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BOOK OF ABSTRACTS

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FOREWORD

Dear Members,

This Book of Abstracts provides details of the 70 posters presented at the General Assembly and Annual Conference of the Marie Curie Alumni Association (2nd and 3rd February 2018, in Leuven, Belgium).

Each poster includes an abstract, making reference to the author(s), organisation(s), and are themed across seven areas of study:

- Life Sciences
- Engineering
- Chemistry
- Physics
- Environmental Sciences
- Economics
- Social Sciences & Humanities

The MCAA once again thanks everyone that showcased their posters at the 2018 event. They continue to encourage members and non-members to submit posters for future Annual Conferences and General Assemblies. Do not hesitate to contact the author of the abstract using the MCAA web-portal.

Yours,
The MCAA Communications team

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Impact of lipid composition on in vivo performance of celecoxib formulations

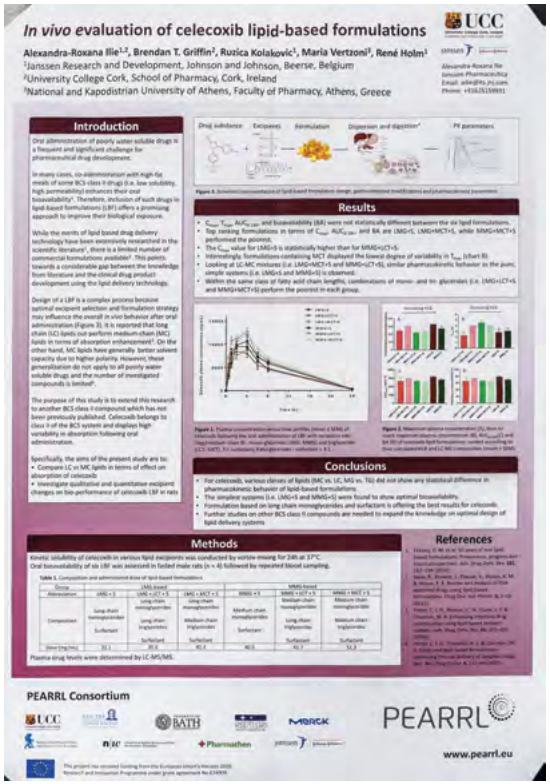
Erratic absorption and variable bioavailability of poorly-water soluble drugs (PWSD) challenge the robust formulation of oral dosage forms, especially at high doses. Overcoming such challenges can be done by solubilizing PWSD in lipid-based formulations (LBF). While this bio-enabling approach has been successful in bringing several drug molecules to market, systematic studies into the optimal excipient composition for LBF are lacking.

This study investigates the influence of composition changes on in vivo performance of LBF. It is reported in literature that long-chain (LC) lipids out-perform medium-chain (MC) lipids concerning absorption enhancement of certain PWSD, whereas for some compounds the differences are negligible. Considering higher solubility in medium-chain lipids, it is interesting to evaluate the LC-MC combination as bio-performance enhancer for high-dose formulations.

Six oral formulations of celecoxib with variations with respect to long-chain triglycerides (LCT), medium-chain triglycerides (MCT), long-chain monoglycerides (LMG), medium-chain monoglycerides (MMG) and a surfactant (S) were tested in a pharmacokinetic rat study. Formulations were grouped into two categories: 1) LMG-based: LMG+S, LMG+LCT+S, LMG+MCT+S and, 2) MMG-based: MMG+S, MMG+LCT+S, MMG+MCT+S.

Statistical analysis did not reveal any significant differences between the formulations regarding relevant PK parameters (i.e. Cmax, Tmax, AUC0-t, and bioavailability); however, a trend was observed towards better in vivo performance in terms of Cmax, AUC0-t, and bioavailability for the LMG+S formulation, whereas MMG+MCT+S performed less well.

Although it has been previously suggested that formulation design principles depend both on the compound's physico-chemical properties and excipient types and ratio, in the case of celecoxib the bio-performance was independent of lipid excipient type and ratio. These observations are not in accordance with data for other compounds, demonstrating that LBF design cannot be generalized at present.



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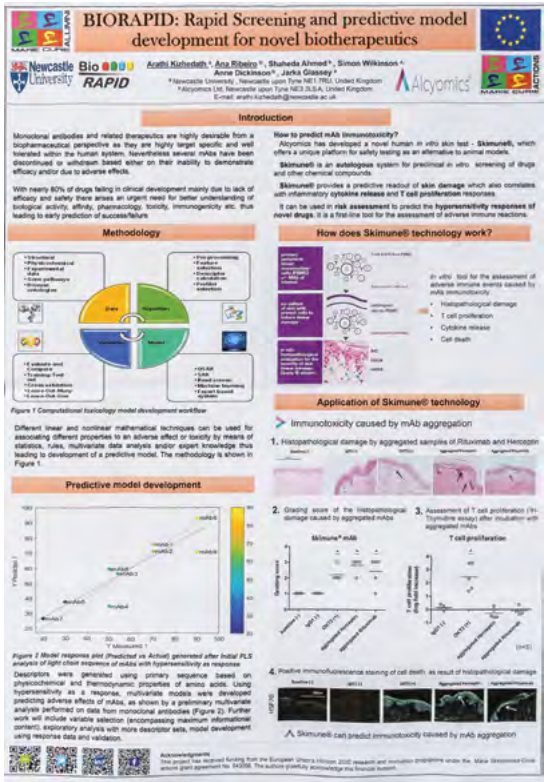
Organisation:
Janssen Research and Development, Johnson & Johnson

Skimune® as a new in vitro assay for detection of immunogenicity by aggregated monoclonal antibodies

Alcyomics has developed a novel human in vitro skin test – Skimune®, which offers a unique platform for safety testing as an alternative to animal models. Skimune® is an autologous system for in vitro screening of drugs and other chemical compounds. Skimune® provides a predictive readout of skin damage which also correlates with inflammatory cytokine release and T cell proliferation responses. It can be used in risk assessment to predict the sensitization potential of novel drugs. It is a first-line tool for the assessment of skin sensitization.

In this work, we present Skimune® as a tool for the assessment of adverse immune reactions to monoclonal antibodies (mAbs). Aggregation of mAbs is a very common event during industrial process, long-term storage (temperature), handling and administration (shaking). Considering the panoply of current protein-based therapeutics, there is a large concern for protein aggregation as potentially immunogenic for humans. While the extent of immunogenicity in patient populations is uncertain, reports show that it can lead to immune activation by cell activation and cytokine release.

In this experimental study, mAb aggregation was forced by exposure of different commercially available mAbs to a heat-stress protocol (up to 65°C). Resulting adverse immune events were measure by the Skimune® assays – T cell activation, cytokine release and histopathological damage. Protein characterization of the heat-exposure mAb samples was carried though analytical ultra-centrifugation (protein content), SDS-Page (molecular weight) and Transmission Electron Microscopy (aggregate formation). Our results show that exposure to temperature can, in fact, cause conformational changes in the mAb structure that, ultimately, cause adverse immune reactions. The aggregates formed provoked cell death by histopathological damage of the skin and activation of cell death pathways, rather than just overall immune activation. Ultimately, Skimune® can be used as a valid tool for assessment of immunogenicity by mAb aggregation.



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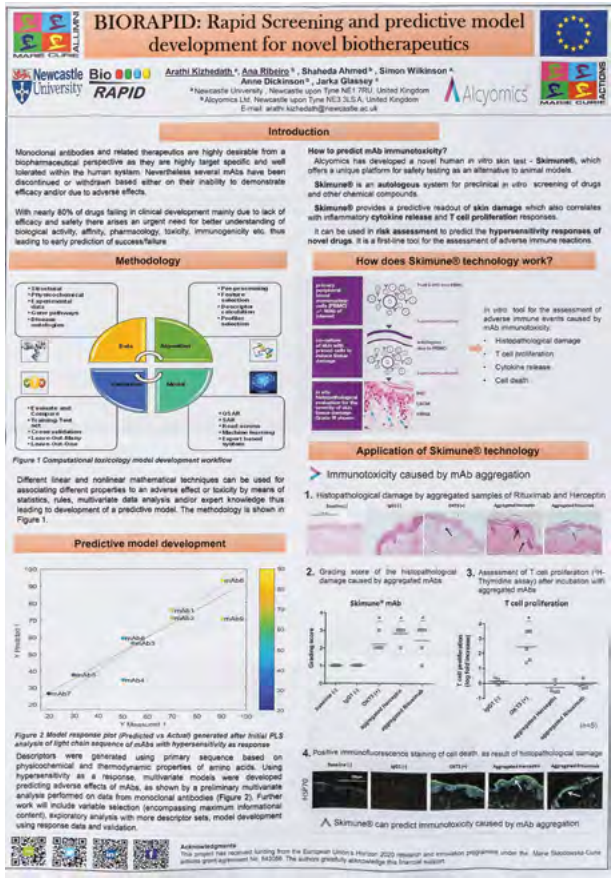
BIORAPID : Rapid early stage screening and predictive model development for novel biotherapeutics

Biologic drugs are structurally complex and very difficult to characterize and produce than small molecule drugs. With nearly 80% of drugs failing in clinical development mainly due to lack of efficacy and safety there arises an urgent need for smarter preclinical development using quality by design based approaches as identified by ICH Q8(R2) guidelines on Pharmaceutical development This contribution describes research undertaken in order to develop a modelling approach enabling the prediction of adverse effects of potential drug candidates by correlating the properties of selected biologic drugs with experimentally determined toxicity and hypersensitivity or allergic reactions. Intrinsic toxicology of bioactive pharmaceuticals was reported using a panel of in vitro methods including effects on cell viability and/or proliferation, genotoxicity and reactive oxygen species production due to oxidative insult. Hypersensitivity reactions were assessed using Skimune™, a non-artificial human skin explants based assay for safety and efficacy assessment of novel compounds and drugs, developed by Alcyomics Ltd. Using Skimune™ as a response, multivariate models were developed for small molecules to demonstrate the applicability of this assay for developing predictive models. Its use has been extended to predicting adverse effects of biologics as well, as shown by a preliminary multivariate analysis performed on data from monoclonal antibodies. The applicability of these in vitro and in silico methods and their benefits in rapid screening of prospective drug candidates in terms of potential hypersensitivity, toxicity and mode of action based on their inherent physical, chemical and/or biological properties as well has been discussed. The key impact of this research is on lowering of attrition rates, faster development of potential drug candidates as well as facilitate continued positive pipeline development for rapid bioprocesses. In the long term it would also help to reduce prices of potentially lifesaving biopharmaceutical products.



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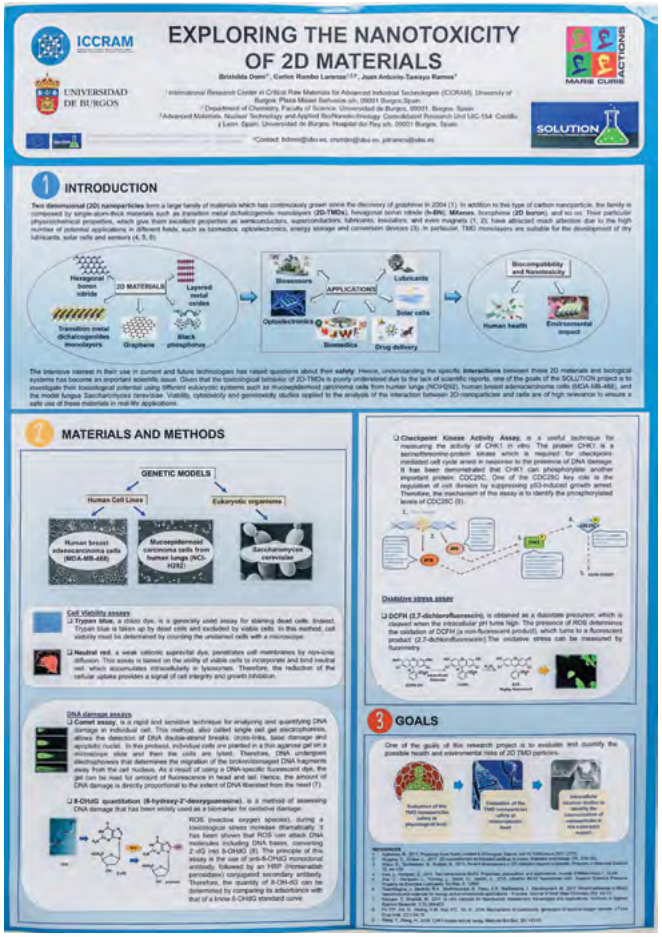
Exploring the nanotoxicity of 2D materials

Two dimensional (2D) nanoparticles form a large family of materials which has continuously grown since the discovery of graphene in 2004. In addition to this type of carbon nanoparticle, the family is composed by single-atom-thick materials such as transition metal dichalcogenide monolayers (2D-TMDs), hexagonal boron nitride (h-BN), MXenes, borophene (2D boron), and so on. Their particular physico-chemical properties, which give them excellent properties as semiconductors, superconductors, lubricants, insulators, and even magnets, have attracted much attention due to the high number of potential applications in different fields, such as biomedics, optoelectronics, energy storage and conversion devices. In particular, TMD monolayers are suitable for the development of dry lubricants, solar cells and sensors. The intensive interest in their use in current and future technologies has raised questions about their safety. Hence, understanding the specific interactions between these 2D materials and biological systems has become an important scientific issue. Given that the toxicological behaviour of 2D-TMDs is poorly understood due to the lack of scientific reports, one of the goals of the SOLUTION project is to investigate their toxicological potential using different eukaryotic systems such as mucoepidermoid carcinoma cells from human lungs (NCIH292), human breast adenocarcinoma cells (MDA-MB-468), and the model fungus Saccharomyces cerevisiae. Viability, cytotoxicity and genotoxicity studies applied to the analysis of the interaction between 2D-nanoparticles and cells are of high relevance to ensure a safe use of these materials in real-life applications.



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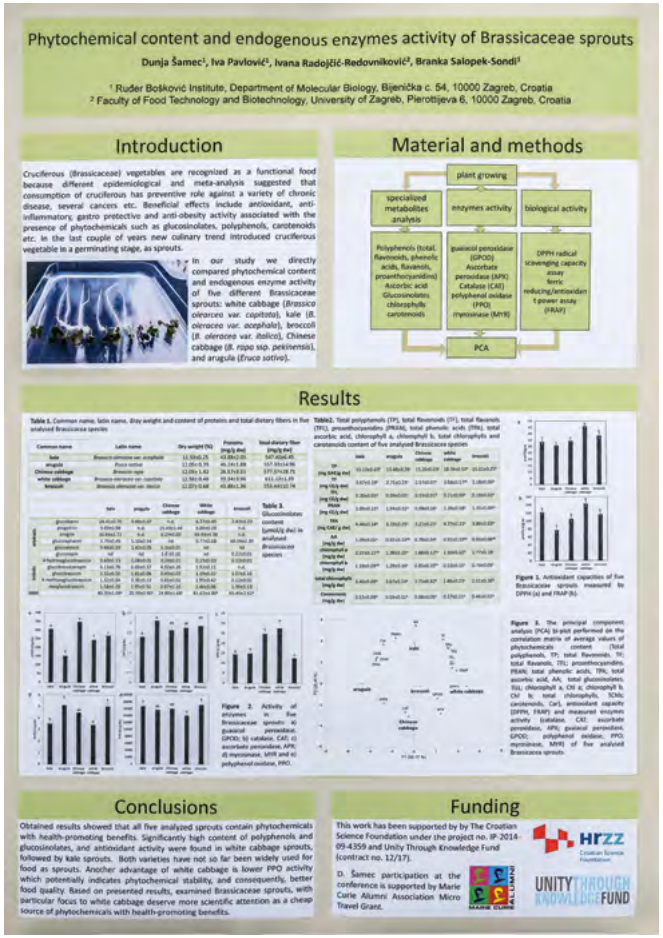
Phytochemical content and endogenous enzymes activity of Brassicaceae sprouts

Brassicaceae (cruciferous) vegetables are recognized as a functional food because different epidemiological and meta-analysis suggested that their consumption has preventive role against a variety of diseases. In the last couple of years new culinary trend introduced cruciferous vegetable in a germinating stage, as sprouts. Consumption of such as vegetables provide unique taste, and additional health benefits due to the fact that during extensive period of growth and development, seedlings and young plantlets accumulate more phytochemicals than vegetables in mature stage. In our study, five Brassicaceae sprouts (white cabbage, kale, broccoli, Chinese cabbage, aragula) were comparatively analyzed based on phytochemicals content and accompanying enzymes associated with phytochemical stability and bioavailability that consequently impact food quality. Significantly high content of polyphenols and glucosinolates, as well as a high antioxidant activity were found in white cabbage, followed by kale sprouts, two Brassicaceae sprouts which, so far, have not been widely consumed for food. Another advantage of white cabbage is lower polyphenol-oxidase activity which potentially indicates prevention of browning and better sprout quality. On the other side, kale, arugula and broccoli possessed lower ascorbate peroxidase activity, and higher ascorbic acid (vitamine C) content. In addition, arugula and broccoli showed significantly higher activity of myrosinase that may result in higher bioavailability of active glucosinolates forms.



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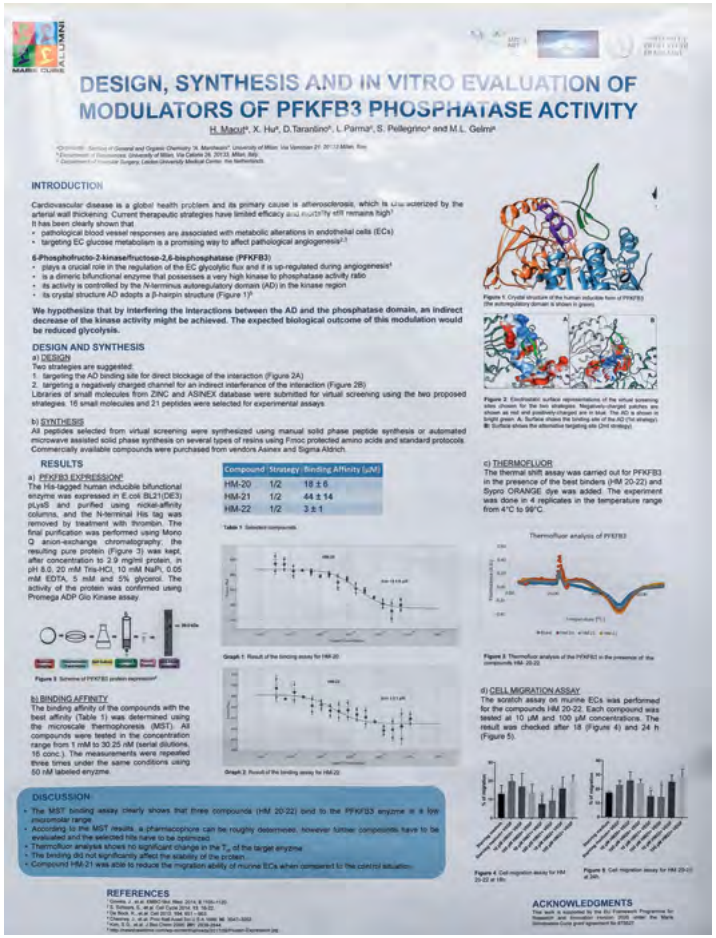
Design, synthesis and in vitro evaluation of modulators of PFKFB3 phosphatase activity

Cardiovascular disease is a global health problem and its primary cause is atherosclerosis, which is characterized by the arterial wall thickening. Current therapeutic strategies have limited efficacy and mortality still remains high. Recent research has shown that targeting dysregulated endothelial cell (EC) metabolism could be a new therapeutic strategy. In the scope of MSCA Moglynet EJD we aim to further explore the possibilities for an improved treatment of this serious disease.

EC glycolytic flux is up-regulated during angiogenesis and it is controlled by 6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase (PFKFB3), which is therefore an innovative target for atherosclerosis therapy. PFKFB3 is a dimeric bifunctional enzyme that has a very high kinase to phosphatase activity ratio. Its activity is controlled by the N-terminus autoregulatory domain (AD) in the kinase region, which adopts a β-hairpin shape in the crystal structure.

We performed virtual screening on the targeted allosteric binding site and here we present the synthesis and biological evaluation of the selected library of PFKFB3 phosphatase modulators. In vitro activity and binding assays were performed on the isolated recombinant enzyme and cell tests were carried out on murine ECs.



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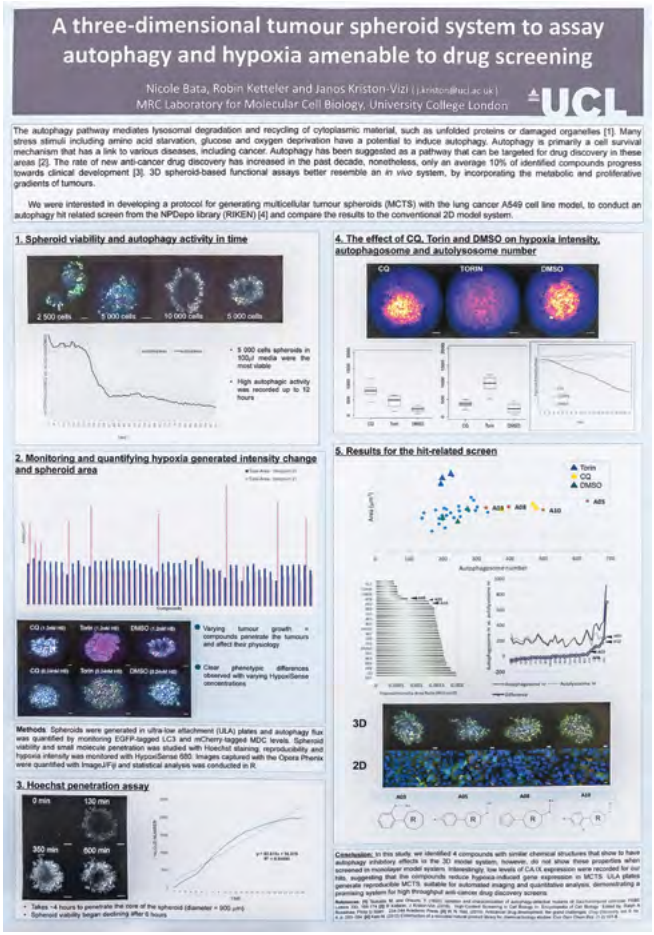
A three-dimensional tumour spheroid system to assay autophagy and hypoxia amenable to drug screening

The autophagy pathway mediates lysosomal degradation and recycling of cytoplasmic material, such as unfolded proteins or damaged organelles. Many stress stimuli including amino acid starvation, glucose and oxygen deprivation have a potential to induce autophagy. Autophagy is primarily a cell survival mechanism that has a link to various diseases, including cancer. Autophagy has been suggested as a pathway that can be targeted for drug discovery in these areas. The rate of new anti-cancer drug discovery has increased in the past decade, nonetheless, only an average 10% of identified compounds progress towards clinical development. 3D spheroid-based functional assays better resemble an in vivo system, by incorporating the metabolic and proliferative gradients of tumours.

