis of solid solutions of the compounds to study, through the methods of chemical vapor transport, molten flux crystal growth and solid state reaction.

2. Determination of structural, thermodynamic and electronic properties through:

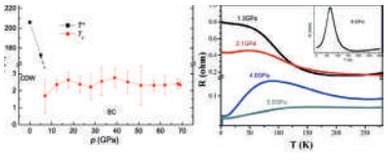
- Transport measurements as a function of temperature (1.5 K to 300 K) and magnetic field (up to 14 T; and up to 45T-DC or 100T-pulsed by submitting proposals to high magnetic field facilities).
- X-ray diffraction measurements.
- Magnetic susceptibility.
- Specific heat and resonant ultrasound spectroscopy (RUS).
- Microscopy characterization (AFM, SEM and FIB);
- Collaborative measurements with other groups: STM, ARPES, TEM, etc.

3. Summarize properties of compounds in **electronic phase diagrams**.



EXPECTED RESULTS

Evidence suggests that the families of superconductors with the highest critical temperatures might exhibit quantum critical points (QCP) under the superconducting dome, associated with the suppression of a line of phase transitions to T=0. How fluctuations associated with such QCP optimizes or even, give rise to the superconductivity (SC) itself, is one of the most important open questions in materials research We plan, on one hand, to suppress lines of phase transitions to T=0 by chemical doping to bring



SC to atmospheric pressure in systems where SC has been observed at high pressures. How does this correlate with possible QCP? We will start with the q-1D TMC's systems of $NbTe_4$, $TaTe_4$ and $HfTe_3$.

On the other hand, we will also use chemical doping to bring as close as possible to room temperature electronic properties of materials associated with topological states. We will start with systems in which transitions to these topological states have been tuned by pressure. For example, $HfTe_5$ and $ZrTe_5$.

CONCLUSION

q-1D TMD's are ideal systems to perform optimization studies, due to their large electronic susceptibility to changes in different physical parameters (strain, pressure, chemical doping, etc.). This projects aims at bringing promising electronic properties of these compounds such as superconductivity, and topological states as close as possible to ambient conditions. This will be done through a combination of chemical doping, single crystal synthesis, characterization of physical parameter, and construction of electronic phase diagrams.

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Phys. Rev. Lett. **109** (2012) 176403.
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Sci. Rep. **7** (2017) 44367.

Dr Vida Engmann

MATERIAL ENGINEERING

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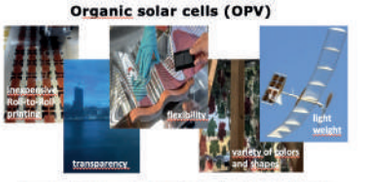
ADDITIVE-ASSISTED STABILIZATION OF NON-FULLERENE ACCEPTOR BASED ORGANIC SOLAR CELLS

INTRODUCTION

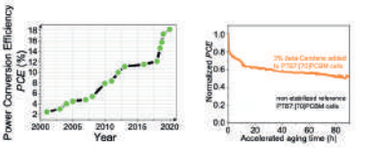
Main problem of tomorrow:

- reduce CO2 emissions
- but ensure electricity to maintain a good quality of life for the increasing world population

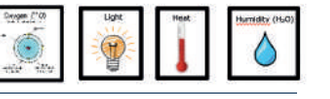
- Solar energy - abundant on Earth and sufficient to power the whole planet



Energy Source / Technology	Energy Payback Time [years]	CO2 emission [kg/kWh]
Wind	0.39	0.027
Mono and poly Si solar cells	1.12	0.032 - 0.36
Amorphous Si cells	1.13 *	0.011 - 0.226
CdTe solar cells	0.44 *	0.025
Organic solar cells	0.08 *	0.01 - 0.06
Hydropower	0.5	0.013 - 0.04
Geothermal	0.54	0.041
Biomass	5 - 10	0.045
Natural gas	–	0.751



- Rapid rise in OPV record efficiencies due to invention of non-fullerene acceptors -> 18% approaching Si PV
- Main issue: photooxidative stability



MATERIALS AND METHODS

1. Preparation of the organic solar cells, **ISOS accelerated lifetime testing**, as well as **UV-visible** and **Fourier Transform Infrared (FTIR) spectroscopy** analysis of structural changes will be carried out at the University of Southern Denmark.