We were interested in developing a protocol for generating multicellular tumour spheroids (MCTS) with the lung cancer A549 cell line model, to conduct an autophagy hit related screen from the NPDepo library (RIKEN) and compare the results to the conventional 2D model system.



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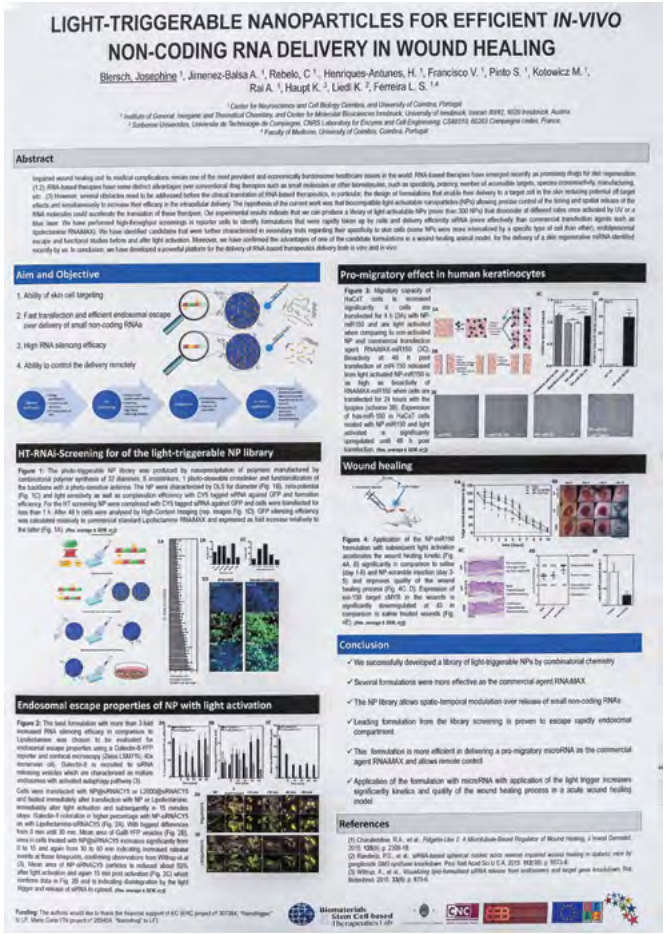
HT-Screening identifies light triggerable NP formulation for efficient in vivo non-coding RNA delivery in wound healing

Impaired wound healing and its medical complications remain one of the most prevalent and economically burdensome healthcare issues in the world. RNA-based therapies have emerged recently as promising drugs for skin regeneration. RNA-based therapies have some distinct advantages over conventional drug therapies such as small molecules or other biomolecules, such as specificity, potency, number of accessible targets, species crossreactivity, manufacturing, etc. However, several obstacles need to be addressed before the clinical translation of RNA-based therapeutics, in particular, the design of formulations that enable their delivery to a target cell in the skin reducing potential off-target effects and simultaneously to increase their efficacy in the intracellular delivery. The hypothesis of the current work was that biocompatible light-activatable nanoparticles (NPs) allowing precise control of the timing and spatial release of the RNA molecules could accelerate the translation of these therapies. Our experimental results indicate that we can produce a library of light-activatable NPs (more than 300 NPs) that dissociate at different rates once activated by UV or a blue laser. We have performed high-throughput screenings in reporter cells to identify formulations that were rapidly taken up by cells and delivery efficiently siRNA (more effectively than commercial transfection agents such as lipofectamine RNAiMAX). We have identified candidates that were further characterized in secondary tests regarding their specificity to skin cells (some NPs were more internalized by a specific type of cell than other), endolysosomal escape and functional studies before and after light activation. Moreover, we have confirmed the advantages of one of the candidate formulations in a wound healing animal model, for the delivery of a skin regenerative miRNA identified recently by us. In conclusion, we have developed a powerful platform for the delivery of RNA-based therapeutics delivery both in vitro and in vivo.



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BIORAPID: Bioprocess scale up/down strategies for rapid development of novel bioactive molecules

Biotechnological applications demand large amounts of high-quality products, which are produced at considerably low costs. Cell physiology and, in many cases, product yield and quality strongly depend on suitable production conditions. However, oscillatory environmental conditions due to gradient formation in the liquid phase in large scale production, lead to cell stress and productivity losses.

The aim of this research is to efficiently mimic various large scale process conditions in lab scales, which provides the possibility of fast, reliable, cheap and consistent optimization of bioprocesses. Hence, robust scale up strategies are developed in order to speed up the development of processes for new bioactive molecules. With this perspective, we simulated the conditions experienced by insulin-producing Escherichia coli cells in large scale bioreactors by performing pulse-based nutrient feeding and starvation experiments in parallel with multiple cultivations. This strategy was tested on mammalian cell cultures in miniaturized bioreactors, ideal for high-throughput screening, by following optimal experimental designs, with the main focus on protein quality. Furthermore, we applied multi-compartment scale down reactors to study the consequences of heterogeneous conditions in lactic acid bacteria (LAB) fermentation in lab scale by pH gradients. A special focus was put on the application of novel online activity and single-cell based monitoring. Finally, we developed a model to describe the dynamics of freeze-drying of LAB with computational fluid dynamics, for future optimization and scale up.

These novel scale up/down strategies may have a crucial role in the pharmaceutical and food industry, since product quality is pivotal for commercialization. At the same time, our approaches are useful to optimize the production of starter cultures for dairy products.

Acknowledgments

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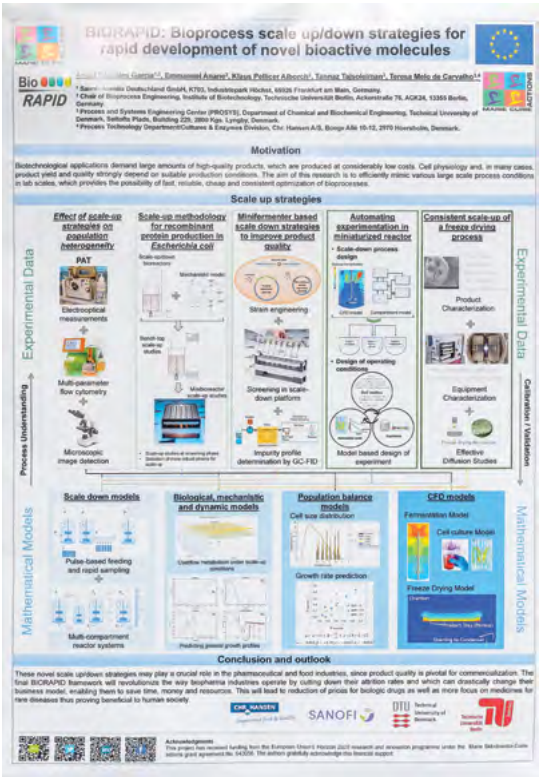

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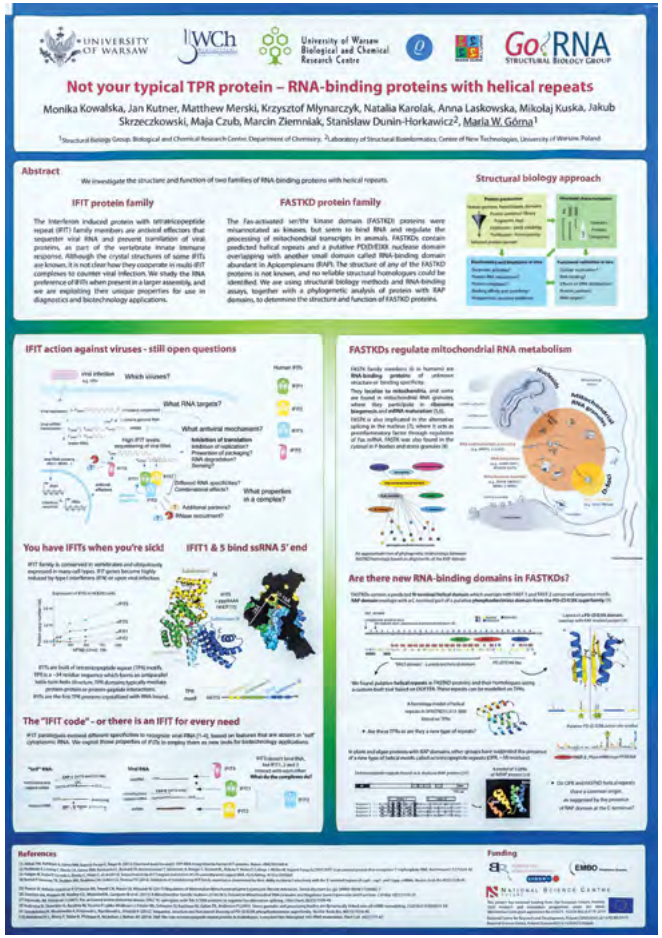
Organisation:
Technische Universität Berlin (TU Berlin)

Not your typical TPR protein – RNA-binding proteins with helical repeats

We investigate the structure and function of two families of RNA-binding proteins with helical repeats. One group is the Interferon induced protein with tetratricopeptide repeat (IFIT) family, which are antiviral effectors that sequester viral RNA and prevent translation of viral proteins, as part of the vertebrate innate immune response. Although the crystal structures of some IFITs are known, it is not clear how they cooperate in multi-IFIT complexes to counter viral infection. We study the RNA preference of IFITs when present in a larger assembly, and we are exploiting their unique properties for use in diagnostics and biotechnology applications.

The second group of our interest are the Fas-activated serine threonine kinase domain (FASTKD) proteins, which were misannotated as kinases, but seem to bind and regulate the processing of mitochondrial transcripts in animals. FASTKD proteins contain predicted helical repeats and a putative PD(D/E)XK nuclease domain overlapping with another small domain called RNA-binding domain abundant in Apicomplexans (RAP). The structure of any of the FASTKD proteins is not known, and no reliable structural homologues could be identified. We are using structural biology methods and RNA-binding assays, together with a phylogenetic analysis of protein with RAP domains, to determine the structure and function of FASTKD proteins.



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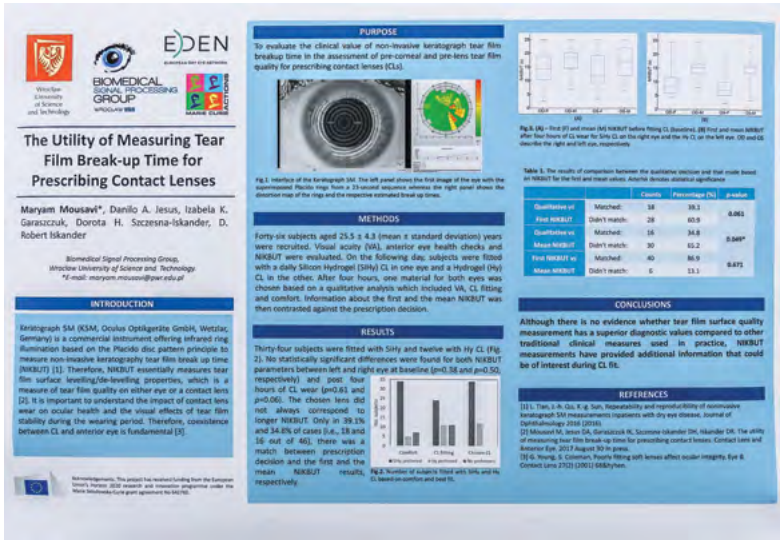
The Utility of Measuring Tear Film Break-up Time for Prescribing Contact Lenses

Purpose: To evaluate the clinical value of non-invasive keratograph tear film breakup time in the assessment of pre-corneal and pre-lens tear film quality for prescribing contact lenses (CLs).

Methods: Forty-six subjects aged 25.5 ± 4.3 (mean ± standard deviation) years were recruited. Visual acuity (VA), anterior eye health checks and NIKBUT were evaluated. On the following day, subjects were fitted with a daily Silicon Hydrogel (SiHy) CL in one eye and a Hydrogel (Hy) CL in the other. After four hours, one material for both eyes was chosen based on a qualitative analysis which included VA, CL fitting and comfort. Information about the first and the mean NIKBUT was then contrasted against the prescription decision.

Results: Thirty-four subjects were fitted with SiHy and twelve with Hy CL (Fig. 2). No statistically significant differences were found for both NIKBUT parameters between left and right eye at baseline (p=0.38 and p=0.50, respectively) and post four hours of CL wear (p=0.61 and p=0.06). The chosen lens did not always correspond to longer NIKBUT. Only in 39.1% and 34.8% of cases (i.e., 18 and 16 out of 46), there was a match between prescription decision and the first and the mean NIKBUT results, respectively. Conclusions: Although there is no evidence whether tear film surface quality measurement has a superior diagnostic values compared to other traditional clinical measures used in practice, NIKBUT measurements have provided additional information that could be of interest during CL fit.



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Metabolic adaptations of astrocytes to physiological oxygen levels in the presence of neurons

Our current knowledge on neuronal metabolism and its regulation are mainly derived from experimental culture conditions that do not fully resemble the physiological situation. Amongst the main drawbacks, we highlight (i) the absence of neighbour astrocytes in close interaction with neurons, and (ii) the occurrence of atmospheric (21%) O2 tension, given that these factors may strongly impact on neuronal oxidative metabolism (1). Regarding oxygen tensions, it has been estimated that neural cells in vivo are exposed to O2 concentrations ranging from 1 to 10%, depending on the distance from the brain vessels (2). In order to ascertain the impact of these factors on neuronal metabolism, here we have established a co-culture system of cortical neurons and astrocytes in primary culture, chronically (6 days) grown under different O2 concentrations (21-2%) in an oxygen-monitored CO2-incubator chamber. Analyses of mitochondrial membrane potential, mitochondrial reactive oxygen species (mROS) generation, and survival, revealed that neurons were healthiest at 5% O2. Furthermore, neurons co-cultured with astrocytes for 6 days showed, at 5% O2, higher mROS production, glycolytic rate, and survival, than those at 21% O2. To explore these metabolic adaptations with a wider perspective, we performed a whole transcriptome differential expression analysis of neurons co-cultured with astrocytes, grown either at 5% or at 21% O2, using a microarray strategy. Our results show significant changes in the expression of several genes encoding proteins limiting for essential metabolic routes, thus revealing the impact of physiological O2 concentrations, in the presence of astrocytes, on neuronal energy adaptations. The currently ongoing validation of these targets regulated by physiological conditions may contribute to ascertain novel mechanisms of neuronal control of metabolism.

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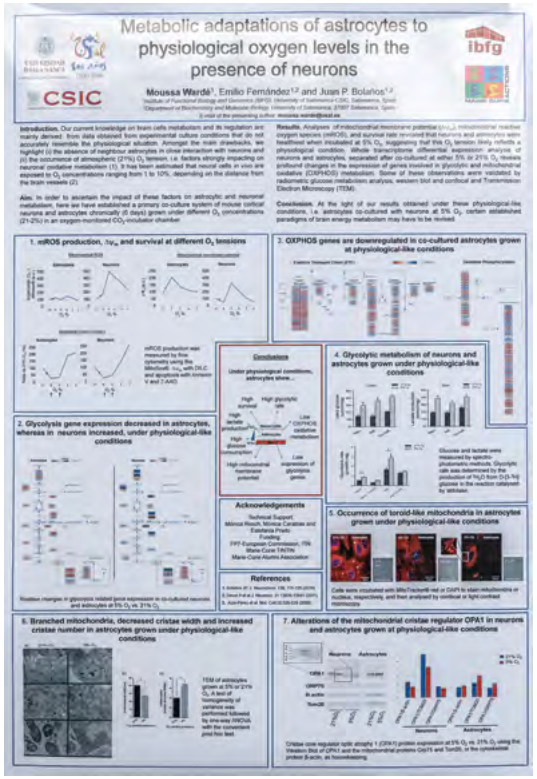
2. Devor A et al.. “Overshoot” of O2 Is Required to Maintain Baseline Tissue Oxygenation at Locations Distal to Blood Vessels. J. Neurosci. 31:13676-13681 (2011).



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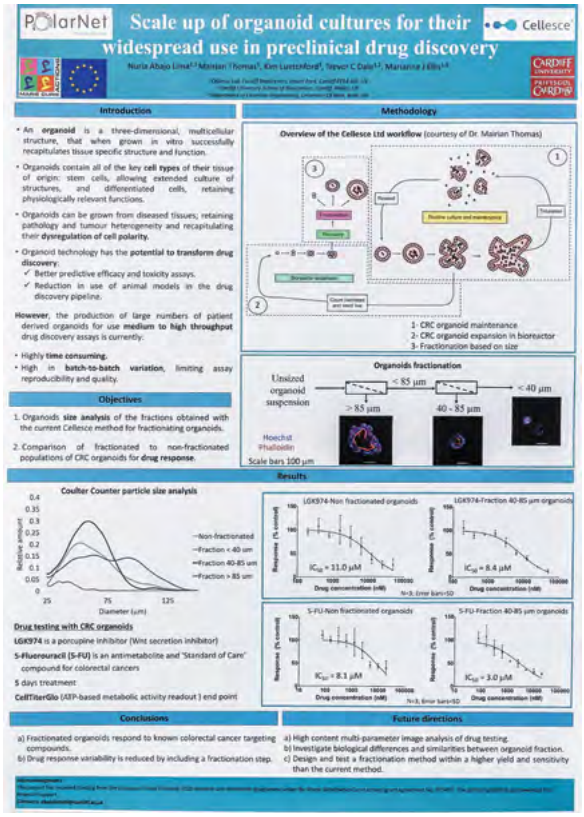
Scale up of organoid expansion and fractionation for their widespread use in preclinical drug discovery

Recent studies showing that cancer organoids recapitulate the biology of primary cancers have driven tremendous excitement in their potential to revolutionize drug discovery and personalized medicine. Tumor heterogeneity at the genetic and phenotypic level drives differential responses to therapeutic agents, and this heterogeneity is preserved in organoids grown from colorectal cancers. Using organoids as an alternative to 2D cultures is growing in popularity but there is a bottleneck to their widespread utilization. Organoids need to be produced on a large enough scale to adequately supply end users, from university researchers to pharmaceutical companies; importantly batch-to-batch variation needs to be minimized. Currently, manual processing results in organoids of varied size and while the majority are suitably functional, they range from too small to polarize, to too big with necrotic cores. Cellesce Ltd has developed a new bioprocessing technology by semi-automating the process of organoid culture, thus improving the control of the process conditions, which yields a more desirable range of organoid sizes.

The aim of this research is to fractionate distinct organoid subpopulations based on their size using chemical engineering technologies. Fractionated populations of colorectal cancer organoids from biopsies that show different phenotypes and mutational backgrounds are separated using the technology, and will be used to study differences in organoid subtypes, i.e. function and polarity, and to relate genetic and phenotypic differences back to drug response and primary tumor heterogeneity. A broad spectrum of inhibitors of signaling pathways are used to demonstrate the importance of the fractionation process and the identification of the organoid size that satisfactorily recapitulates the drug response of the native organ.

This approach will enable the use of biophysically-purified organoid subpopulations to study the molecular mechanisms underlying organoids' phenotypic heterogeneity, together with the efficiency of novel anti-cancer drugs before their use in Phase II clinical trials.



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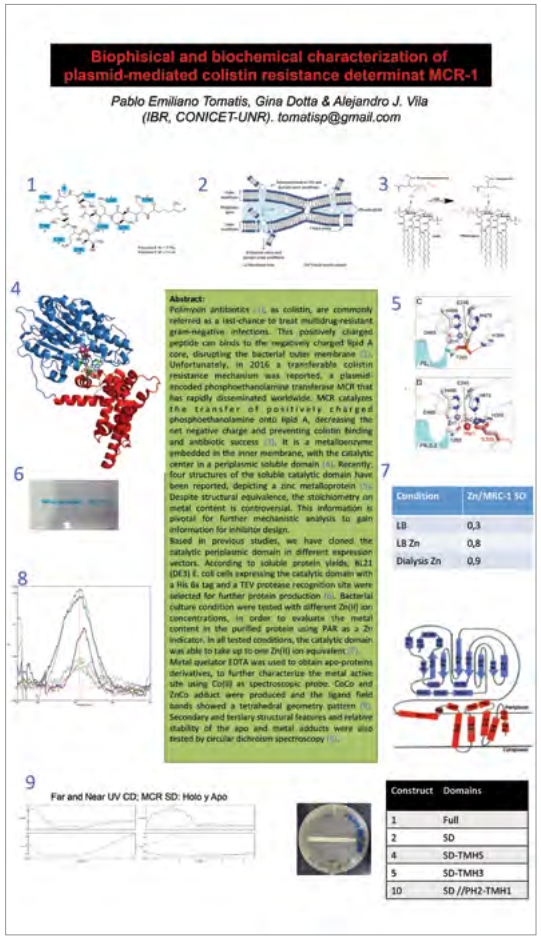
Biophisical and biochemical characterization of plasmid-mediated colistin resistance determinat MCR-1

Polimyxin antibiotics, as colistin, are commonly referred as a last-chance to treat multidrug-resistant gram-negative infections. This positively charged peptide can binds to the negatively charged lipid A core, disrupting the bacterial outer membrane. Unfortunately, in 2016 a transferable colistin resistance mechanism was reported, a plasmid-encoded phosphoethanolamine transferase MCR that has rapidly disseminated worldwide. MCR catalyzes the transfer of positively charged phosphoethanolamine onto lipid A, decreasing the net negative charge and preventing colistin binding and antibiotic success. It is a metalloenzyme embedded in the inner membrane, with the catalytic center in a periplasmic soluble domain. Recently, four structures of the soluble catalytic domain have been reported, depicting a zinc metalloprotein. Despite structural equivalence, the stoichiometry on metal content is controversial. This information is pivotal for further mechanistic analysis to gain information for inhibitor design.