2. Quantification of radical defects in the cells will be investigated in collaboration with Russian Academy of Sciences, using **Electron Spin Resonance (ESR) spectroscopy.**

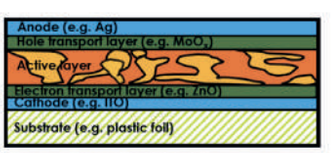
3. The presence of highly reactive singlet oxygen, which is essential for the photo-oxidation of organic materials, will be investigated by **Singlet Oxygen Phosphorescence** in collaboration with Aarhus University.

4. Nanoscopic variations in morphology and related electronic properties during degradation will be investigated using **Low-Electron Energy Microscopy (LEEM)** in collaboration with Lawrence Berkeley National Laboratory, a leader in this technique.

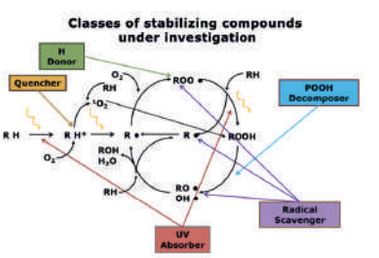
5. **Outdoor testing** of stabilized solar cells will be carried out in collaboration with Ben Gurion University of the Negev, to measure cell life under changing outdoor environmental stresses (daily and seasonal variations in lighting, temperature and humidity).

RESULTS

My newly developed method, **additive-assisted stabilization,** will be employed to extend lifetimes of **non-fullerene acceptor (NFA)** based solar cells, by incorporating extra stabilizing components into the active layer.



Organic Solar Cell (OPV)



- Photooxidative mechanisms of novel highly efficient NFA-based OPV systems will be identified
- Stabilizing compounds, that quench singlet oxygen and interrupt radical chain oxidation, will be identified for the novel NFA systems
- As a result, highly efficient NFA cells with drastically improved lifetimes and accumulated power generation factors will be developed

CONCLUSION

NFA materials have drastically increased the efficiency of OPV. However, due to the oxidation of organic materials, these efficiencies decay over time. The NFA cells stabilization method that will be developed in this project, will, combined with their unique properties – sustainability, flexibility, and ease of integrability - give rise to a wide range of novel applications, thus radically increasing the share of electricity produced from solar energy everywhere on the planet.

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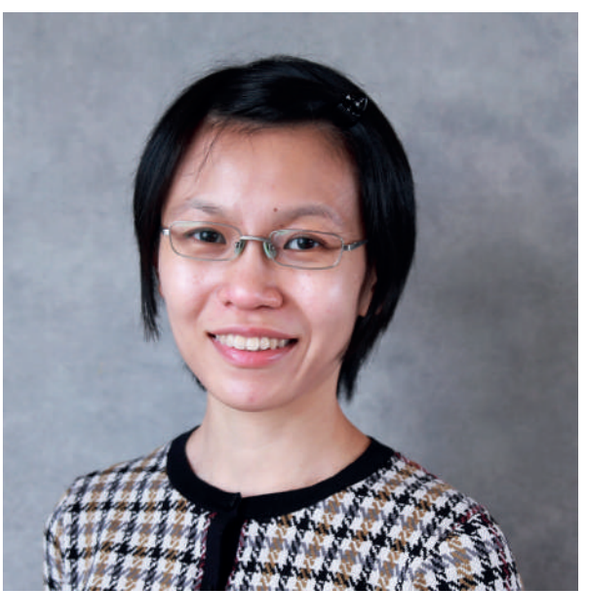
For Women in Science

FONDATION L'OREAL

Dr Huanqian Loh

PHYSICS



National University of Singapore

Singapore

RECONFIGURABLE TWEEZER ARRAYS OF ULTRACOLD MOLECULES FOR QUANTUM SIMULATION OF ADVANCED MATERIALS

INTRODUCTION

Grand challenge:

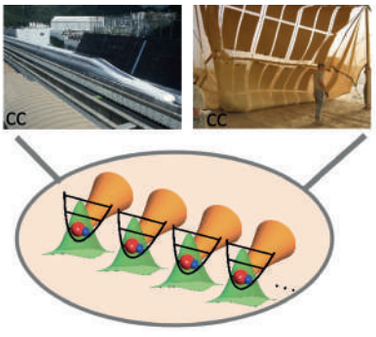
Advanced materials like flexible solar cells and superconductors are important for managing the world's rising energy needs. An improved understanding of these materials would revolutionize energy transport and storage, yet their microscopic behavior remains poorly understood. This is because advanced materials are often based on many interacting quantum particles, which cannot be easily simulated on classical computers.

Using quantum simulators:

Ultracold polar molecules have been proposed as ideal analog quantum simulators that can model strongly-correlated materials.

Project aim:

To achieve single-molecule, single-quantum-state control for quantum simulation.



MATERIALS AND METHODS

Single-atom control:

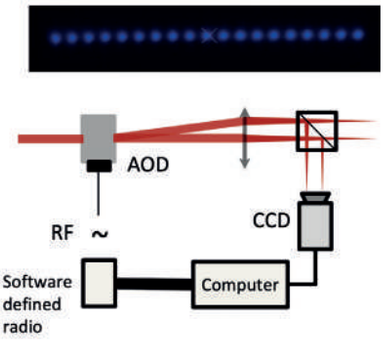
Trap laser-cooled Na and K atoms in reconfigurable tweezer arrays

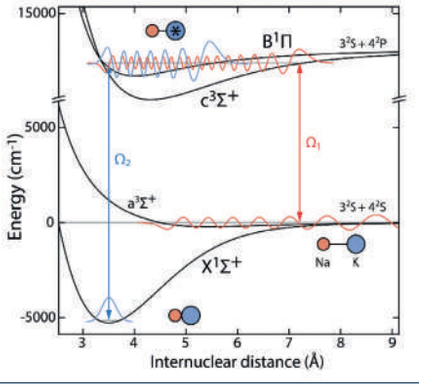
Merge tweezers to bring the atoms together in a controlled way

Single-molecule control:

Form Feshbach molecules (loosely bound molecules) from atoms in merged tweezers

Stimulated Raman adiabatic passage (STIRAP) to reach the ground molecular state



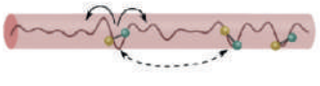


EXPECTED RESULTS

Key features of this work:

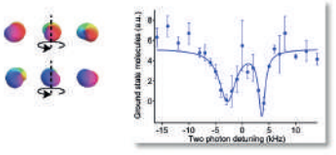
- Scalable generation of tweezer arrays
- Array size
- Dimensionality
- Doping fraction
- Site-to-site potential

} Arbitrarily programmed

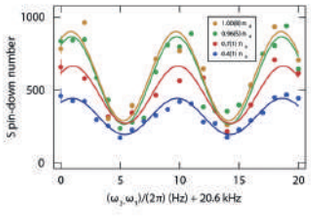


To induce interactions, we can apply:

- Static laboratory electric fields (induce up to 0.8 Debye)
- Microwaves (induce rotating dipole moments of up to 1.5 Debye.)



The NaK molecules are expected to exhibit long nuclear spin coherence times, as previously observed in the bulk.



CONCLUSION

Establishing single-molecule control would overcome an important hurdle to realizing molecules as analog quantum simulators.
The quantum simulators will in turn be used to study complex many-body phenomena such as the interplay between interactions and localization.
They will also be used to explore out-of-equilibrium dynamics, modelling energy transport in advanced materials.

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ENVIRONMENTAL SCIENCE

Group 4

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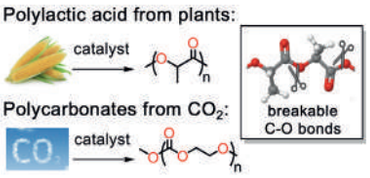
SUSTAINABLE ALTERNATIVES TO CONVENTIONAL PLASTICS

INTRODUCTION

Plastics are ubiquitous in modern day life and have transformed our way of living, with applications in healthcare, electronics, transport and construction. Yet of the 8300 million metric tonnes (Mt) of plastic produced since 1950, an estimated 5700 Mt has been sent to landfill or leaked into the natural environment. Furthermore, over 99% of plastics are currently made from fossil fuels. This is unsustainable.

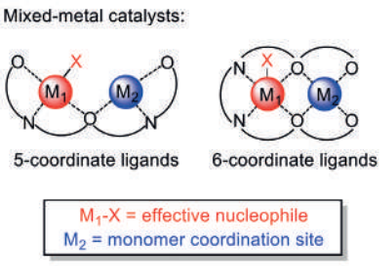
What would true sustainability look like? Ideally, plastics would be made from renewable feedstocks (e.g. plants) or industrial waste (e.g. carbon dioxide, CO_2). These resources would be efficiently converted into useful materials through inexpensive, fast and low energy processes, which typically requires the use of a suitable catalyst. The resultant materials should then be recyclable and/or degradable at their end-of-life.



This project aims to address these challenges by developing novel materials from renewable resources, underpinned by tailored catalyst design.