Based in previous studies, we have cloned the catalytic periplasmic domain in different expression vectors. According to soluble protein yields, BL21 (DE3) E. coli cells expressing the catalytic domain with a His 6x tag and a TEV protease recognition site were selected for further protein production. Bacterial culture condition were tested with different Zn(II) ion concentrations, in order to evaluate the metal content in the purified protein using PAR as a Zn indicator. In all tested conditions, the catalytic domain was able to take up to one Zn(II) ion equivalent.

Metal quelator EDTA was used to obtain apo-proteins derivatives, to further characterize the metal active site using Co(II) as spectroscopic probe. CoCo and ZnCo adduct were produced and the ligand field bands showed a tetrahedral geometry pattern. Secondary and tertiary structural features and relative stability of the apo and metal adducts were also tested by circular dichroism spectroscopy.



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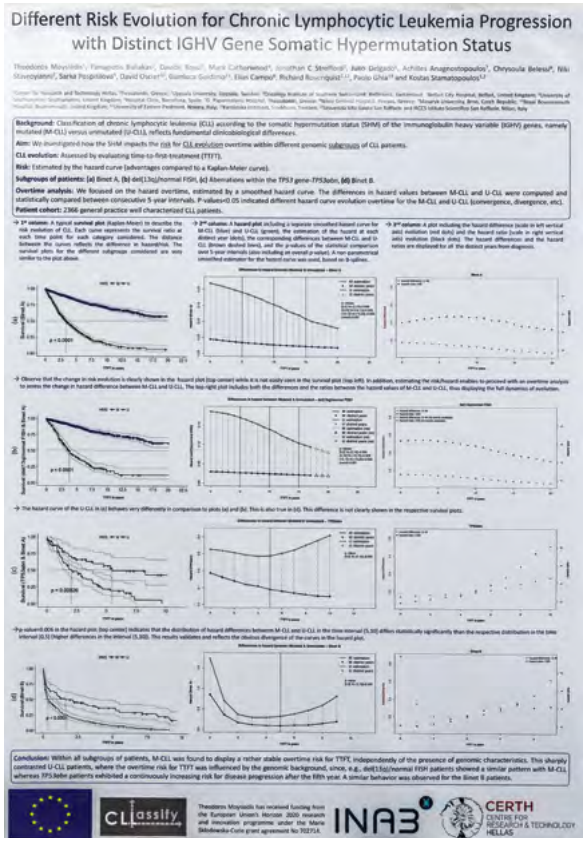
Different Risk Evolution for Chronic Lymphocytic Leukemia Progression with Distinct IGHV Gene Somatic Hypermutation Status

Chronic lymphocytic leukemia (CLL) is the most common adult leukemia in the West and exhibits remarkable clinicobiological heterogeneity. A great challenge for CLL patients is to determine if and when they will experience disease progression requiring treatment. Nowadays, immunogenetic and genomic features are considered essential for accurate prognostic assessment in CLL. When utilizing such biomarkers, the prognosis is assessed assuming stable predictability over the disease course. Here, we assessed the risk evolution for CLL progression overtime by evaluating time-to-first-treatment (TTFT) in 2366 CLL patients not requiring treatment at the time of diagnosis. Based on the somatic hypermutation status (SHM) of the immunoglobulin heavy variable (IGHV) genes, the patients were classified as mutated (M-CLL) and unmutated CLL (U-CLL). Our analysis focused on different genomic subgroups within each SHM category.

Initially, the overtime risk was estimated by the hazard curve. This enables to better visualize changes in risk evolution compared to the typical Kaplan-Meier curve, which is the current gold-standard tool for risk evolution in survival-analysis, by showing the "instant" risk for treatment initiation at a specific time point. We then performed an interpolation method to estimate, for both the M-CLL and the U-CLL patients, the specific values of their hazard curves at each distinct year from the time of diagnosis, and the corresponding hazard differences. The follow-up was divided in 5-year intervals, and the distributions of the hazard differences were statistically compared between consecutive 5-year intervals. P-values less than 0.05 would indicate different hazard curve evolution for the M-CLL and the U-CLL patients.

We observed significant differences in risk evolution between the different genomic subgroups in each SHM category. In particular, while M-CLL patients were found to display a rather stable overtime risk for TTFT, in U-CLL patients, the risk evolution was clearly influenced by the genomic background.



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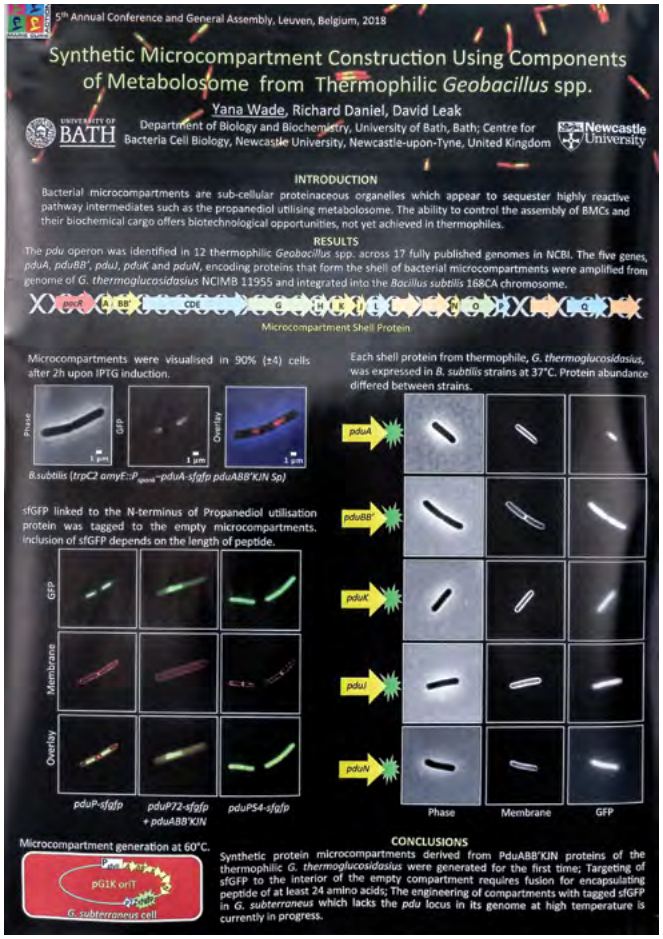
Microcompartment construction using components of the propanediol utilisation metabolosome from thermophilic Geobacillus spp.

Bacterial microcompartments (BMCs) are sub-cellular proteinaceous organelles which appear to sequester highly reactive pathway intermediates such as the propanediol utilising metabolosome (Pdu). The ability to control the assembly of BMCs and their biochemical cargo offers biotechnological opportunities, not yet achieved in thermophiles.

The pdu operon in the genome of thermophilic G. thermoglucosidasius NCIMB 11955 was examined. The five genes, pduA, pduBB', pduJ, pduK and pduN, encoding proteins that form the shell of BMCs were amplified. Initially, the empty BMCs were assembled by expression of the pduABB'JKN proteins in Bacillus subtilis 168CA. Circular structures with clear boundaries were visualised by TEM in thin-sectioned cells. Superfolder GFP (sfGFP) fused to the sequence of the Propanediol utilisation protein PduP was incorporated into the lumen of BMCs. Given the Bacillus-based observations, the pduABB'JKN and pduP72-sfGFP were placed under the control of both a maltose inducible promoter and a synthetic strong constitutive RplsI promoter for simultaneous co-expression in Geobacillus spp. The fragments were cloned into shuttle vectors capable of conjugative transfer from Escherichia coli S17-1 and will be transferred into Geobacillus strains lacking the pdu operon, such as G. subterraneus.

These results show for the first time the generation of synthetic protein compartments derived from components of the Pdu organelle of thermophilic G. thermoglucosidasius and targeting of enzymes to their lumen. The engineering of BMCs with tagged sfGFP in G. subterraneus, which lacks the pdu locus in its chromosome, is currently in progress.



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Scleral and soft contact lens wear alters ocular surface

Scleral contact lenses are oxygen permeable rigid contact lenses that rest entirely on the sclera, without touching the cornea. Their diameter is consequently larger than that of soft contact lenses. Traditionally, scleral lenses have been used for visual correction in compromised eyes, when spectacles or soft contact lenses could not help and also as therapeutic device in cases of ocular surface disease. However, in the last decade scleral contact lens prescription has significantly increased and nowadays scleral lenses are progressively being considered for refractive error correction also in healthy eyes. Independently of the type of contact lens worn, the interaction between the contact lens and the ocular surface is a crucial factor in assuring the safety and comfort of the fit. The aim of this work was to compare how the ocular surface is altered as a consequence of soft lenses and hard scleral lenses wear. 20 volunteer subjects participated in the study, half wore a soft contact lens and half a scleral lens during a 5-hours period. Measurements with a non-contact corneo-scleral topographer (Eye Surface Profiler) were always conducted before lens insertion and immediately after lens removal. Limbal radius (the edge between cornea-sclera) was the parameter chosen as indicator of ocular surface alteration. Limbal radius was determined from 3-dimensional corneo-scleral maps using a custom made algorithm. The mean limbal radius increment of the volunteers wearing a hard scleral lens was larger (220 ± 130 µm) than that of those wearing a soft lens (160 ± 60 µm). The large standard deviation obtained implies a high subject dependency regarding limbal radius increment after contact lens wear, remarking the importance of the lens-subject biocompatibility. The results from this study suggest that even though scleral lenses do not directly touch the cornea they greatly alter the corneo-scleral transition and consequently ocular surface shape.

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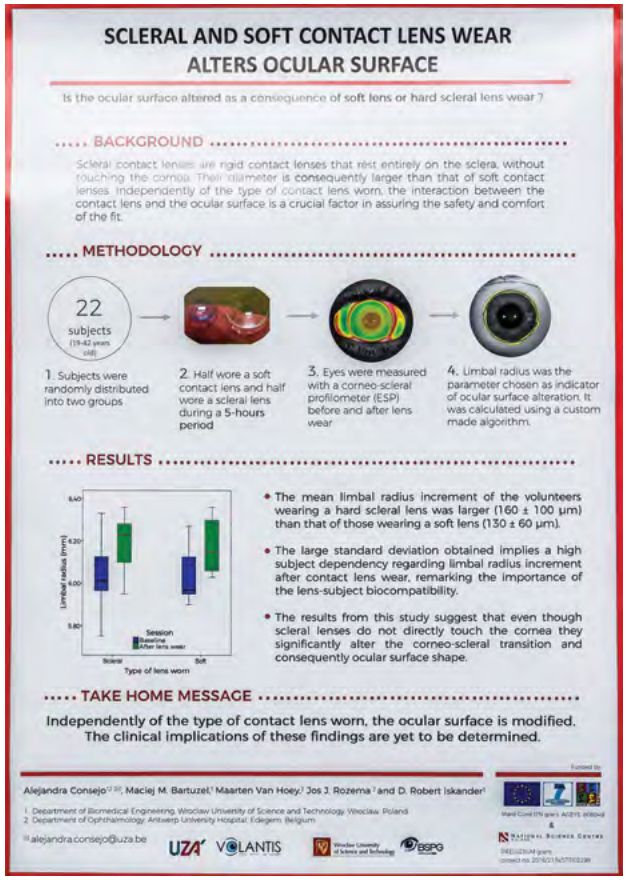

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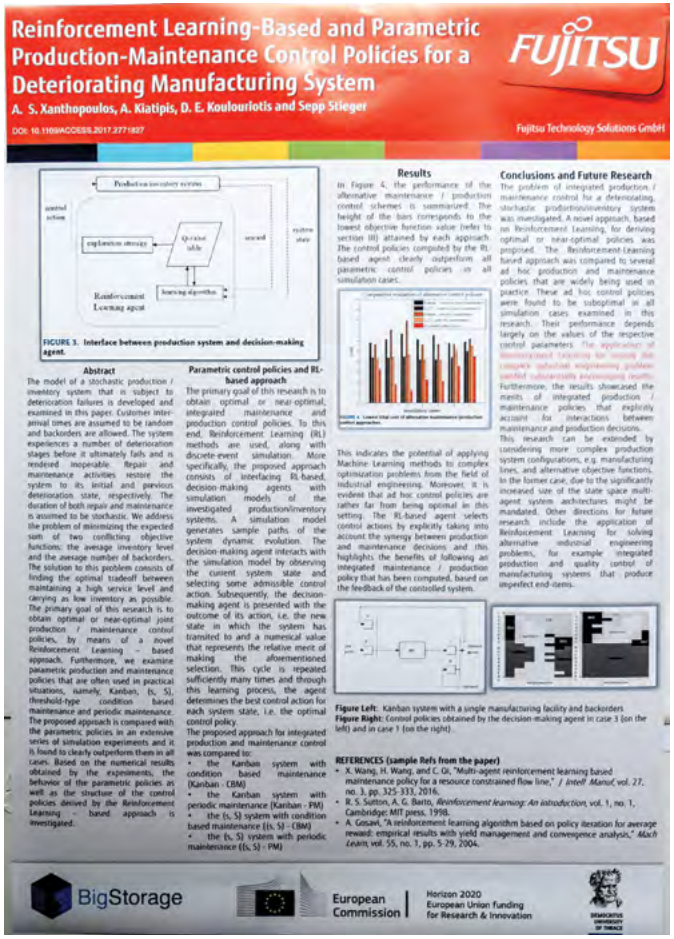
Reinforcement Learning-Based and Parametric Production-Maintenance Control Policies for a Deteriorating Manufacturing System A.

The model of a stochastic production/inventory system that is subject to deterioration failures is developed and examined in this paper. Customer interarrival times are assumed to be random and backorders are allowed. The system experiences a number of deterioration stages before it ultimately fails and is rendered inoperable. Repair and maintenance activities restore the system to its initial and previous deterioration state, respectively. The duration of both repair and maintenance is assumed to be stochastic. We address the problem of minimizing the expected sum of two conflicting objective functions: the average inventory level and the average number of backorders. The solution to this problem consists of finding the optimal trade-off between maintaining a high service level and carrying as low inventory as possible. The primary goal of this research is to obtain optimal or near-optimal joint production/maintenance control policies, by means of a novel Reinforcement Learning-based approach. Furthermore, we examine parametric production and maintenance policies that are often used in practical situations, namely Kanban, (s, S), threshold-type condition based maintenance and periodic maintenance. The proposed approach is compared to the parametric policies in an extensive series of simulation experiments and it is found to clearly outperform them in all cases. Based on the numerical results obtained by the experiments, the behavior of the parametric policies as well as the structure of the control policies derived by the Reinforcement Learning-based approach is investigated.



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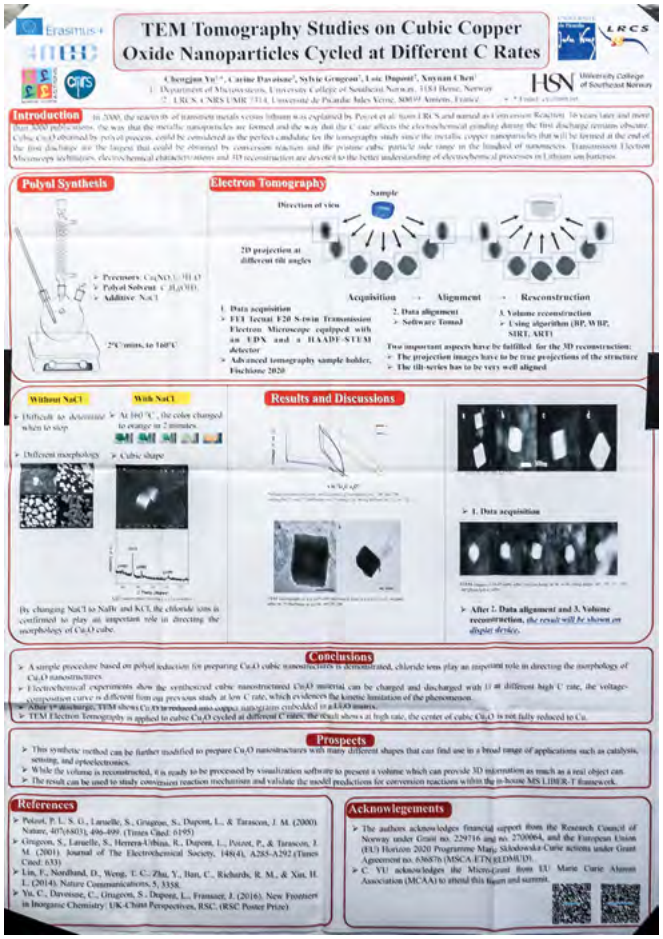
Towards the development of novel carbon based materials for on-chip supercapacitor

In this project, the key challenges by self-assembling carbon nanotube (CNT), graphene and other carbon materials with engineered nanoarchitectures are addressed. The innovative materials approach is the use of silicon nano-taper array decorated with nano particles (NPs) for catalytic growth to construct functional 3D templates, and of low dimension carbons in the form of CNT or graphene to construct 3D nanoarchitectures. Our hypothesis is that silicon nano-taper array with engineered density and shape will prove to be the most effective functional structure for template-assisted self-assembling the electrodes of supercapacitors. The resulting electrodes exhibit optimized configuration of pores, quantitative electrochemical accessibility, and the use of maximized active material sustaining fast charging rates. Moving from on-chip to large-size supercapacitors, the wafers with the 3D nanoarchitecture stack together via interconnection to fabricate the large-size supercapacitors. At the same time, the R&D on on-chip supercapacitors emphasis should be put on developing package material system and process suitable for IC compatibility and high reliability. We will design both in-plan and sandwich supercapacitor configurations, and electrical interconnections for a compact integration on chip and on printed circuit board. The application of liquid or solid electrolyte request chemical stable package materials. Implementing the separator between two electrodes against electron short-circuit, especially in the liquid electrolyte supercapacitors, is another challenge requiring obstacle-free for ion diffusion. We will use glass-to-silicon anodic bonding or silicon-to-silicon direct bonding to encapsulate electrolyte. The wafer level package will be investigated for both supercapacitor chips and wafer-stacked supercapacitors of large-scales. The demonstrator application will focus on medium power and energy storage systems.



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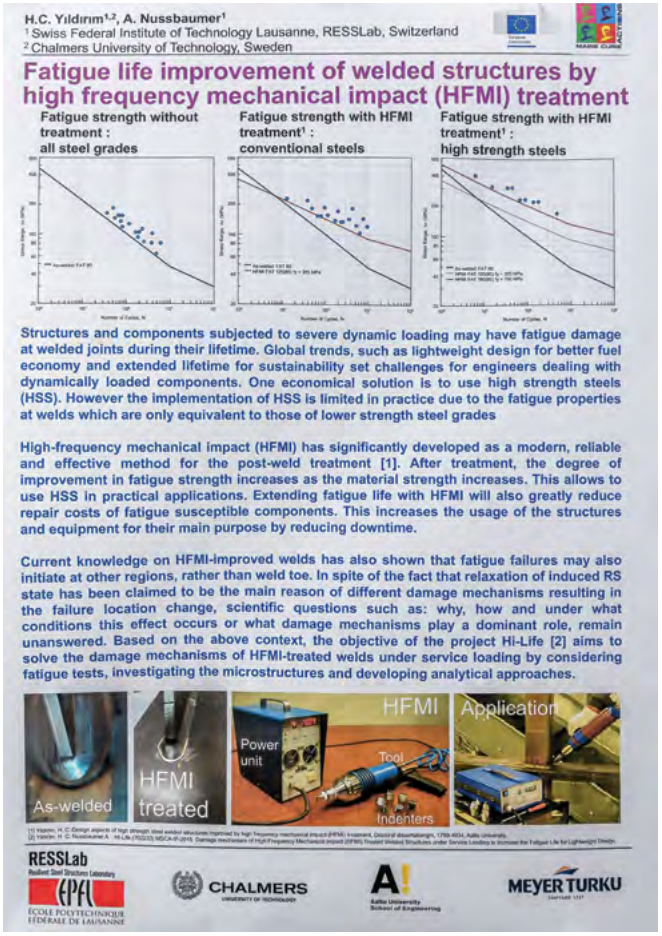
Fatigue life improvement of welded structures by high frequency mechanical impact (HFMI) treatment

Structures and components subjected to severe dynamic loading may have fatigue damage at welded joints during their lifetime. Global trends, such as lightweight design for better fuel economy and extended lifetime for sustainability set challenges for engineers dealing with dynamically loaded components. One economical solution is to use high strength steels (HSS). However the implementation of HSS is limited in practice due to the fatigue properties at welds which are only equivalent to those of lower strength steel grades

High-frequency mechanical impact (HFMI) has significantly developed as a modern, reliable and effective method for the post-weld treatment [1]. After treatment, the degree of improvement in fatigue strength increases as the material strength increases. This allows to use HSS in practical applications. Extending fatigue life with HFMI will also greatly reduce repair costs of fatigue susceptible components. This increases the usage of the structures and equipment for their main purpose by reducing downtime.

Current knowledge on HFMI-improved welds has also shown that fatigue failures may also initiate at other regions, rather than weld toe. In spite of the fact that relaxation of induced RS state has been claimed to be the main reason of different damage mechanisms resulting in the failure location change, scientific questions such as: why, how and under what conditions this effect occurs or what damage mechanisms play a dominant role, remain unanswered. Based on the above context, the objective of the project Hi-Life [2] aims to solve the damage mechanisms of HFMI-treated welds under service loading by considering fatigue tests, investigating the microstructures and developing analytical approaches.



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Investigation of 2D Magnetic Resonance Thigh Muscle Image Segmentation using a Convolutional Neuronal Network

Purpose: Musculoskeletal disorders as pulmonary disease or osteoarthritis have a high prevalence among the population and are the most frequently cause for pain, limitation and a loss of quality in life. Automated segmentation of muscles is an important step towards investigating the impact of muscle morphology towards clinical outcome from large available datasets and cohort studies as the osteoarthritis initiative (OAI). Therefore we investigate a 2D state-of-the-art Convolutional Neuronal Network (CCN) for the automated cross-sectional area segmentation of the quadriceps, hamstrings, subcutaneous fat (SCF) and the femoral bone.

Methods: The 2D segmentation method was implemented in Python 3.4 using a fully convolutional segmentation network (FCN) widely used for natural images. Semi-automatically segmented MRI slices located at approximately 33% of the thigh (from distal to proximal) in axial non–fat-suppressed T1-weighted thigh MRIs from the OAI (n=1499) were randomly divided into training (N=1449) and validation sets (N=50). All MRI slices where cropped (256x256 pixels) and centered towards the femoral bone of the right knee to simplify the segmentation problem for the FCN architecture. We evaluated the segmentation accuracy achieved in the validation set using the Dice Similarly Coefficient (DSC).

Results: A high accuracy was observed for all evaluated structures (DSC: quadriceps: 0.98 ± 0.00, hamstrings: 0.98 ± 0.01, SCF: 0.99 ± 0.01 and femoral bone: 0.97 ± 0.02).

Conclusion: The evaluated 2D state-of-the-art CCN architecture appears to be suitable for the task of fully automatic thigh cross-sectional area segmentation. The performance of the method compares favorably to the performance of previously used (semi-) automated methods, but still needs to be extended to all anatomical thigh structures (i.e., adductors, sartorius muscle, inter-muscular fat).

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Monitoring of biopharmaceutical production

With increasing demand for biopharmaceuticals, the production and development of new biopharmaceuticals faces new challenges. The production consists of upstream where the biopharmaceutical material is produced and downstream where the product is purified. Assuring high quality products and high yields is key, and can be facilitated by real time monitoring. Challenges faced are the specific adjustment of the production based on the nutritional needs of the production organism, distinguishing between the product and process- and product-related impurities throughout the process.

These challenges are addressed from different angles, one of them is developing disposable, printed biosensors. Such sensors could be enzyme-based or with a passive biorecognition element to detect the product. Another approach is to combine multiple sensor signals into mathematical models to estimate unknown variables. Mechanistic understanding can be incorporated as well to describe the physical phenomena of the production process.

By combining biosensors and soft sensors into a framework to monitor the production of biopharmaceuticals, process understanding can be improved and real-time process control can promote high yield and quality of biopharmaceutical products.

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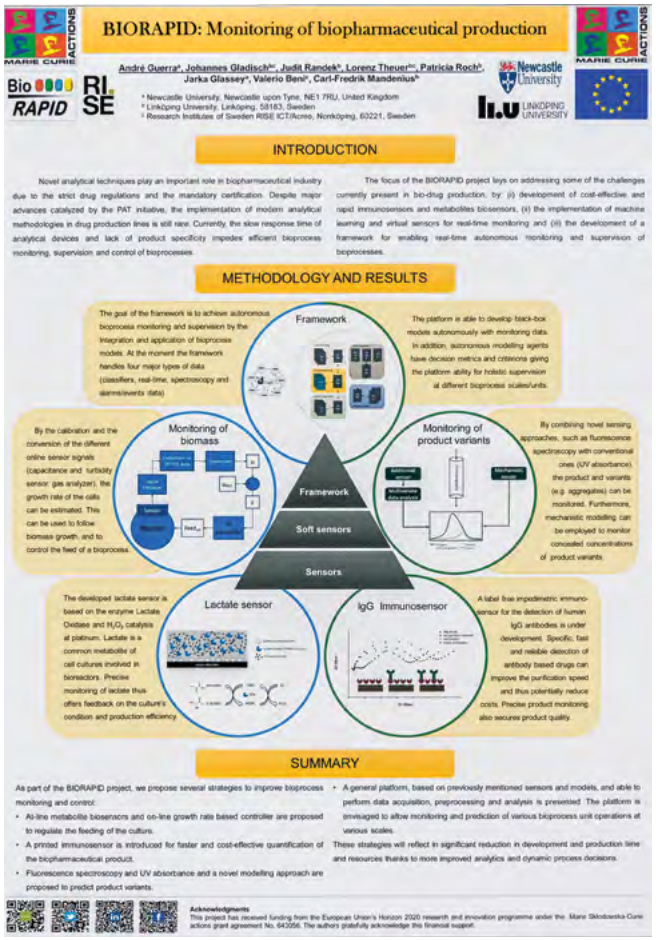

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Model-based Distributed Sensor Fusion for MAGV State and Parameter Estimation

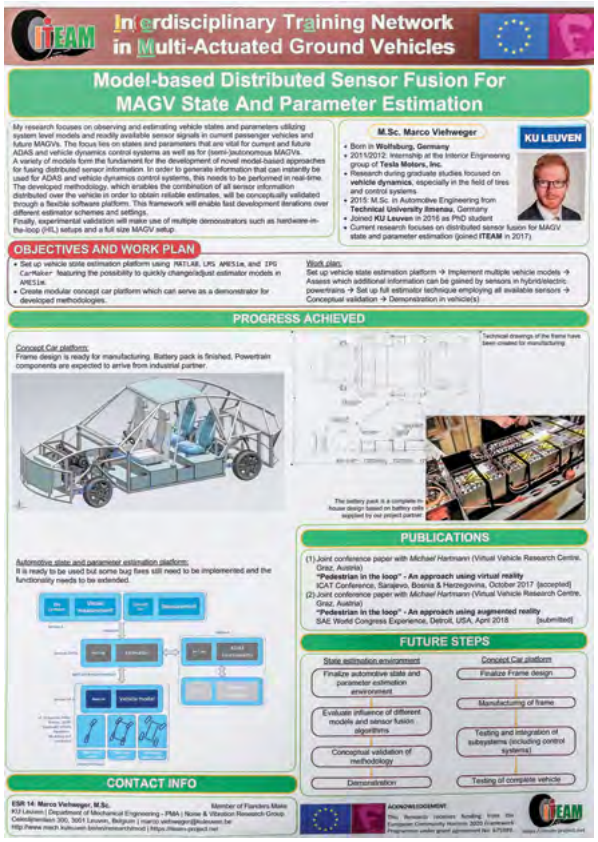
This project is part of the Interdisciplinary Training Network in Multi-Actuated Ground Vehicles (ITEAM). ITEAM is aiming at establishing and sustainably maintaining the European training network with a high grade of interdisciplinarity by training strong specialists to research and develop cutting-edge technologies in the field of multi-actuated ground vehicle (MAGV). In this framework, the ITEAM consortium sets out to foster the development of new hardware and software solutions to enhance the driving performance, to improve the vehicle safety, and to reduce the pollutants emissions.

Within the ITEAM project, my research focuses on observing and estimating vehicle states and parameters utilizing system level models and readily available sensor signals in current passenger vehicles and future MAGVs. The focus lies on states and parameters that are vital for current and future ADAS and vehicle dynamics control systems as well as for (semi-)autonomous MAGVs.

A variety of models form the fundament for the development of novel model-based approaches for fusing distributed sensor information. In order to generate information that can instantly be used for ADAS and vehicle dynamics control systems, this needs to be performed in real-time.

The developed methodology, which enables the combination of all sensor information distributed over the vehicle in order to obtain reliable estimates, will be conceptually validated through a flexible software platform. This framework will enable fast development iterations over different estimator schemes and settings.

Finally, experimental validation will make use of multiple demonstrators such as hardware-in-the-loop (HIL) setups and a full size MAGV setup.



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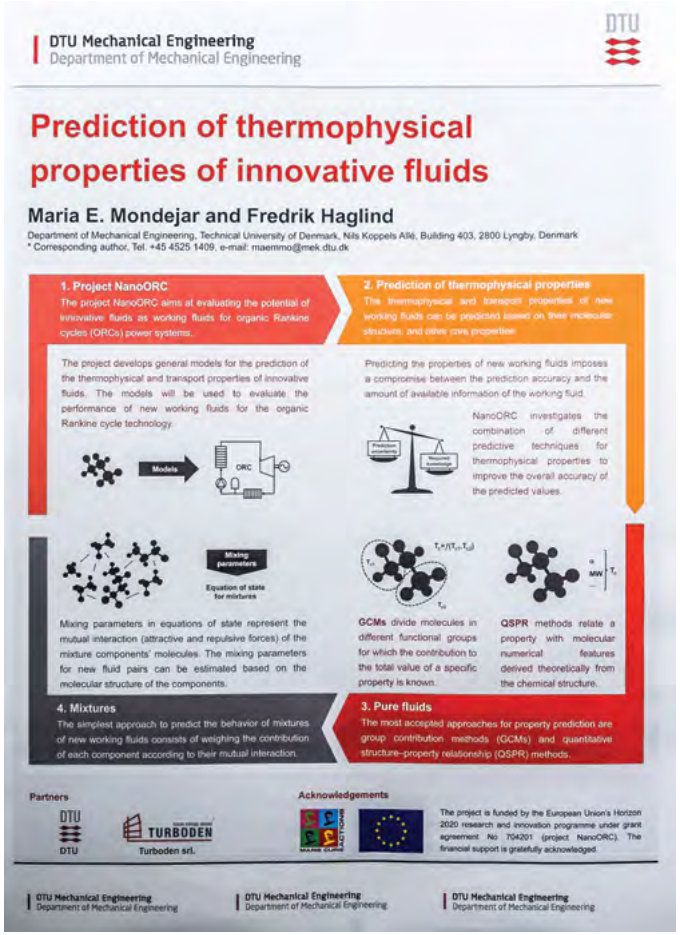
Prediction of thermophysical properties of innovative fluids

The introduction of new working fluids for organic Rankine cycle power systems requires the estimation of their performance based on the available knowledge about the fluids thermophysical properties. A good accuracy in the prediction of the thermophysical properties of the fluid will reduce the uncertainty in the simulation results, thereby providing more reliable results.

However, predicting the properties of new working fluids is complex, especially when only the molecular structure of the fluid is known. Generally, predictive models with higher accuracy require more knowledge about the fluid, and vice versa. This fact imposes a compromise between the accuracy of the prediction and the amount of information needed for the working fluid.

In the project NanoORC, the combination of different predictive techniques for thermophysical properties of fluids is investigated with the aim of improving their accuracy. The objective is to customize the predictive models depending on the nature of the fluid, minimizing the prediction uncertainty. This approach is also followed to extend the prediction capability of the models to mixtures of new working fluids. Based on this work, a number of tools will be developed for the study of the potential of new working fluids for organic Rankine cycle power systems.



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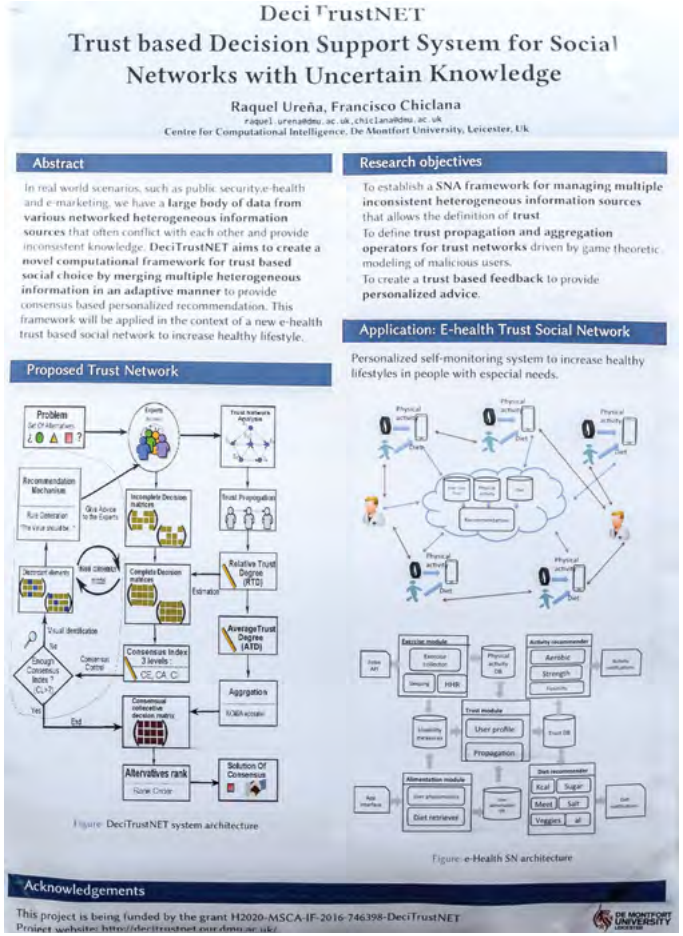
DeciTrustNET

In real world decision-making, such as public security, social choice or recommender systems, we have a large body of data from various networked heterogeneous information sources or individuals that often conflict with each other and provide inconsistent knowledge. It is a challenging task to yield an optimal consensus decision, given the range of individual decisions obtained in terms of these knowledge sources. This research proposal aims to create a novel mathematical and computational framework for trust based social choice in networks and with uncertain knowledge by merging multiple individuals' preferences in an adaptive manner to reduce the disagreements among them, and automatically seek a decision or provide a recommendation with a maximal consensus. To achieve our goal, we propose to bring together, for the first time, four previously disparate strands of research: social network analysis, fuzzy preference modelling, multiple attribute group decision-making and game theoretic modelling of malicious users. As a showcase the proposed framework will be incorporated to an e-health recommender platform to increase healthy lifestyle.



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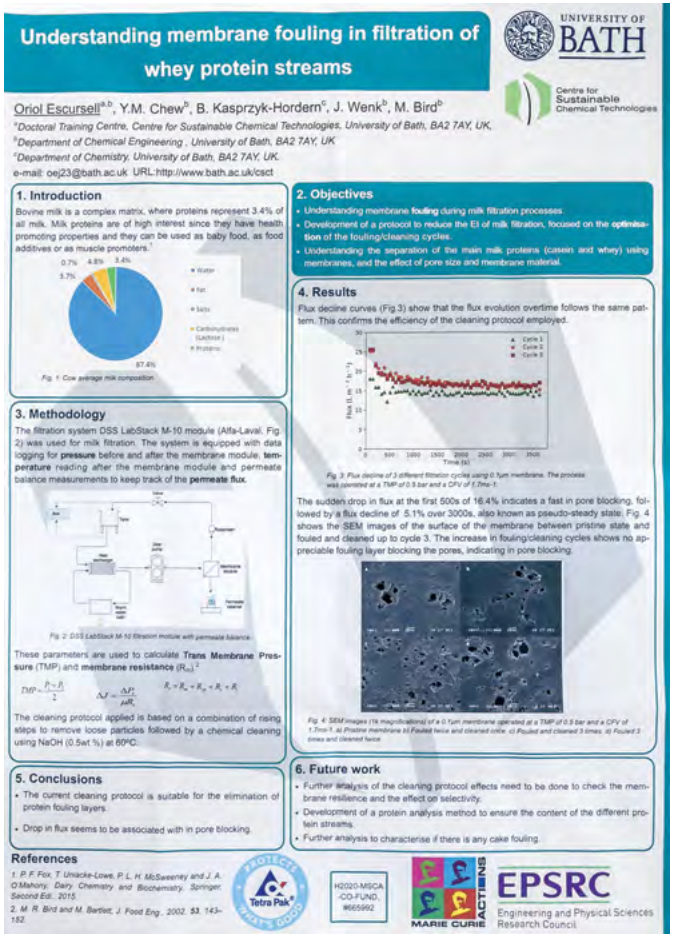
Membrane fouling during microfiltration of casein and whey fractionations

Environmentally friendly, economical and sustainable methods of food processing are required due to the projected growth in global population, and the current environmental impacts linked to food production. In the case of dairy products, the need to separate the main milk proteins - casein and whey, has led to the development of several technologies. The potential advantages of using membranes over chemical separation techniques has made them an attractive option for the food industry. However, it is important to be able to understand the fouling present, and being able to use it in the best way to optimize both fractionation and flux.

The two main aspects to consider for membrane separations are the selectivity of the process and the flux. Both of these parameters are affected by fouling. To determine membrane performance, fouling patterns have been studied by running pasteurized skimmed milk through two sets of commercially available polymeric PVDF membranes (800 kDa and 0.1 µm nominal pore size respectively, Synder Filtration). Filtration was carried out using a DSS M10 apparatus with four flat sheet membranes with a combined area of 336 cm2



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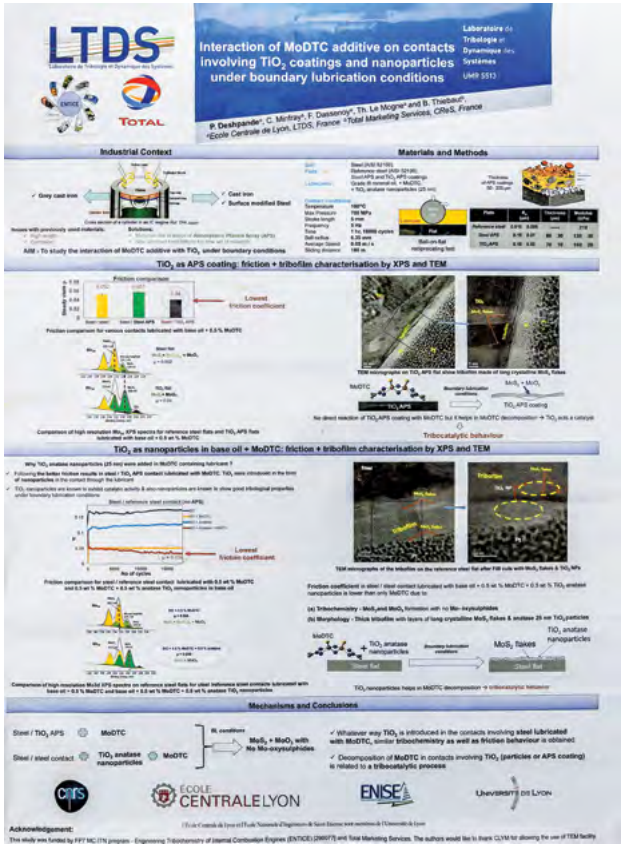
Interaction of MoDTC additive on the contacts involving TiO2 based coating & nanoparticles under boundary lubrication conditions

Nowadays, to reduce weight, gas emission and oil consumption of the passenger car engines, Atmospheric Plasma Spray (APS) coatings like TiO2 APS coating are used on cylinder liner. For such coatings, fused and crushed micron sized powders of TiO2 are used in APS process to obtain 70 µm thick coatings on steel substrates with specific surface roughness parameters. MoDTC (Molybdenum Di-Thiocarbamate), an organometallic friction modifier additive, has been extensively used to reduce friction coefficient in engine components under boundary lubrication conditions. In this study, tribochemical interaction of MoDTC with TiO2 APS coating was investigated. MTM tribotests were carried out for steel / steel and steel / TiO2 APS contacts in presence of lubricant containing MoDTC. Tribofilms generated on the steel and TiO2 discs were analysed by XPS (X-ray Photoelectron Spectroscopy) and TEM (Transmission Electron Microscopy).
Steel / TiO¬2 APS contact showed significant friction reduction compared to steel / steel contact due to specific tribochemistry and morphology of the tribofim obtained. Following the lower friction coefficients obtained in case of steel / TiO2 APS contact and also to further investigate the interaction of MoDTC with TiO2 substrate, TiO2 was introduced in the form of anatase nanoparticles via a lubricant containing also MoDTC in the steel / steel contact. A blend was prepared with anatase nanoparticles and MoDTC in base oil and used as a lubricant in steel / steel contact. Further investigation of tribofilms was again done using XPS and TEM. TiO2 introduced in any form (APS coating or nanoparticles) in the contact showed similar trends of tribological behavior due to similar tribochemistries observed inside the tribofilms. The results obtained are discussed in detail and conclusions are made regarding the decomposition of MoDTC.

Keywords: Atmospheric Plasma Spray coatings, MoDTC, TiO2 APS and TiO2 anatase nanoparticles



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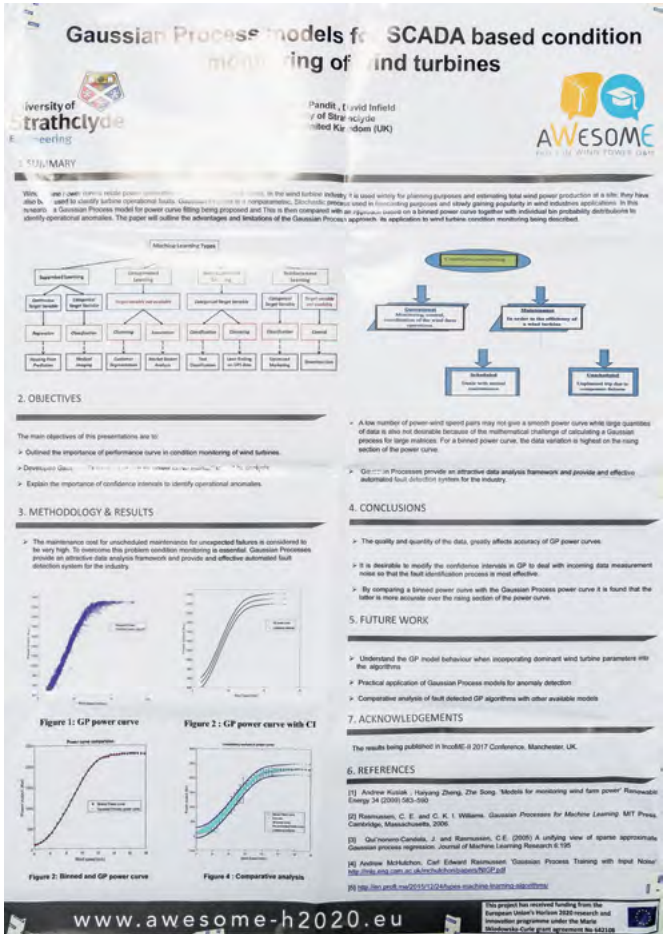
Gaussian Process models for SCADA based condition monitoring of wind turbines

Wind turbine power curves relate power generation to the hub height wind speed. In the wind turbine industry it is used widely for planning purposes and estimating total wind power production at a site; they have also been used to identify turbine operational faults. Gaussian Process is a nonparametric, Stochastic process used in forecasting purposes and slowly gaining popularity in wind industries applications. In this research, a Gaussian Process model for power curve fitting being proposed and This is then compared with an approach based on a binned power curve together with individual bin probability distributions to identify operational anomalies. The paper will outline the advantages and limitations of the Gaussian Process approach. its application to wind turbine condition monitoring being described.