MATERIALS AND METHODS

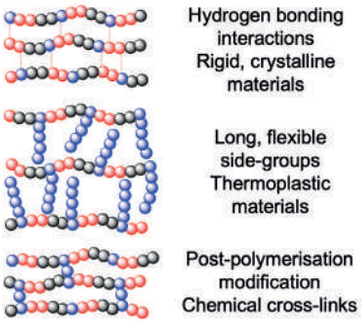
New mixed-metal catalysts designed to give improved performance for the preparation of plastics from plants and/or CO_2 are currently being prepared. This involves specialist air- and moisture-sensitive techniques (Schlenk chemistry and gloveboxes) and catalyst characterisation through a combination of NMR spectrometry, mass spectrometry, elemental analysis and X-ray diffraction.



The catalysts will subsequently be applied in polymerisations. Firstly, they will be investigated for the production of polylactic acid from plants and polycarbonates from CO_2/epoxides Secondly, the epoxide comonomer will be replaced with an alternative comonomer, to derive a novel class of polyurethanes from CO_2. The material properties will be investigated to identify suitable applications.

EXPECTED RESULTS

Mixed-metal cooperativity is an emerging field within polymerisation catalysis. Having two different metals in close proximity has advanced catalyst performance in terms of activity, selectivity and control over the polymer microstructure. The complexes developed in this project are expected to enhance performance as well as enable the synthesis of a new family of polyurethanes from CO_2. Through varying the comonomer, different functional groups will be incorporated into the polymer chain, enabling inter-chain interactions that will tailor the materials properties. For example, long side chains will reduce the packing efficiency, which introduces flexibility into the structure, whereas reactive functional groups will be cross-linked to produce rigid materials.



CONCLUSION

There is a pressing need to develop new sustainable materials that are both fit-for-purpose and designed for end-of-life. Converting biomass and/or CO_2 into oxygenated polymers is an exciting opportunity to valorise waste and create new degradable plastics. Designing bespoke mixed-metal polymerisation catalysts enables activities up to 50 times faster than the single-metal analogues.

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UNCONVENTIONAL FOOD PLANTS: THEORETICAL CHALLENGES FOR BIOCULTURAL CONSERVATION

INTRODUCTION

Unconventional food plants (UFPs) are edible plants unknown to most people in a certain region. Because most UFPs are wild, they may be available in situations where conventional crops are not (Samant and Dahar 1997), and their popularization usually benefits small farmers and extractors because they have access to such products and possess the traditional knowledge associated with them.

However, despite the increasing number of studies that nutritionally characterize UFPs, few studies address the barriers and opportunities in terms of popularizing them. Therefore, this research seeks to provide theoretical basis for popularizing UFPs and promoting biocultural conservation. Our main research questions (RQs) are:

1) Which UFPs are known and are used by rural communities in Piaçabuçu?

2) Which UFPs have the greatest diffusion potential? 3) Do socioeconomic factors influence the sensory evaluation and economic valuation of UFPs? 4) What is the influence of the label "UFP" on sensory evaluation and economic valuation? 5) Do socioeconomic factors and food neophobia influence the perception of barriers and advantages in UFP consumption by potential consumers?

MATERIALS AND METHODS

To answer RQ 1, we will record UFPs known by residents of rural communities in the county of Piaçabuçu (NE Brazil), as well as the local perception on the most promising species. The chosen species will face a series of ecological, propagation, sensory and economic valuation studies (RQ2). Species with good results will be indicated for popularization (Fig. 1). To answer RQs 3 and 4, different food types will be prepared, which will be subjected to tasting by volunteers They will perform an acceptability test (Lawless e Heymann 2010). A contingent valuation technique known as willingness-to-pay will also be performed. For RQ3 we will use linear models to search for socioeconomic predictors of UFP sensory and economic acceptance. We will also analyze, with students t-tests, whether people, knowing the food they are tasting is UFP, respond differently in terms of acceptability and willingness-to-pay than those that taste the food without knowing it (RQ4). To answer RQ 5 potential consumers will be interviewed to identify how willing they would be to include different plants in their diet, as well as the perceived risks, barriers, and opportunities arising from the consumption of these species. We will also employ the food neophobia scale to access the respondents degree of food neophobia. Socioeconomic (and neophobia) influence on the attribution of risks, barriers, and opportunities will also be investigated with linear models.