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BIORAPID: Modelling tools in bioprocess development

Knowledge- and data-driven modelling methods are applied for early process development of microbial and mammalian manufacturing processes in work package 2 of the BioRapid project (www.bio-rapid.eu). Advanced process modelling together with rapid data acquisition methods are needed in the biotechnological industry for e.g. process development, on-line process monitoring and control, and the evaluation of high-throughput (HT) experiments. Machine learning (ML) algorithms are promising for data analysis since they are automatic, efficient, and fast, which is especially relevant for large amounts of data from HT experiments. ML algorithms (e.g. partial least square (PLS) regression) were established as scripts to be used on dedicated data sets. In our first case study, HT ambr250 bioreactor data was used to evaluate the impact of critical process parameters (CPP) on key process indicators (KPI). In the second case study, a knowledge-driven model was applied as software sensor in bacterial fermentations. It read the available on-line measurements, and predicted among other things the microbial growth. These software sensors allow plant operators a risk-based decision-making since the probability of achieving the critical quality attributes (CQA) is calculated in real time. In the third case study, data-driven models were used to design the processing routes in the manufacturing of pharmaceuticals. The models incorporated the information about the antibody structures and process knowledge in order to predict e.g. the stability of the protein, and the probability of aggregation under different operation conditions. The developed models and toolboxes aim to support the risk assessment in the existing bioprocess development frameworks, e.g. Quality by Design (QbD), and to reduce the development costs by reducing the necessary number of experiments.

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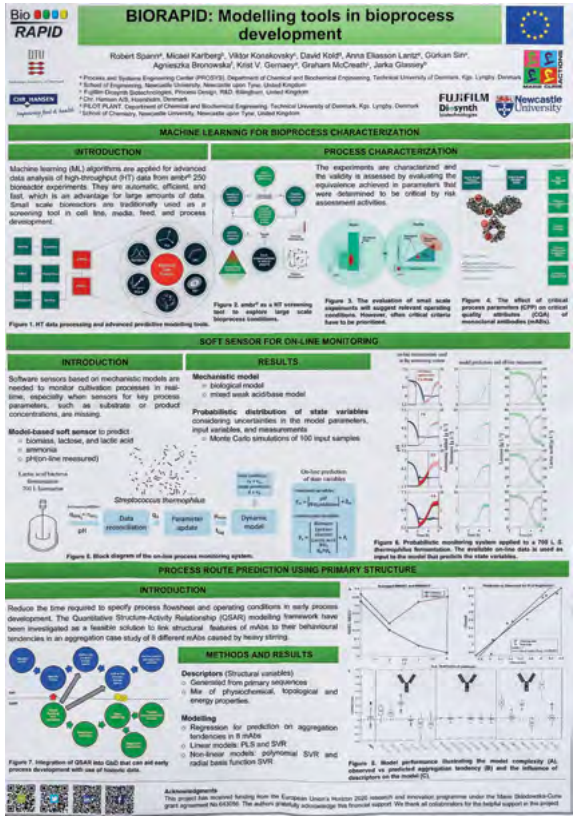

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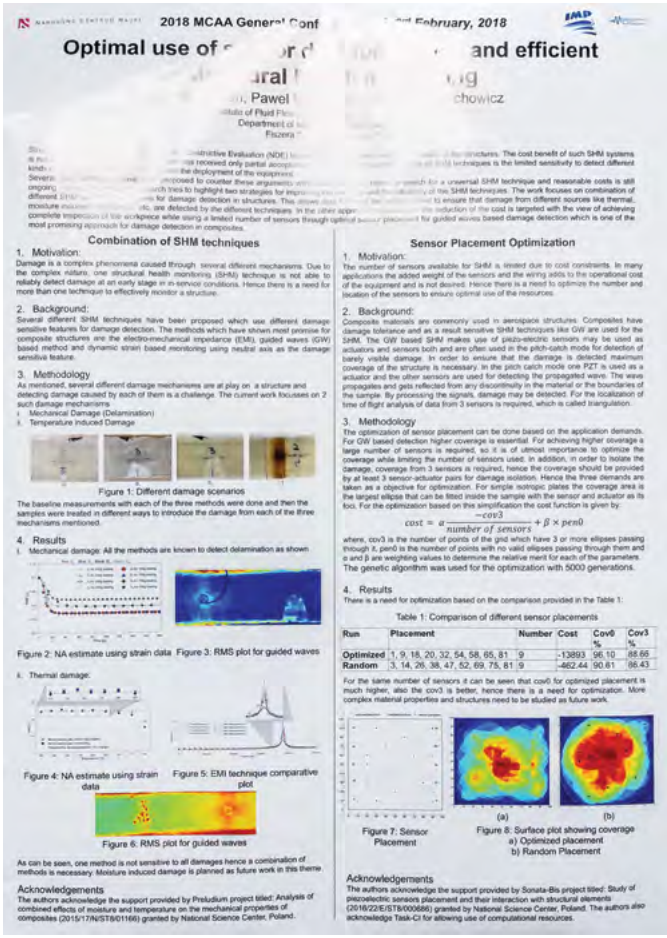
Optimal use of sensor data for reliable and efficient structural health monitoring

Structural Health Monitoring (SHM) and Non Destructive Evaluation (NDE) techniques improve the safety and reliability of the structures. The cost benefit of such SHM systems is not always apparent and hence the field has received only partial acceptance. The arguments against the use of SHM techniques is the limited sensitivity to detect different kinds of damage and relatively high cost of the deployment of the equipment.

Several SHM techniques have been proposed to counter these arguments with limited success. Hence a search for a universal SHM technique and reasonable costs is still ongoing. Hence the proposed research tries to highlight two strategies for improving the reliability and the efficiency of the SHM techniques. The work focuses on combination of different SHM and NDE techniques for damage detection in structures. This allows data fusion at the decision level to ensure that damage from different sources like thermal, moisture induced, mechanical, etc. are detected by the different techniques. In the other approach the issue with the reduction of the cost is targeted with the view of achieving complete inspection of the workpiece while using a limited number of sensors through optimal sensor placement for guided waves based damage detection which is one of the most promising approach for damage detection in composites.



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Using Social Paradigms In Smart Cities Mobile Context-Aware Computing

Mobile context-aware computing is an essential component of the smart cities infrastructure. Attempts were made to develop a model that can effectively represent a system in device to support context-aware behavior. My research is aimed to contribute with a model enabling a dynamic integration of mobile devices into a context-aware system. A software prototype is being built to demonstrate the model's plausibility.

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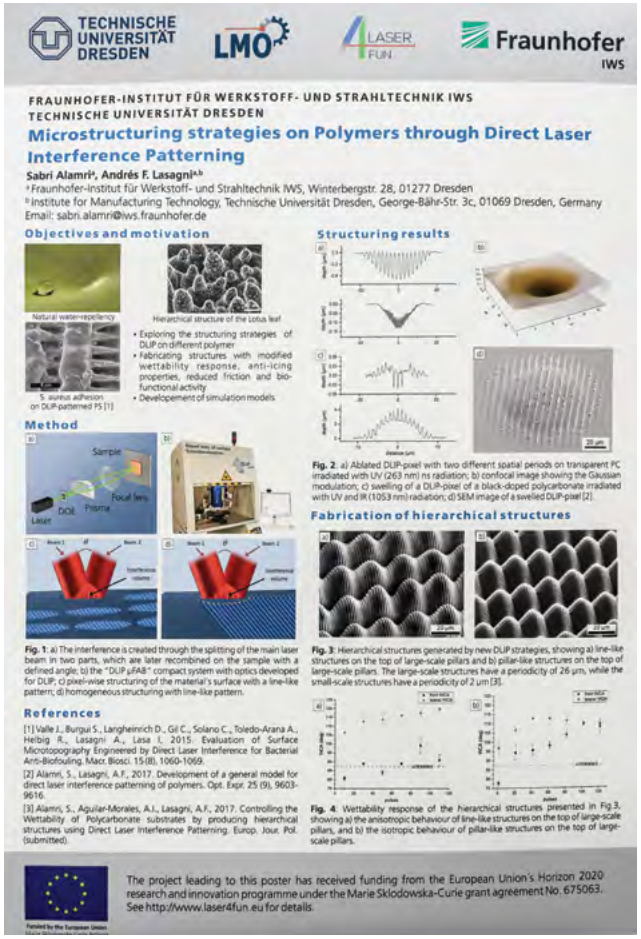
Microsctructuring strategies on Polymers through Direct Laser Interference Patterning

The control of the wettability can be performed either by changing the surface chemical composition or by modifying its roughness. In addition, it has also been demonstrated that the presence of hierarchical micro- and nano-structures allows radically changing the material wetting behavior, especially for reaching the super-hydrophobicity regime. Moreover, highly oriented structures permit controlling the wetting in a desired direction, property of great interest in the micro-fluidics sector.

In this study, we demonstrate how Direct Laser Interference Patterning (DLIP) can be employed to fabricate hierarchical structures on polycarbonate. In particular, new strategies for interference structuring are presented, in which high depth hierarchical microstructures with selective wetting properties can be created within a single step process. The experimental setup consists of a compact system designed for a two-beams DLIP, operating at the wavelength of 263 nm and producing line-like structures with a spatial period of 2 µm. Polycarbonate sheets have been selected due to its stable and characteristic structuring behavior with UV radiation and the structuring method can be extended to other materials which behave similarly. Combining common structuring strategies employed for Direct Laser Writing and DLIP, hierarchical structures with diverse depth, shape and pattern orientation have been fabricated. The results have been characterized by confocal microscopy, scanning electron microscopy, and the wettability behavior by the static water contact angle. The assessment showed a clear correlation between structure geometry and wettability response, in terms of structure height and directionality of the droplet shape. Moreover, due only to the laser processing, the static water contact angle has been increased from 87.8° ± 0.4° to 117.6° ± 1.8°.



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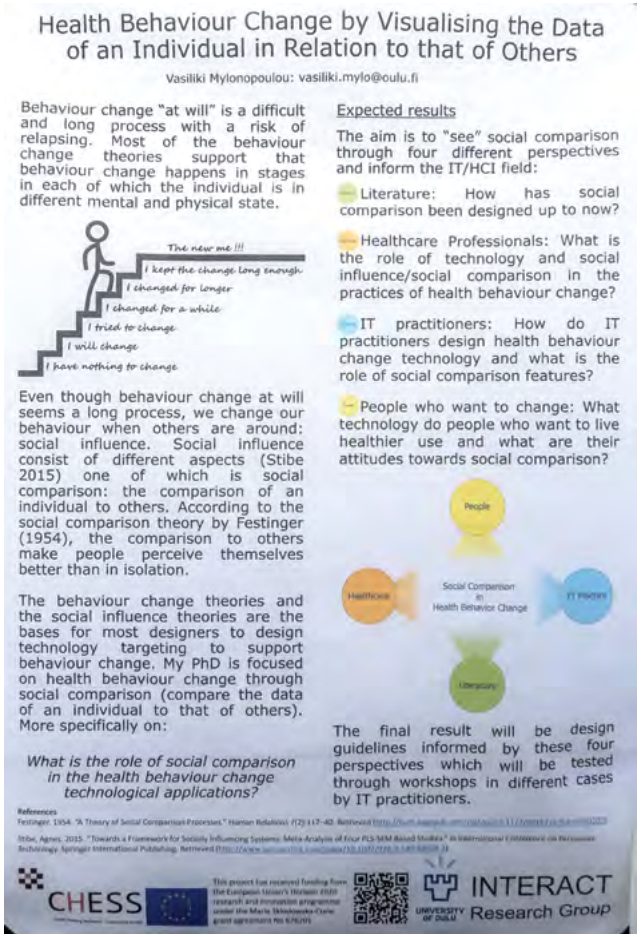
Health Behaviour Change by Visualising the Data of an Individual in Relation to that of Others

Behaviour change is a long and difficult process. However, we change our behaviour subconsciously when other people are around. Technological applications targeting behaviour change include features that facilitate social influence: the other people's influence on our behaviour. The social influence features have been designed - until recently (2015) - as a whole, without taking into consideration the different aspects of social influence (e.g. social comparison, social learning, cooperation etc.).

This research focuses on the social comparison aspect and the design of social comparison features in technological applications targeting to support health behaviour change. The methodology used is qualitative (participant observations, and interviews). The result will be a tool for designing social comparison features on health behaviour change technological applications, informed by four perspectives:

- how the current literature presents the design of social comparison features
- how the designers currently design social influence features (focused on social comparison)
- what is the healthcare professionals opinion on social comparison and relevant health behaviour change technology
- what kind of data the users want to compare, and how they want to compare them



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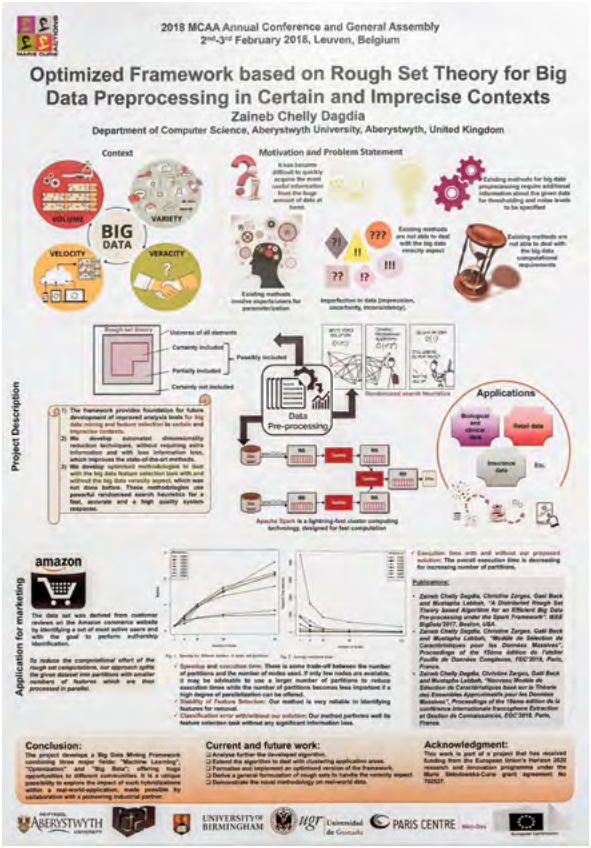
Optimized Framework based on Rough Set Theory for Big Data Preprocessing in Certain and Imprecise Contexts

Over the last decades, the amount of data has increased in an unprecedented rate, leading to a new terminology: “Big Data”. Big data are specified by their Volume, Variety, Velocity and by their Veracity/Imprecision. Based on these 4V specificities, it has become difficult to quickly acquire the most useful information from the huge amount of data at hand. Thus, it is necessary to perform data (pre)processing as a first step. To achieve this task, several state of the art methods were proposed. However, most of them require additional information about the given data for thresholding, specify some noise level, and are neither able to deal with the big data veracity aspect nor with their computational requirements. Therefore, this project’s overarching aim is to fill these major research gaps with an optimized framework for big data (pre)processing in certain and imprecise contexts. To achieve this, we propose innovative techniques capable of discovering data dependencies using the data alone requiring no additional information. These novel proposed solutions are based on Rough Set Theory for data (pre)processing and Randomized Search Heuristics for optimization.

The project combines the expertise of the experienced researcher Dr Zaineb Chelly Dagdia in machine learning, rough set theory and information extraction with the knowledge in optimization and randomized search heuristics of the supervisor Dr Christine Zarges at Aberystwyth University, UK. Further expertise is provided by internal and external collaborators from academic and non-academic institutions, namely Prof Lebbah (University of Paris 13, France), Prof Shen (University of Aberystwyth, UK), Prof Tino (University of Birmingham, UK), Prof Merelo (University of Granada, Spain) and an industrial partner from France to ensure that real-world requirements are met throughout the development of the framework.



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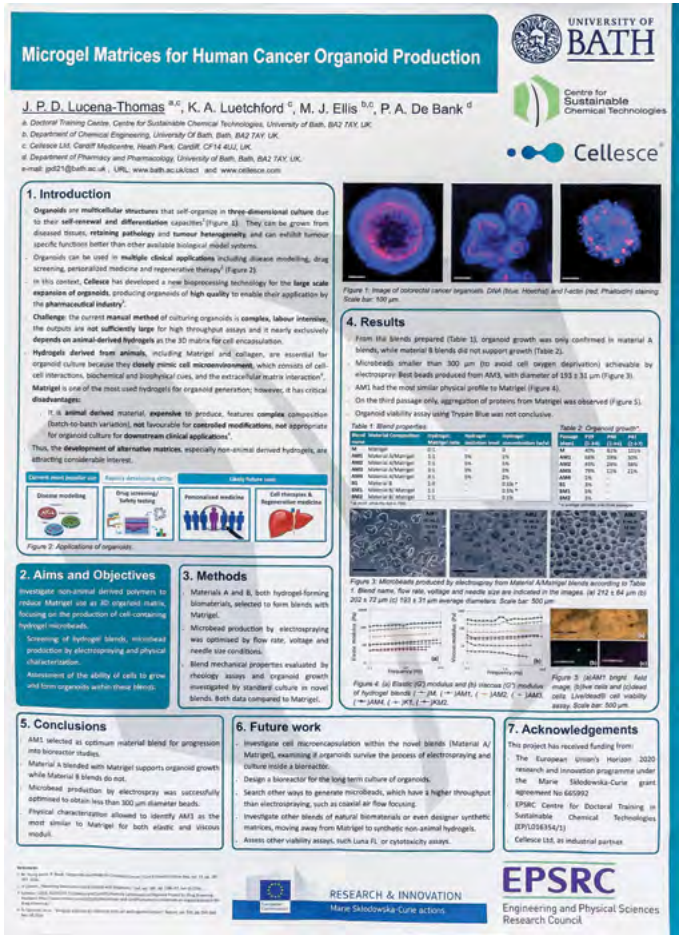
Microgel Matrices for Human Cancer Organoid Production

Organoids are three-dimensional multicellular structures capable of mimicking tissue structure and tumour heterogeneity better than other available biological model systems. They are a powerful new enabling technology in drug discovery because they can give more accurate test results while enabling high throughput screening of drug candidates. However, traditional manual culture and expansion of organoids is labour intensive and expensive. In order for organoids to be widely used in industrial and clinical applications, their robust production must be scaled up efficiently. Cellesce Ldt has developed a process to grow large numbers of organoids for commercial drug screening but the methods rely heavily on very expensive animal-derived matrix scaffolds for organoid encapsulation, mainly Matrigel. These materials are both expensive to produce and are prone to batch-to-batch variations in the bioactive molecules which they contain. In this research, non-animal derived polymers were investigated to reduce Matrigel use as 3D organoid matrix, focusing on the production of cell-containing hydrogel microbeads. Alginate and carrageenan, both seaweed derived hydrogel-forming biomaterials, were selected to form blends with Matrigel, thus providing a more sustainable and cost-effective means of organoid generation. The microbeads were produced by electrospraying and compared in terms of their physical properties. Finally, the ability of the cells to grow and form organoids within these blends was assessed and compared with the current method using Matrigel. This study concluded that the oxidised alginate-based blends were the only ones that supported organoid growth, with the 2% (w/v) 5% oxidised alginate/Matrigel (1:1) being the optimum blend among the others. The main outcome of this research will be the basis for future bioreactor and scale-up studies.



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Adaptable Games that Support the Delivery of Mental Health Interventions to Children

Growing evidence suggests that appropriately designed computer games can support effective and engaging mental health interventions for young adolescents. But to have widespread impact, games need to be adaptable. During my research project, I will conduct user studies and an in-depth literature review about the design process and current state of the art of supporting technology for mental health for youth. Subsequently, my focus will shift to exploring ways to add adaptability to mental health games such as Pesky gNATs, a 3D computer game that implements cognitive behavioural therapy (CBT) that clinicians and children can play together during therapy sessions. The goal is to re lease a game that is widely applicable and can be used across a wide range of client groups, disorders, intervention models and intervention intensities by introducing flexibility in game design and gameplay. For example, clinicians could be allowed to adjust the game to individual needs of the children and the therapy context.

As part of the training, I will undertake two secondments: a 3-month secondment at the Anna Freud Centre will provide me with practical knowledge on topics related to children's mental health issues and the applied intervention models. I will also use the secondment to engage in participatory design and prototyping sessions with children. Subsequently, I will engage in a 3-month secondment at Opposable Games to build on my knowledge and skills that are required to develop games. After finishing the secondments, the game development phase starts after which the result will be assessed through prototype demos and interviews with therapists. The knowledge gained before, during and after the research and development will be added to the PhD thesis.

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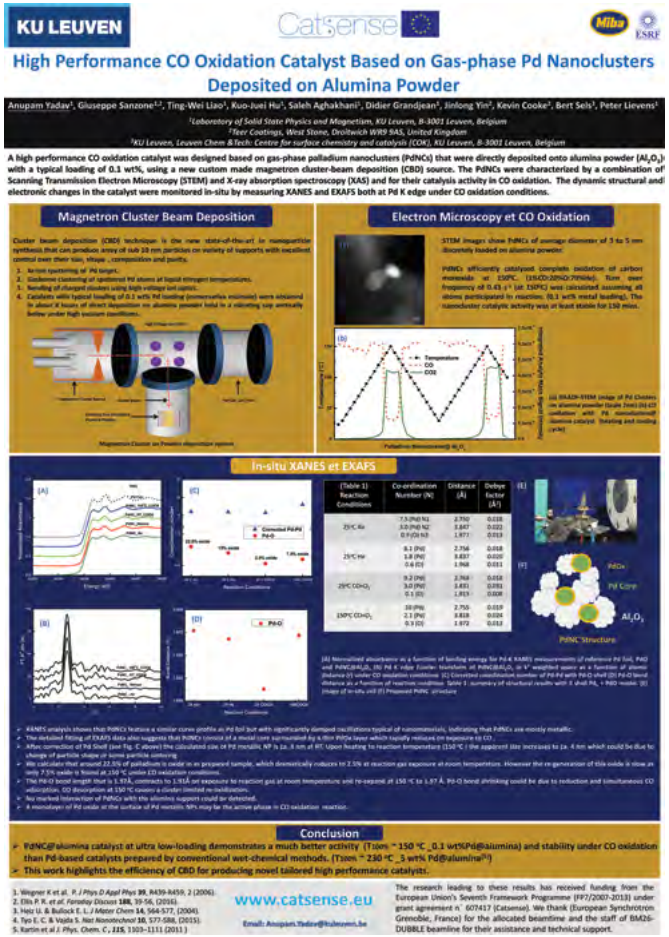
High Performance CO Oxidation Catalyst Based on Gas-phase Pd Nanoclusters Deposited on Alumina Powder

A high performance CO oxidation catalyst was designed based on gas-phase palladium nanoclusters (PdNCs) that were directly deposited onto alumina powder (Al2O3) with a typical loading of 0.1 wt%, using a new custom made magnetron cluster-beam deposition (CBD) source. The Pd-NCs were characterized by a combination of Scanning Transmission Electron Microscopy (STEM) and X-ray absorption spectroscopy (XAS) and for their catalysis activity in CO oxidation. STEM investigations confirmed that ligand free PdNC's with an average size of 3-5 nm were discretely loaded on alumina powder. The dynamic structural and electronic changes in the PdNC catalyst were then monitored in-situ by measuring XANES and EXAFS both at Pd K edge under CO oxidation conditions and it revealed that PdNCs possess a unique PdOx@Pd structure, interacting weakly with the alumina support. PdNC's catalyst demonstrates a much better activity and stability under CO oxidation, in comparison to Pd catalysts prepared by conventional wet-chemical methods.



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Arsenolipids are not evenly distributed within brown macro-algae Saccharina Latissima

Seaweed and seafood have naturally high concentrations of total arsenic compared to agricultural produce. Arsenic is thought to accumulate in seaweed because of structural similarities of arsenate and phosphate as phosphate transporters can mistake arsenate for phosphate due to lack of specificity. However, arsenic is not found in the form of toxic arsenate in seaweed but mainly as arsenosugars. Seaweed has also been shown to contain a significant proportion of arsenic in the form of arsenolipids (AsLp), i.e. hydrocarbons (AsHC), fatty acids (AsFA) and phospholipids (AsPL). Arsenic is often grouped as either inorganic arsenic (iAs: arsenate & arsenite) or organic arsenic, where iAs is a class I carcinogen but the organic arsenic has been considered less toxic. However, recent studies show that arsenolipids can be as toxic as the iAs. To date little is known about AsLps in seaweed, partly due to difficulties associated with the measurements of these compounds, and more information is urgently needed. Here over 50 individuals of Saccharina Latissima were collected and pooled together, partitioned into different parts of the seaweed (holdfast, stipe, old frond, young frond, sporangia) and analysed for AsLps and arsenosugars.

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Structural and Functional Comparison of Low-Molecular-Weight Thiols

Low-molecular-weight (LMW) thiols play a key role in many biochemical processes and can be found in a wide variety of organisms including prokaryotes, plants and, mammals [1-3]. These special species protect living organisms against free radicals and participate in signal transduction, and the regulation of gene expression. As sulfur-containing natural compounds they can also serve as S-donors. One of the most important small molecule weight thiol is glutathione (GSH, γ-glutamyl-L-cysteinylglycine), a linear γ-tripeptide containing glutamic acid, cysteine and glycine. It is widespread in mammals and indispensable for the oxidative stress protection of the central nervous system of the living organisms.

The main purpose of this study is to determine the most important structural and functional properties of LMW thiols. For a selected set of species, a detailed comparison is presented based on the calculated properties of the molecules.

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Acknowledgements:

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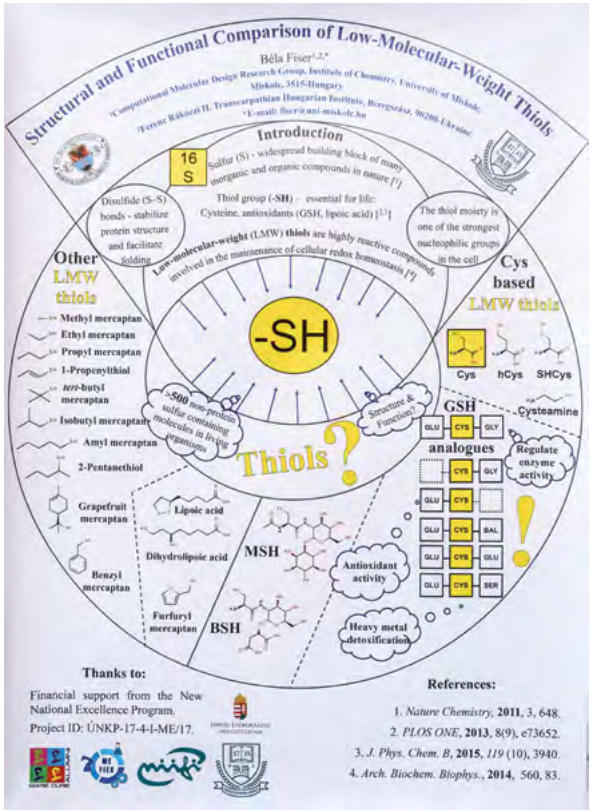

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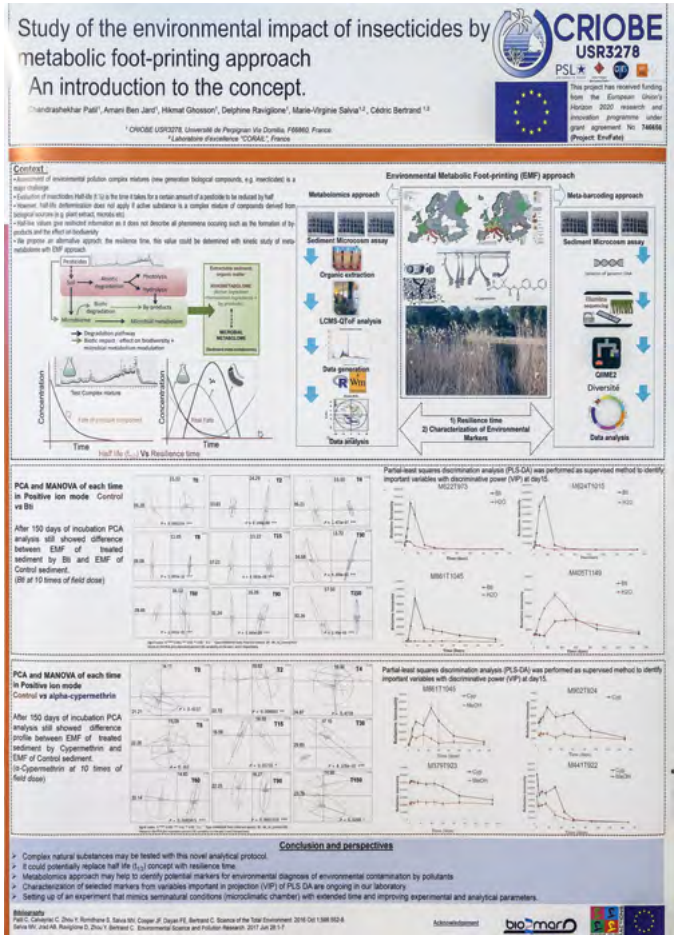
Study of the environmental impact of insecticides by metabolomic foot-printing approach - An introduction of the concept.

The European Directive in 1998 led to the increasing use of biological insecticides such as cry proteins produced by the bacterium Bacillus thuringiensis israelensis (Bti) that kill mosquito larvae after being ingested. Considering the interest in Bti as more environmentally sustainable biocide, it is important to examine environmental fate and impact of Bti especially taking into account the need of this information to fulfil the REACH criteria. The project 'EnvFate' aims to employ an innovative 'Environmental Metabolic Footprinting' approach, that spans the interface between chemistry and biology. To dynamically characterize biomarkers of Bti pollution found among metabolites issued from the sediment matrix meta-metabolome will require to develop and optimize detection protocols using LC-MS platform. In addition, metabarcoding approach will allow to understand microbial community responses to the Bti pollution. Emphasis will be placed on better standardisation, data interpretation and evaluation that will build confidence in the value of "omics technologies – this being essential to increase their (regulatory) use. These activities will advance our understanding of environmental risks associated with Bti, and pave the way for the development and adaptation to new environmental monitoring tool. EnvFate will thus increase the European research visibility to promote sustainable development, ensure the protection of environment, one of the priority areas of the H2020 program.

Here we are presenting sensible preliminary findings to convince the application of concept to evaluate the environmental impact of complex insecticide mixtures.



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NMR analysis of cyclodextrins as stability enhancers for chiral pyrethroids

Malaria, Zika virus, dengue fever and yellow fever are mosquito transmitted diseases for which vaccines either do not exist or are not widely available. Prevention control is the main way to reduce their spread, and the World Health Organisation recommends the use of insecticides as a key prevention measure.

Pyrethroids are one of the best insecticides for public health use, but they suffer from stability issues mainly related to the occurrence of hydrolysis and photodegradation, which particularly involve the chiral centers. There is a strong correlation between the enantiomeric composition and the biological activity of pyrethroids, it is therefore very important to find a way for improving their stability.

In the attempt of enhancing both chemical and stereochemical stability of chiral pyrethroids over time, cyclodextrins were tested as stability agents, thanks to their tendency to host molecules within their cavity. Cyclodextrins are already known as pyrethroids solubility and stability enhancers [1-3], but at the best of our knowledge this interaction was not investigated via NMR spectroscopy so far. Native cyclodextrins and b-cyclodextrin derivatives were then tested as stability and solubility enhancers of deltamethrin, which was chosen as probe among the other pyrethroids for its high insecticidal activity and its low stereochemical stability.

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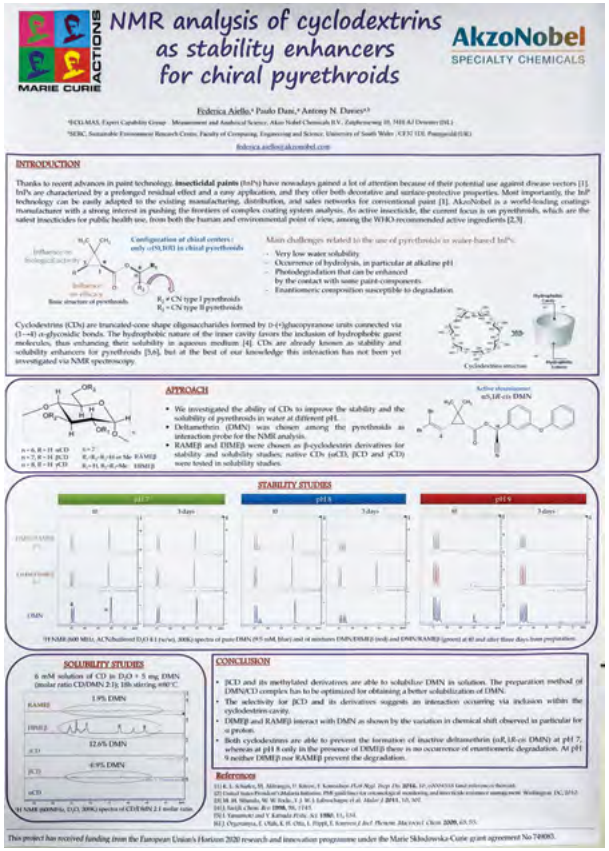

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Halide perovskites for photovoltaic applications

More than 80% of the world's primary energy still comes from fossil fuels [1]. Tackling renewable energy sources is one of the first significant solution to achieve a sustainable development. The sun is the primary source of energy on our planet Earth and it can be directly converted into electricity through photovoltaic systems. One of the most exiting discoveries in photovoltaic research right now are halide perovskite solar cells.

Since the emergence of halide perovskite solar cells in 2012 [2,3], improvements in film morphology and fabrication techniques have led to a power conversion efficiency (PCE) of 22.1% [4]. What prevents halide perovskites to be already available on the market are toxicity issues and lack of stability. Perovskite materials suffer from very fast degradation when exposed to water or even moisture in the air. Ensuring the long term stability of perovskite solar cells under ambient conditions remains a big challenge in the field.

My PhD looks at different ways to improve the stability of the device. On the one hand, different hydrophobic interlayers that delay the degradation have been investigated. On the other hand, the long-term stability of the device was improved by changing the chemistry of the absorber layer. The stability of devices stored in ambient conditions was enhanced by the presence of an extra cation (tetrabutylammonium – TBA) and cells with high mol% TBA were found to have reasonable efficiencies while being semi-transparent [5].

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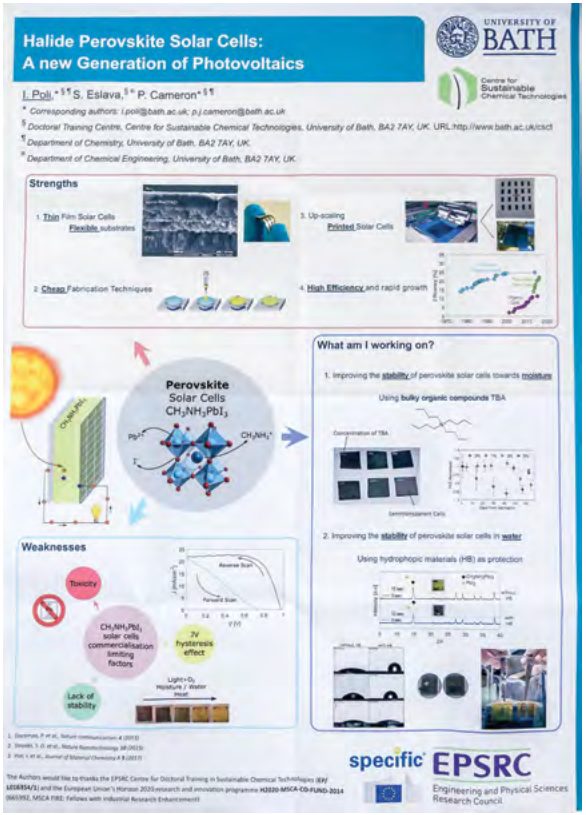

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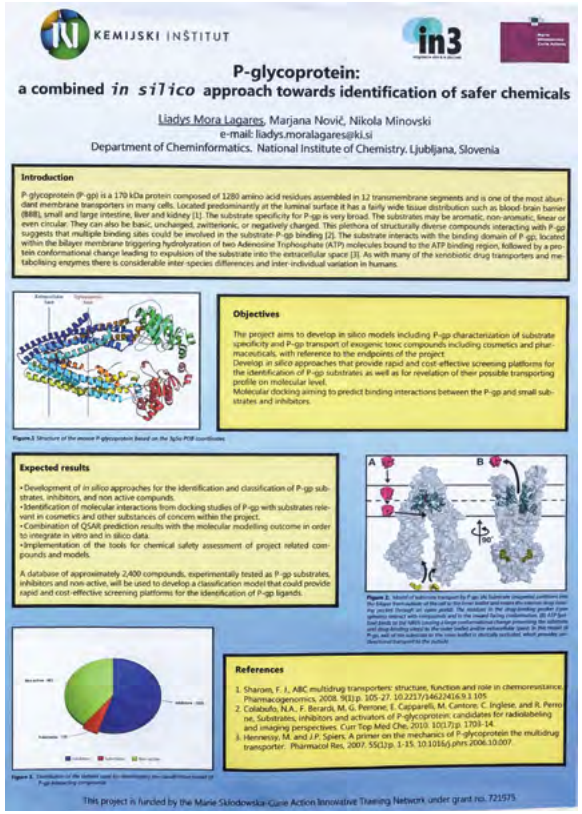
P-glycoprotein modelling: New methodology of combining molecular modelling with in silico models for safer chemicals

P-Glycoprotein (P-gp) is a transmembrane protein, playing significant roles in the process of drug discovery. P-gp affects absorption, distribution, and elimination of different compounds and is mainly expressed in intestines, liver, kidneys, heart, colon, and placenta. The expression of P-gp in the blood-brain barrier has been associated with the restricted access of many compounds to the central nervous system. P-gp is responsible for resistance of cells to exogenous agents, particularly the anticancer drugs, giving rise to the multidrug resistance phenomenon by mediating the active transport of these drugs from the intracellular to the extracellular compartment. Increased expression of P-gp is also implicated in decreased HIV drug availability at certain intracellular sites. Moreover, studies showed that P-gp contributes to resistance to pesticides in certain pest species, and to decrease toxicity by removing compounds from cells in mammals. Due to the previous reasons, it is advisable in the drug discovery process to pay attention to the likelihood of a compound under development being transported by P-gp, since this contributes to whether a compound actually reaches its intended target or is removed from the cell before exerting its action.

The project aims to develop improved in silico models including P-gp characterization of substrate specificity and transport of exogenous chemicals. The development of in silico approaches could provide rapid and cost-effective screening platforms for the identification of P-gp substrates or inhibitors. Theoretical models of P-gp transport mechanism involve pharmacophore modelling and molecular docking aiming to predict the binding interactions between the protein and small substrates and inhibitors. The outcome of the molecular modelling is going to be combined with the predictions resulting from QSAR models developed within the project. The in vitro studies performed by project partners are going be used and compared with the in silico results for generating a two way optimization.



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Methotrexate analogues ecodesigned for programmed self-destruction

Due to the high increase of medicines consumption during the last century, active pharmaceutical ingredients (APIs) are commonly found in the environment. Indeed, wastewater treatment plants (WWTP) are not generally prepared to deal with the tremendous variety of APIs and their metabolites, which allows them to reach natural aqueous environments and soils. Once released in the environment, APIs are likely to provoke toxic effects on organisms due to their intrinsic properties, wide variety, presence as a mixture, and chronic exposure. Anticancer drugs, being cytotoxic, genotoxic, mutagenic, carcinogenic, and/or teratogenic, are targeted as potential ecological stressors.[1] One strategy to reduce persistent APIs in the environment is to replace them with rationally designed molecules programmed to self-immolate after fulfilling their therapeutic purpose.[2]

Bearing all this in mind, methotrexate (MTX) was selected as the starting point of our novel approach of ecodesigned drugs. This compound, also used as a treatment for autoimmune diseases, is one of the most widely prescribed antitumor agents worldwide since the 40's. MTX is a folic acid analogue that competitively inhibits dihydrofolate reductase, interfering in the synthesis of DNA and cell replication. Because of its intensive usage and hydrophilicity, MTX has been detected in hospital and WWTP effluents in several countries.[3] The synthesis of eco-designed analogues of MTX and metabolites, together with their stability and biological studies will be presented.

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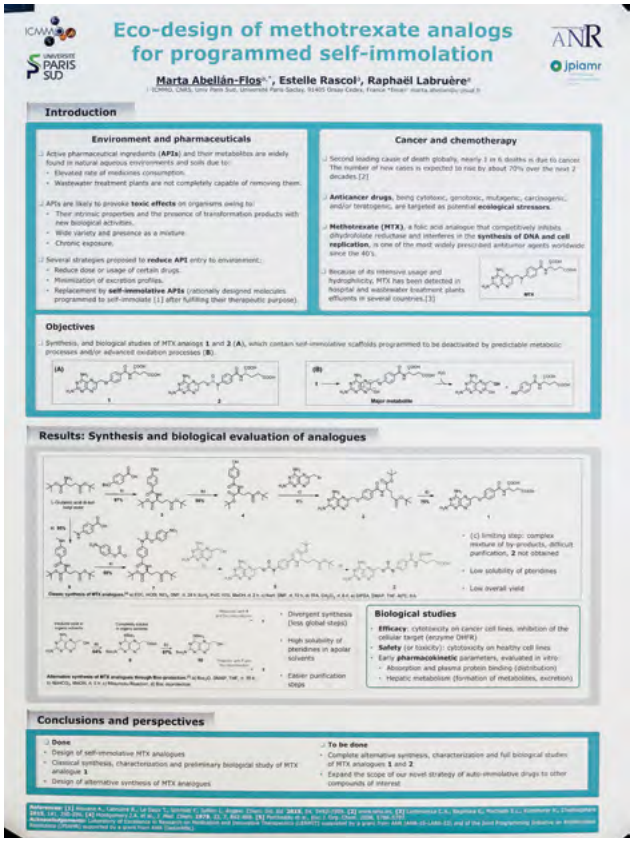

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Bio–nano convergence and science policy

The field of bio–nano science is at a crossroads. The last decade has seen tremendous advances in the development of new materials and in our understanding of biological interactions. Despite this, there is a growing realisation that "research as usual" may not be enough; that our current approach is neither the best way for facilitating impactful and robust exploratory research, nor for accelerating translational work. Moving forward we should ask: will "research as usual" get us to where we want to be? Encouragingly, there is an ongoing energetic discussion—involving researchers, funders, policy makers, and publishers—on how we can address these challenges. In this discussion, several key topics have emerged as part of research "convergence" [1–3]. Examples include areas such as: (i) the advantages of cumulative research; (ii) the necessity of aligning projects with research priorities; (iii) the value of transparent science; (iv) the opportunities presented by "dark data"; and (v) the importance of establishing bio-nano standards. Pursuing and adopting these areas require adjustments across research strategy and science policy, but we believe they are central for accelerating scientific discovery and translational research.
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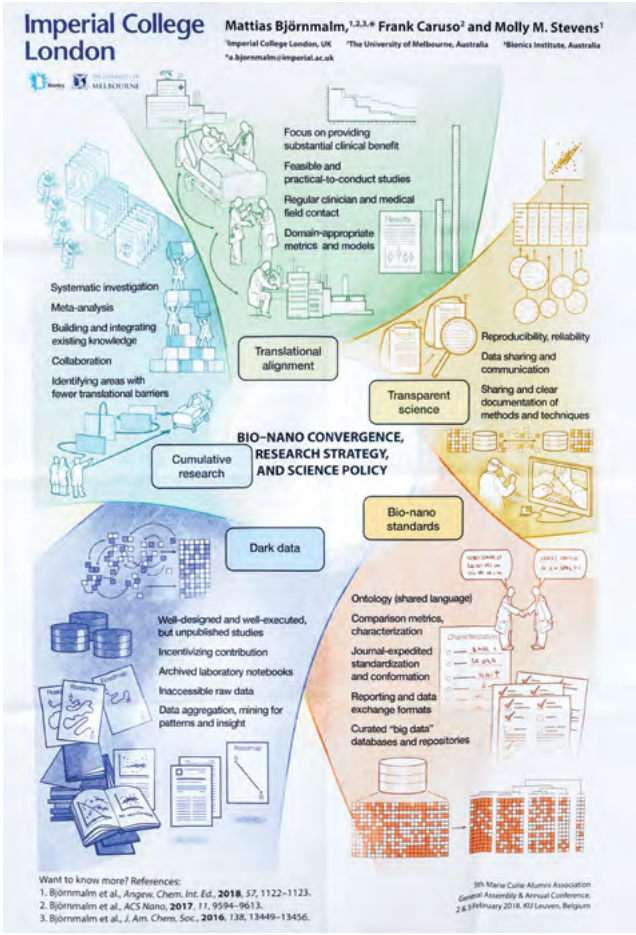

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Molecular design strategy for PH responsive two-component gel based on thermally activated delayed fluorescence emitter

Recently, OLEDs employing metal-free thermally activated delayed fluorescence (TADF) emitters have emerged as a cheaper alternative to phosphorescent OLEDs and biological application.1-5 Here we present an in-situ formation of two-component hydrogels from pyridine decorated benzophenone TADF compound and tartaric acid. The two component system (4PyCz + acid) undergoes aggregation, leading to a fibrillar-type self-assembly in THF-water mixture along with green (534 nm) emission. A new method is proposed to enhance the emission of the organic compound by supramolecular assembly. Interestingly colour and rigidity of the gel can be tuned by varying the additives (acid) and ratios of additives.