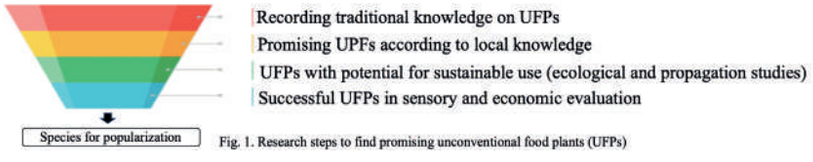

Fig. 1. Research steps to find promising unconventional food plants (UFPs)

EXPECTED RESULTS

Because of food neophobia, we hope that the label "UFP" negatively influences food acceptance. (Fig. 2) We also expect that socioeconomic factors and food neophobia will predict the willingness-to-consume UFPs.

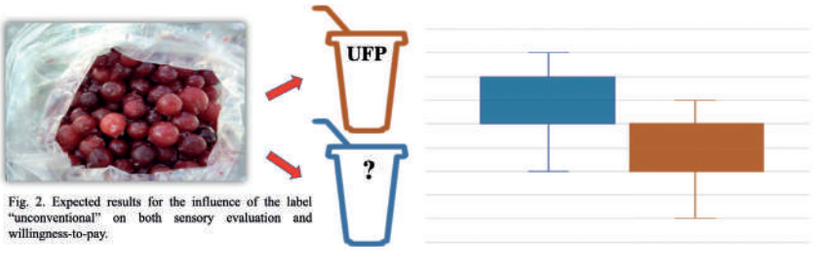

Fig. 2. Expected results for the influence of the label "unconventional" on both sensory evaluation and willingness-to-pay.

CONCLUSION

We will provide additional information on human behavior towards plant resources, usiframeworkng an innovative interdisciplinary. Our study will also have immediate practical contributions, since we will be able to provide farmers and extractors with information on the most promising UFPs, the best ways to introduce them to potential consumers, and the socioeconomic profiles that are more likely to consume UFPs.

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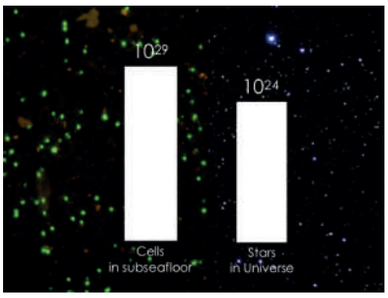
HIDDEN DEPTHS: UNCOVERING NEW GENETIC POTENTIAL IN SINGLE-CELLS RECOVERED FROM MILES BENEATH THE EARTH'S SURFACE

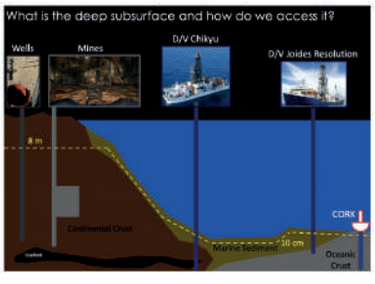
INTRODUCTION

Windows into the Earth's subsurface are few and far between. Yet from what glimpses we have had, there appears to be a boundless capacity for tiny life forms to survive, if not thrive, in this vast underground world. Estimates of the number of cells in the subsurface are literally astronomical, with 10^{28} subsurface cells and only 10^{24} stars in the universe.

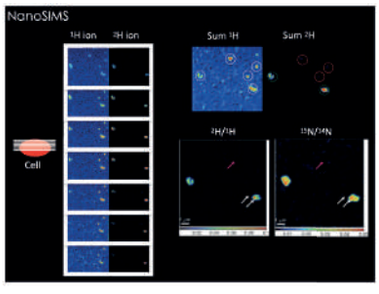


However, since access to these systems are so limited and require massive engineering and technology efforts, we know very little about how these life forms are able to survive without sunlight and in temperatures and pressures three to five times what we experience on the surface of the Earth.