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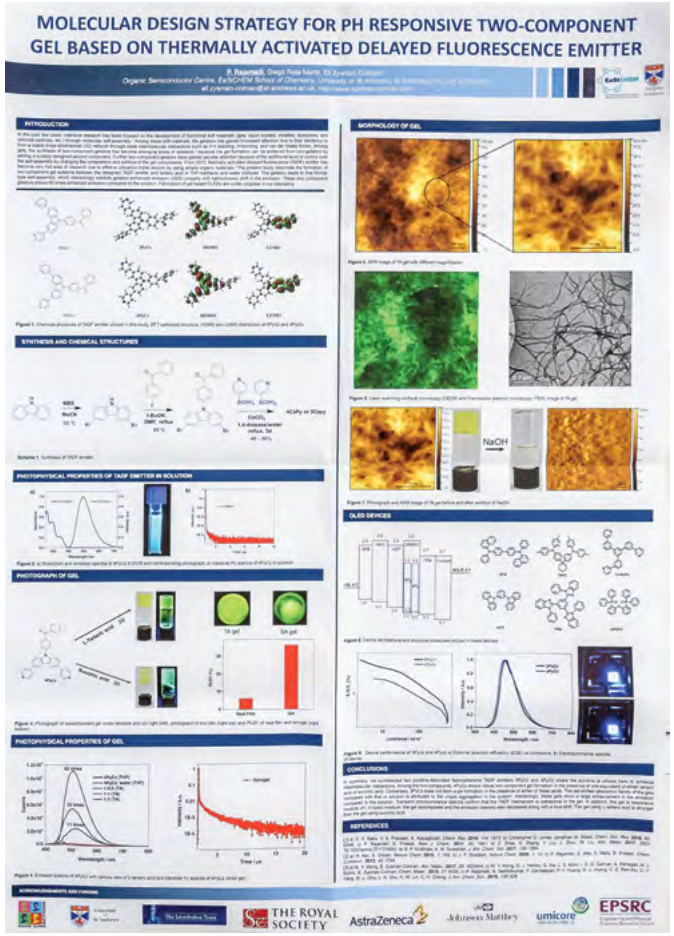

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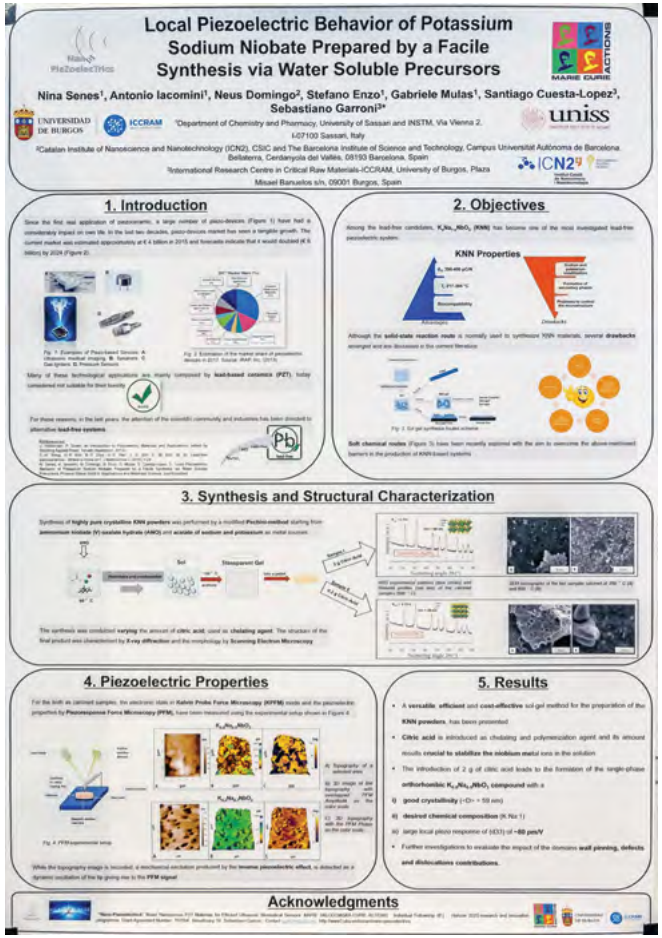
Local Piezoelectric Behavior of Potassium Sodium Niobate Prepared by a Facile Synthesis via Water Soluble Precursors

Due to the ever-increasing restrictions connected to the use of toxic lead-based materials, the developing of lead-free piezoceramics has become one of the most urgent tasks. In this context, potassium sodium niobate materials have attracted many attentions as promising candidates due to their excellent piezo properties and stability. For this reason, many efforts have been addressed to improve the synthesis process now suffering by several drawbacks including the high volatilization of potassium and sodium at the conventional high temperature treatments and the use of expensive metal precursors. To overcome these issues, a new modified Pechini method to synthesize single phase K0.5Na0.5NbO3 powders, from water soluble metal precursors, is here presented. Microstructural and structural parameters have been characterized by X-ray diffraction (XRD). Depending on the amount of citric acid added to the starting reagents, two pure single-phase K0.5Na0.5NbO3 (2g citric acid) and K0.3Na0.7NbO3 (0.2 g citric acid), respectively, were obtained with a good crystallinity at a moderate temperature of 500 °C. The piezo responses of the as calcined systems have been tested by piezoresponse force microscopy (PFM). K0.5Na0.5NbO3 exhibits a much higher response with respect to the other phase, which relates to the larger crystallinity and to the chemical composition.



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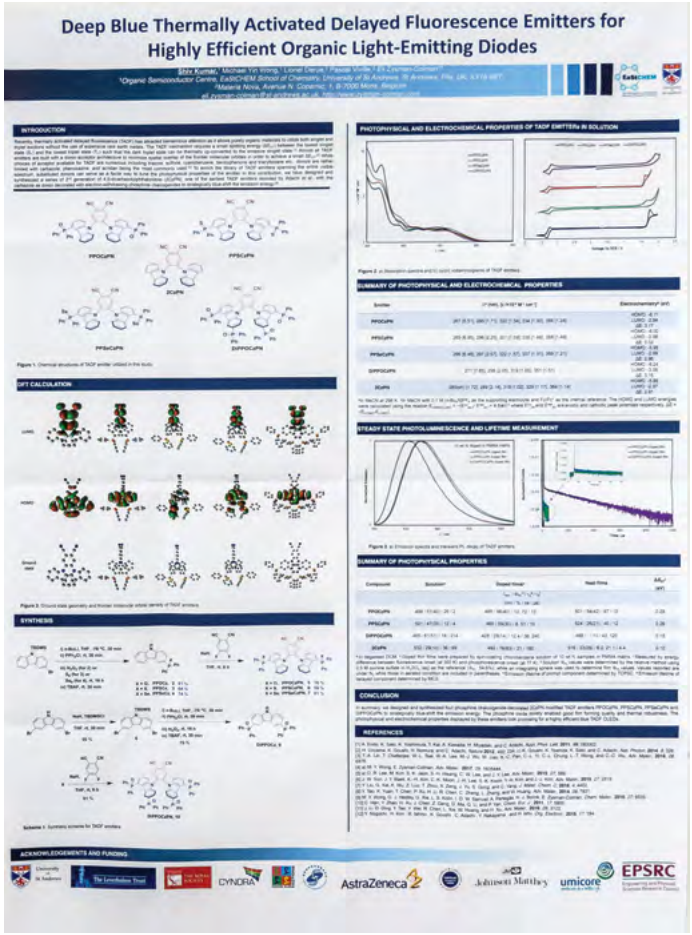
2nd Generation Deep Blue Thermally Activated Delayed Fluorescence Emitters for Highly Efficient Organic Light-Emitting Diodes

In recent years, organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) have emerged as the third-generation of OLEDs for displays and solid-state lightings. The most exciting feature of TADF-OLEDs is the harvesting triplet excitons using a pure-organic dye molecule with an efficient reverse intersystem crossing (RISC). An efficient RISC requires the singlet-triplet splitting (ΔEST) between the first singlet (S1) and triplet (T1) energy level to be small, generally less than 0.2 eV. So far, several sky blue TADF emitters have been reported in literature but the performance of deep blue TADF emitters still must be improved and their development is still in progress. We have employed the carbazole donors with electron-withdrawing phosphine chalcogenides substituents to strategically blue-shift the emission of the known sky blue TADF emitter 4,5-dicarbazolylphthalonitrile (2CzPN). We present calculations, synthesis, photophysical characterization and initial device results.



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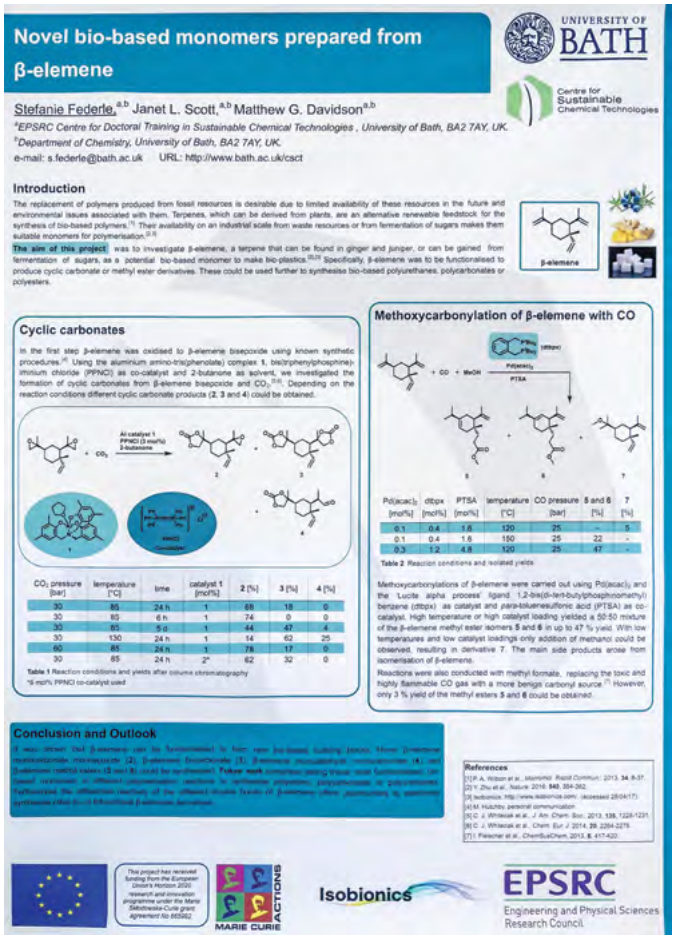
Novel bio-based monomers prepared from β-elemene

The replacement of polymers produced from fossil resources is desirable due to limited availability of this resource in the future and environmental issues associated with it. To address these issues, current research focuses on both the development of polymers from renewable resources and on the generation of biodegradable polymers. Terpenes, which can be derived from plants, have received interest as possible bio-based monomers, because they are abundant and furthermore some terpenes can be gained from waste products on an industrial scale. Their diverse hydrocarbon structures and the occurrence of double bonds offers the possibility for the synthesis of various polyolefins.

This project investigates how the terpene β-elemene can be functionalised to generate novel bio-based monomers for polymerisation. The β-elemene structure bears three double bonds providing a useful starting material for introducing different functional groups via reactions at these alkene moieties. It was shown that different β-elemene derivatives bearing epoxide, cyclic carbonate or methyl ester moieties can be produced. These β-elemene derivatives could be used further for polymerisation reactions to produce polycarbonates, polyurethanes or polyesters.



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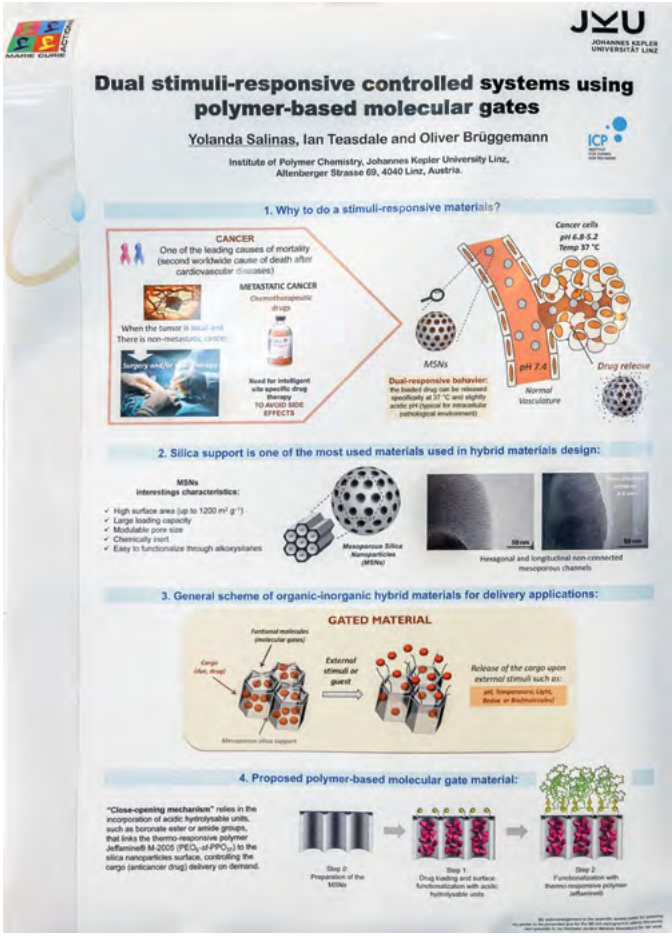
Dual stimuli-responsive controlled systems using polymer-based molecular gates

Multifunctional hybrid materials based on mesoporous silica nanoparticles (MSNs) [1] are promising candidates as drug delivery systems compared to liposomes or emulsions. Their thermally stability and rigid framework prevents premature degradation, and they can be easily functionalized with stimuli-responsive gate-keepers, reducing the unpleasant side effects of conventional systems. Bearing in mind those advantages, in this project is proposed a smart controlled delivery system based on silica nanoparticles capped with a polymer [2] sensitive to both temperature and pH. This dual-responsive behavior is very useful for biological applications as the loaded drug can be released faster at 37 °C and slightly acidic pH (typical for intracellular environment) than at neutral physiological conditions. These two stimuli are very popular in the design of gated systems and in this work, the close/open mechanism relies in the incorporation of acidic hydrolysable units, such as boronate ester or amide groups, that links the thermo-responsive polymer Jeffamine® M-2005 (PEO5-st-PPO37) to the silica nanoparticles surface, controlling the cargo delivery on demand. The preliminary results have shown the promising chances of the system for future dual 'off-on' drug delivery applications such as cancer therapy, as in many types of tumors an acidic microenvironment can be found.

[1] E. Aznar, M. Oroval, L. Pascual, J. R. Murguía, R. Martínez-Máñez, F. Sancenón, "Gated Materials for On-Command Release of Guest Molecules", Chem. Rev. 2016, 116, 561–718.
[2] L. Wei, N. Hu, Y. Zhang, "Synthesis of Polymer-Mesoporous Silica Nanocomposites", Materials 2010, 3, 4066-4079.



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Mechanism of pigment migration in polymer coatings

Polymer coatings are used to protect underlying surfaces, mostly metals and alloys, extending their service life. Because of high costs of corrosion the use of protective coatings is crucial in any application that involves materials processing and manufacturing. A polymer coating applied on protected surface is composed of a binder (cross-linked polymer resin) and additives such as functional pigments including anticorrosive agents and non-functional fillers. Polymer coatings provide passive corrosion protection by forming a barrier for corrosive species and blocking ionic transfer between anode and cathode areas on a metal surface; active corrosion protection is provided by anticorrosive additives (pigments). Effective pigments exhibit limited solubility in water which prevents excessive leaching and results in long-term release to guarantee anti-corrosion performance during the entire lifetime. The most efficient anticorrosive systems involve chromate-based pigments. However, due to toxicity concerns, there is a need to search for more environmentally-friendly yet equally or better-performing alternatives. One of key obstacles for the effective design of novel anti-corrosive coatings is the lack of understanding of fundamental transport phenomena of pigments in such systems.

This work aims at investigating the migration mechanism of pigments through model polymer coatings (i.e. epoxy films filled with different pigments and fillers). Advanced analytical methods such as SEM-EDX (scanning electron microscopy/energy dispersive X-ray spectroscopy), STEM (scanning transmission electron microscopy)-EDX and FIB (focused ion beam)/SEM are used to track the location of pigments and analyse structural changes in the coatings after exposition in water or electrolyte solutions which triggers the migration process.

Acknowledgements:

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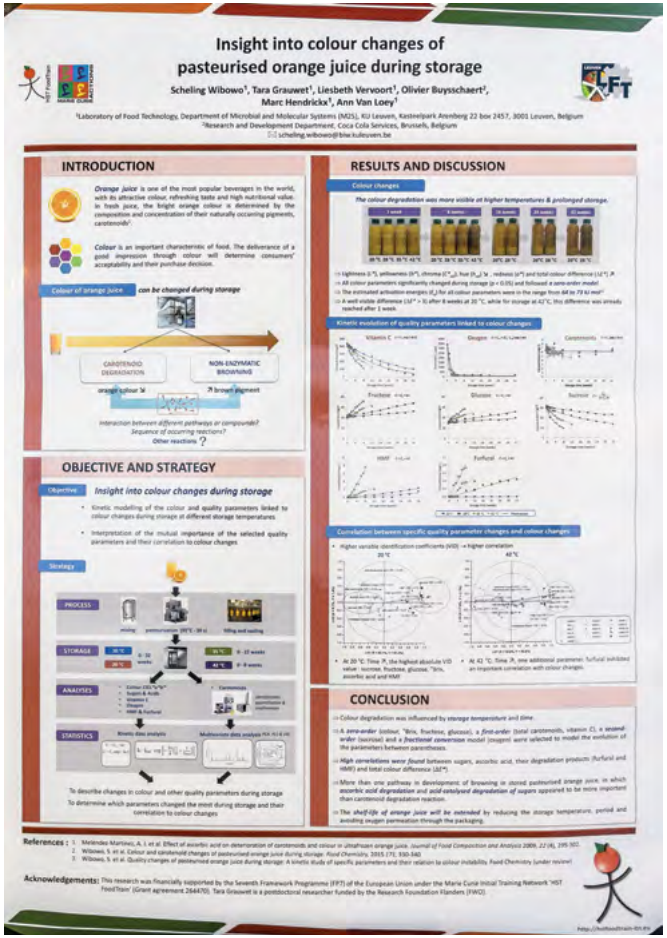
Insight into colour changes of pasteurised orange juice during storage

For shelf-stable pasteurised orange juice, colour degradation (browning) is a known problem, which is, however, scientifically still not completely understood. Besides colour, also other chemical changes can occur in the juice during shelf life, thereby affecting consumer acceptance. In this project, pasteurised orange juice samples were stored at four different temperatures, 20 °C and 28 °C for a total of 32 weeks, 35 °C for 12 weeks and 42 °C for 8 weeks. A targeted approach was used to gain insight in the chemical reactions responsible for quality changes, particularly, colour changes. The effect of storage time and temperature on a wide range of quality attributes (colour, carotenoids, acidity, sugars, oxygen, vitamin C, furfural and 5 hydroxymethylfurfural (HMF)) was investigated using a kinetic approach. In addition, multivariate data analysis (MVDA) was applied to describe the correlation between the multiple targeted responses and colour. Browning was clearly observed during storage, particularly at elevated storage temperatures. Concerning changes in carotenoids, the natural pigments responsible for the orange colour of orange juice, a limited decrease of total carotenoid content throughout storage was observed. Moreover, the acidity of orange juice was relatively stable. An increase was observed for fructose, glucose and HMF contents, while ascorbic acid and oxygen contents decreased during storage. Based on MVDA, high correlations were found between, ascorbic acid, their degradation products (furfural and HMF) and total colour difference (ΔE*). Therefore, it can be concluded that there are multiple pathways involved in the development of browning of pasteurised orange juice during storage, in which ascorbic acid degradation and acid-catalysed degradation of sugar appeared to play important roles.