MATERIALS AND METHODS

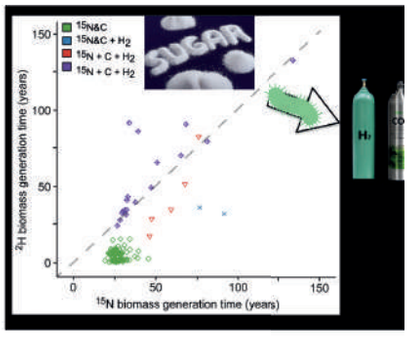


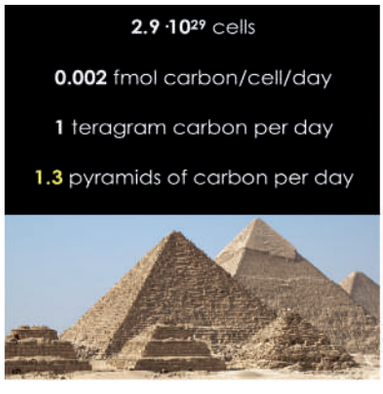
Through the application of highly sensitive methods at single-cell resolution (Nanoscale Secondary Ion Mass Spectrometry; NanoSIMS), I have been able to detect activity in samples kilometers below the surface of the seafloor, including some cells that have not seen the surface for millions of years. I propose to extend the utility of these extremely rare sample sets to gain additional genetic information by amplifying the genomes of these single-cells.



RESULTS

Single-cell rates of activity from this system were some of the slowest measured for life anywhere on Earth (hundreds of years). The dominant metabolism was fermentation of the coal, like how yeast make alcohol from sugar in beer and wine. While these rates are slow, when considering how vast the subsurface environment is, this can still amount to the processing of 1.3 "pyramids" of carbon per day by subsurface microbes.





CONCLUSION

This "high-risk, high-reward" project has the potential to tell stories about the evolution of life on Earth and where it might exist in similar environments elsewhere in our solar system.

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NEW WAYS OF BIODEGRADATION OF MARINE PLASTIC: LIGHT AND MICROBES

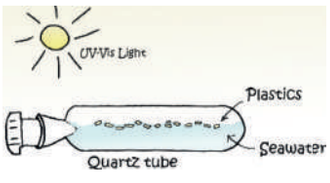
INTRODUCTION

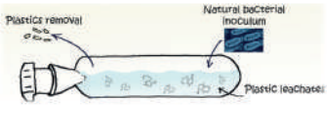
Up to 12.7 million metric tons (MT) of plastic entered the ocean only in 2010[01]. The exposition of plastic litter to solar UV radiation cause its weathering degradation and fragmentation[2]. Commercial plastic contains additives and plasticizers to improve the properties required for it purpose and to make it more resistant to degradation. When in contact with water, these additives can leach out to the aquatic medium[3,4].

Plastic photo-dissolution into DOC and its posterior consumption by marine bacteria could be an alternative way to the **plastic biodegradation** mechanisms proposed so far. For that, we need to know: 1) the conditions enhancing plastic leaching; 2) the bacterial species able to grow and consume plastic leachates. Also, it is important to understand if the DOC released by plastic is harmful for marine microorganisms and if it has a significant impact in the **carbon cycle.**

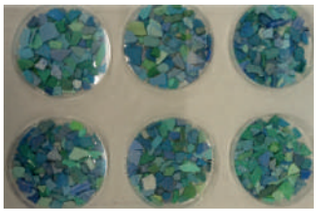
MATERIALS AND METHODS

Plastic leaching (photodegradation)
Plastic pieces added to seawater will be exposed to UV-Vis radiation during different time periods. Organic compounds will be measured to know how much compounds and which will be released.





Biodegradation of plastic leachates
Plastic leachates will be inoculated with a natural bacterial community. Bacterial growth will be followed by flow cytometry. Bacterial groups will be analyzed by CARD-FISH. Bacterial species and genes involved in DOC consumption, will be identified through sequencing of the 16S rRNA marker gene.
These experiments will be performed with different plastic types and at different environmental conditions.



EXPECTED RESULTS

*Production of dissolved organic compounds in plastic treatments after photodegradation. *Higher bacterial growth in plastic treatments. *Specific bacterial species growing on plastic leachates. *Specific genes found in plastic treatments.

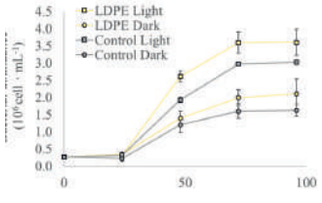


Figure. Bacterial abundance growing in marine plastic leachates. LDPE: low density polyethylene; Control: seawater without plastic leachates.

Photo: Alejandro Durán

CONCLUSION

Knowing the environmental conditions favouring plastic leaching into the seawater, we will know how to degrade plastic waste faster and which materials are the most environmentally friendly. That, together with the identification of the bacterial species consuming such leachates, will allow us to develop an alternative way of plastic biodegradation contributing to a cleaner ocean. This fits into the sustainable development goal (SDG) Nº14 proposed by the United Nations, Life Below Water. By 2025, it pretends to prevent and significantly reduce marine pollution.

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