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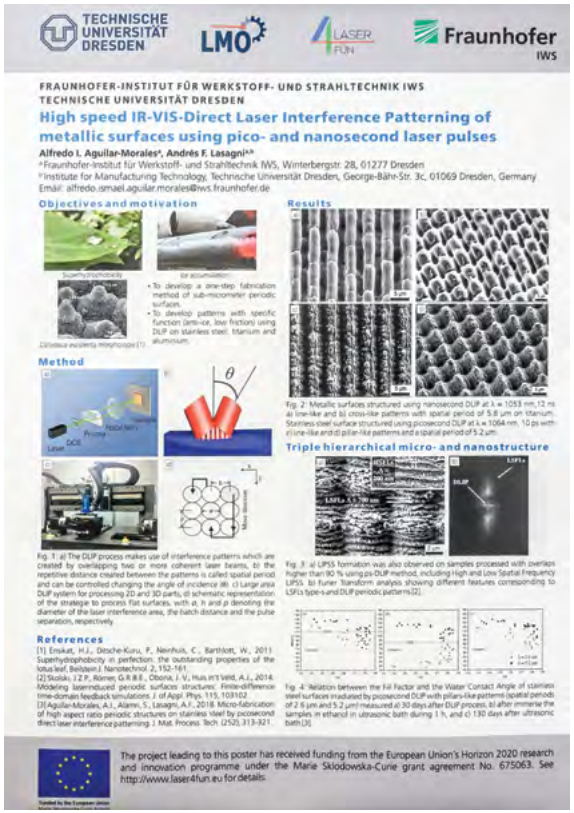
High speed IR-VIS-Direct Laser Interference Patterning of metallic surfaces using pico- and nanosecond laser pulses

Natural surfaces have inspired the development of new material properties based on the superhydrophobicity and self-cleaning. In this context, the leaves of Nelumbo nucifera have attracted attention due to its water repellency based on the micro- and nanostructure. Advanced laser processing technologies such as Direct Laser Interference Patterning (DLIP) can offer the fabrication of functionalized surfaces based on the biomimetic superhydrophobic microstructures.

In this work, surface structuring by picosecond DLIP was used to mimic on stainless steel the morphology observed on natural superhydrophobic surfaces. Structures with spatial periods of 2.6 µm and 5.2 µm were fabricated in the pillar-like pattern exhibiting high aspect ratios periodic structures. These morphologies have demonstrated the increment of the Water Contact Angle (WCA) from 67.6° (untreated surface) up to 145° based on the periodical micro- and nanostructures. Thereby, a triple hierarchical pattern is observed including Low and High Spatial Frequency LIPSS (LSFL and HSFL). Micro and submicrostructures produced using high pulse to pulse overlap were evaluated in relation with its WCA directly after the laser irradiation, revealing values around 20°. However, after 30 days, the morphologies with lower Fill Factor depict higher WCA values (up to 150°). This behavior is well explained due to the increment of carbon content on the surface which is time dependent. An additional wettability response was observed after washing the samples in ultrasonic bath with ethanol during 1h. The results suggest that after the ultrasonic bath, a complete or partial removal of the non-polar carbon layer occurs which is responsible of a drastically decrease in the WCA for the samples with 2.6 µm spatial period. Differently, due to the high aspect ratio (⊠ 2.2) of the produced pillars on the samples treated using 5.2 µm spatial period, the hydrophobic character is kept which means that in this case the surface topography mainly controls the surface wettability.



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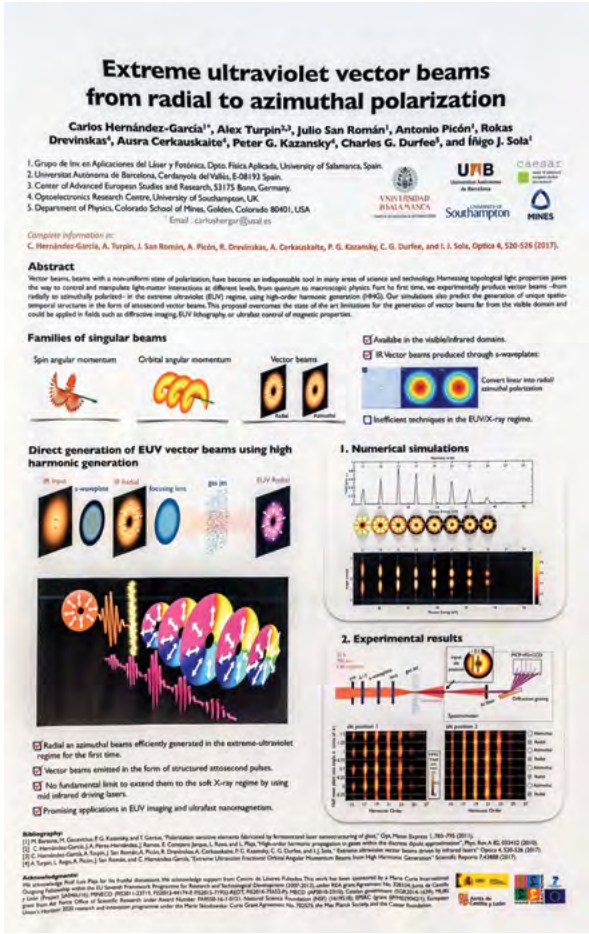
Attosecond extreme ultraviolet vector laser beams from radial to azimuthal polarization

Vector beams –light beams with spatially variant polarization– have become an indispensable tool in many areas of science and technology such as optical trapping, quantum memories, and quantum optics. Radially and azimuthally polarized light beams are especially interesting to sharply focus light below the diffraction limit, and to induce longitudinal magnetic fields, respectively. The spectral limitations of their generation techniques based on linear optics prevent their efficient generation in the extreme-ultraviolet (EUV) and x-ray regimes, which would further extend their applications down to the nanometric scale. In this work EUV vector beams are generated for the first time using the nonlinear process of high harmonic generation (HHG). To do so, an infrared fs radially polarized vector beam –generated with a s-waveplate– is focused into an argon gas jet, whose atoms emit coherent EUV radiation. Our experimental and theoretical results demonstrate that HHG imprints the polarization state of the infrared beam, ranging from radial to azimuthal, into the EUV range. Our numerical simulations also demonstrate that the harmonic beams can be synthesized into EUV/soft x-ray attosecond vector beams, that can carry orbital angular momentum.



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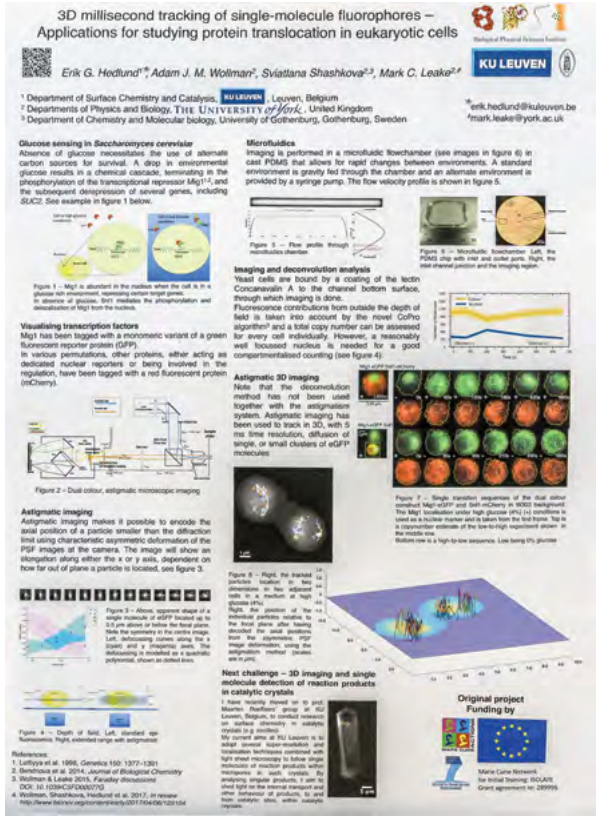
3D millisecond tracking of single-molecule fluorophores – Applications for studying protein translocation in eukaryotic cells

Metabolic processes are the basis of all life. An organism must be able to utilise chemical energy to stay alive and eventually reproduce. These are the central features of life, regardless of organism length scale. To achieve this, an organism must be able to adapt to varying surrounding environmental conditions. Cells respond to external stimuli by releasing kinase cascades along often intricate signalling pathways which regulate cellular function. These chemical signals eventually bring about some cell level response.

In our research on transcription factor dynamics in Brewer's yeast, Saccharomyces cerevisiæ, we have found that a key transcription factor, Mig1, forms functional clusters that translocate between nucleus and cytosol as a response to environmental glucose fluctuations (Wollman et al. 2017). The bulk behaviour of Mig1 glucose sensing in yeast has recently been well characterised (Bendrioua et al. 2014). However, only now have we been able to follow the dynamics and interactions of individual molecules and clusters in the pathways.

Fluorescent optical microscopy techniques are ideal for non-invasive probing of samples that can be placed in such a way that the sample turbidity hampers the image. We use genetically incorporated fluorescent markers which allows functional in-vivo imaging.

By using astigmatic imaging at high speed, we can track in three dimensions, fluorescently tagged proteins translocating in living cells over several tens of milliseconds with a temporal resolution of down to 5 ms, allowing diffusing particles to be tracked under physiological conditions. We used mutant yeast strains with fluorescent protein tags attached to the transcription factor Mig1. Furthermore, a microfluidic flow channel provides a consistent and controllable environment during an experiment.



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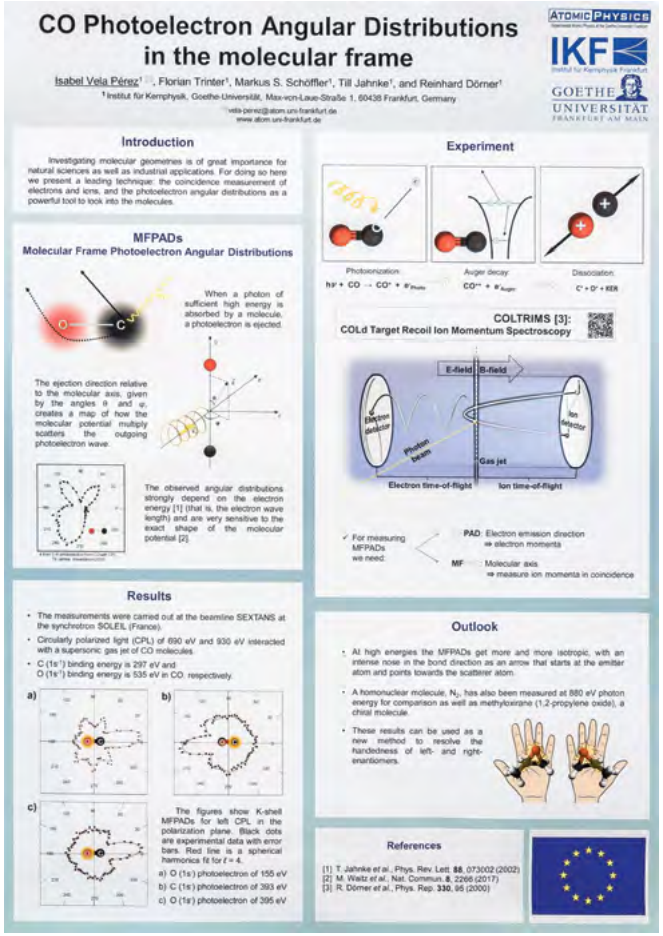
CO photoelectron angular distributions in the molecular frame

Investigating molecular geometries is of great importance for different applications in physics, chemistry, life sciences or the pharmacy industry.

Here we present a photoionization experiment carried out at synchrotron SOLEIL, where a X-ray photon beam was intersected with a CO supersonic gas jet. By absorbing a photon, the K-shell ejects a photoelectron, followed by an Auger decay and finally by a Coulomb explosion. Using the COLTRIMS (COLd Target Recoil Ion Momentum Spectroscopy) reaction microscope, both electrons plus both ions are detected in coincidence.

The photoionization event is determined by the initial state of the system, the properties of the dipole operator, which is responsible for the photoionization, and the final state. At high energies, the continuum electron can be described by a plane wave where the photoionization differential cross section of the electron emission direction (the molecular frame photoelectron angular distribution, MFPAD) is proportional to the square of the Fourier transform of the initial state.

By selecting high photon energies (690 eV), circularly polarized light and restricting the MFPAD to the polarization plane, the effect of the dipole operator can nearly be neglected and thus the initial electronic wave function is in good approximation mapped onto the emitted -and detected- photoelectron.



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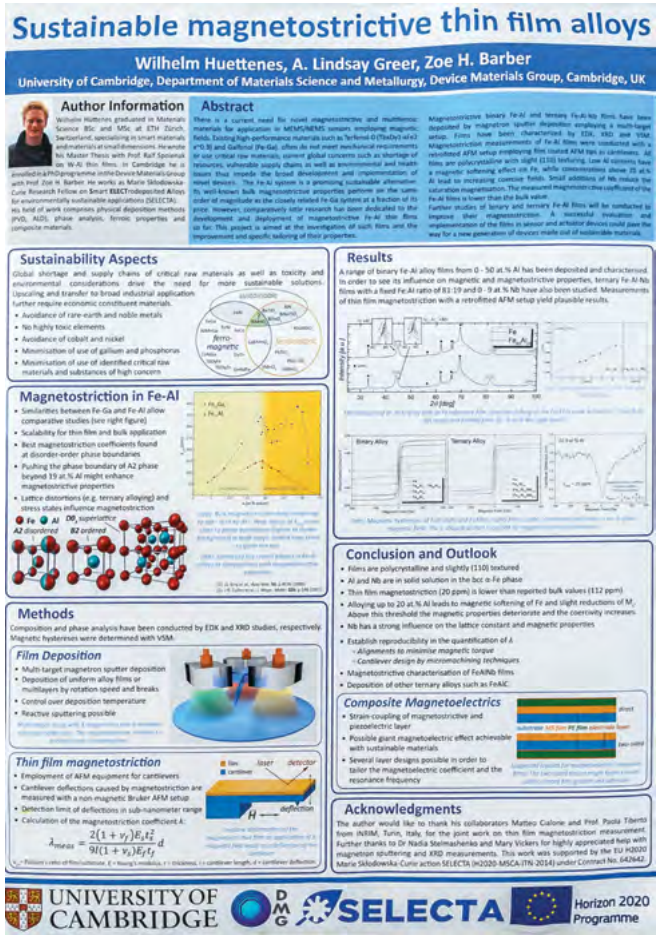
Sustainable magnetostrictive thin film alloys

There is a high demand for novel magnetostrictive and multiferroic materials for application in MEMS/NEMS sensors employing magnetic fields. Existing high-performance materials such as Terfenol-D (TbxDy1-xFe2 x~0.3) and Galfenol (Fe-Ga) have a high magnetostrictive coefficient, but often do not meet mechanical requirements and contain critical raw materials; current global concerns such as shortage of resources, restricted choice in sources of import as well as environmental and health issues thus often impede the broad development and implementation of novel devices. The Fe-Al system is a promising sustainable alternative to these materials. Its well-known bulk magnetostrictive properties perform on the same order of magnitude as the closely related Fe-Ga system at a fraction of its price. However, comparatively little research has been dedicated to the development of magnetostrictive Fe-Al thin films so far. The current study is aimed at the investigation of such films and the improvement and specific tailoring of their properties. Strategies such as metastable phases produced by magnetron sputtering, induced phase transformations and ternary alloying are presented. A novel approach for the measurement of the magnetostrictive effect in very thin films (<500 nm) is introduced. Finally, results on respective binary and ternary Fe-Al alloys are given and put in a broader context.



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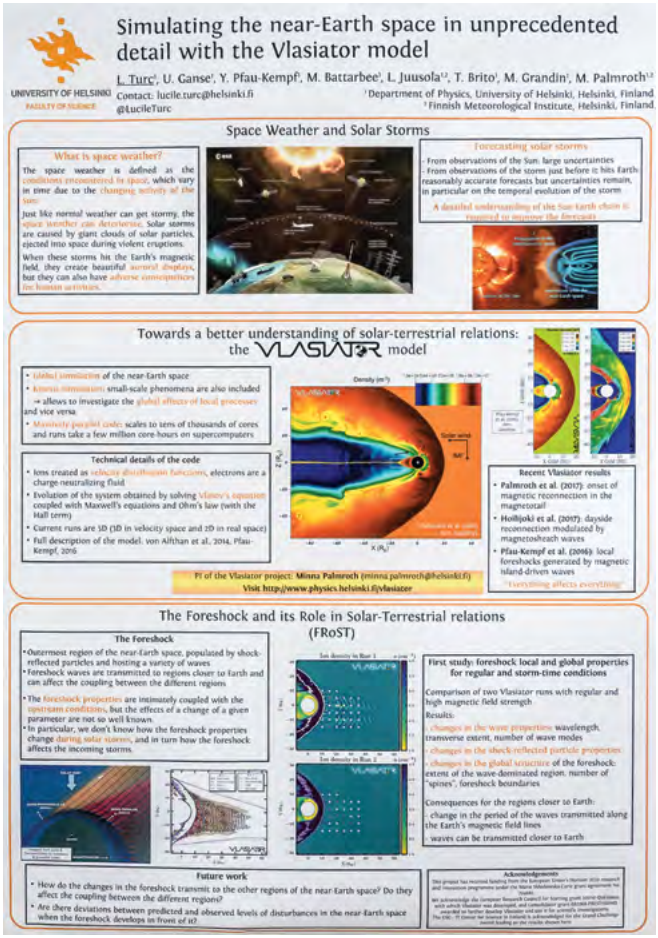
Simulating the near-Earth's space in unprecedented detail with the Vlasiator model

The space around Earth is not as empty as one may think, but is filled with particles escaping from the Sun, called the solar wind. The Earth's magnetic field shields our planet from this flow, forming a protective magnetic bubble around our atmosphere. However, just like normal weather can get stormy, the conditions in space, the space weather, can deteriorate. Solar storms are caused by giant clouds of solar particles, ejected into space during violent eruptions. The most widely-known effects of solar storms are the beautiful auroral displays which can sometimes be witnessed in night skies. Yet stormy space weather can also have adverse consequences for human activities, in space and on the ground, for example damaging spacecraft electronics or disrupting GPS signals. In our modern society, relying ever more on space-based assets, understanding and being able to predict space weather has become crucial. One way to further our understanding of space weather is to develop computer simulations capable of describing the interaction of the solar wind with the near-Earth space. Simulating this is however extremely challenging because of the variety of scales, both temporal and spatial, over which the relevant phenomena take place. At the forefront of numerical space physics, the newly-developed Vlasiator simulation code offers a unprecedented view of the near-Earth space. My Marie Curie-funded project focuses on utilizing this new model to study how incoming solar storms modify one of the outermost regions of the near-Earth space called the foreshock, and whether the foreshock changes in turn how solar storms interact with the Earth's magnetic field. The aim of the project is to assess whether these effects should be taken into account in refined space weather forecasts. In this poster, I will present the Vlasiator model and initial results from my research project.



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Anaerobic degradation of phenanthrene by a novel sulfate-reducing bacterial enrichment culture

Polycyclic aromatic hydrocarbons (PAHs) are widely distributed contaminants that produce hazardous effects on human health. In PAH-contaminated sites, oxygen is rapidly depleted. Thus, microorganisms able to use these compounds as a carbon source in the absence of molecular oxygen are crucial for their consumption. Phenanthrene is a 3-ring PAH mostly found in fossil fuels. This work aims at elucidating the mechanisms for the anaerobic degradation of phenanthrene by a sulfate-reducing enrichment culture (TRIP) obtained from the Pitch Lake in Trinidad-Tobago, the world largest natural asphalt lake.

The metagenome of TRIP was sequenced and annotated at the Microbial Genome Annotation & Analysis Platform, Genoscope. Five bacterial draft genomes were reconstructed from the metagenome sequences. The key player of TRIP belongs to the Desulfobacteraceae family of deltaproteobacteria. Analysis of the metabolic capacity of this bacterium revealed the key enzymes for dissimilatory sulfate reduction, a complete Embden-Meyerhof-Parnas pathway for oxidizing glucose to pyruvate and a complete tricarboxylic acid cycle. This bacterium also presents the key genetic elements of the classical pentose phosphate pathway for NADPH and pentose synthesis and of the Wood-Ljungdahl pathway for the complete oxidation of acetyl-CoA. The predicted metabolic pathways were corroborated by transcriptomics and proteomics analyses of the TRIP culture during growth with phenanthrene. Sequence similarity to genes previously characterized for naphthalene degradation allowed identifying two gene clusters encoding a carboxylase enzyme potentially involved in the activation of phenanthrene and genes encoding reductases potentially involved in subsequent ring dearomatization and reduction steps.

This work provides evidence of the pathway involved in the anaerobic biodegradation of a highly toxic PAH.

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Role of bacterial enzymes in the transition from free living to plant endophytes and the design of efficient biofertilizers

One of the main challenges for humanity is to increase food production while using scarce resources and protecting the environment. Plant's productivity can be enhanced by the activity of Plant Growth-Promoting (PGP) bacteria, applied as biofertilizers. Biofertilizers have been applied during decades, but in many cases bacteria with great potential in lab, fail when applied in natural soils (probably they are out-competed by the native microbiota or unable to adapt to the environmental conditions).

In the Rhizobium-legumes model, bacterial cellulases are crucial in the bacterial entrance into the root. Nevertheless, the implication of these enzymes in the active entrance of bacteria in non-legume crops has not been studied yet. This project aims to research the role of bacterial enzymes in the capability of endophytes to enter non-legume plants, using rapeseed as model. If any enzymes enable active root infection, giving an advantage over passive mechanisms, selection of bacterial strains not only on the base of their PGP capacity, but also on their ability to enter the plant -with less competitors and protected from abiotic stresses-, will allow the design of more efficient biofertilizers.

Preliminary results show that several rapeseed bacterial endophytes with PGP traits are also able to produce hydrolytic enzymes. When inoculated over seedlings, some of them are significantly promoting plant development. Moreover, electronic microscopy shows their ability to greatly colonize roots. These bacteria have been chosen to make a transcriptomic study to compare gene expression in free living bacteria and in those attached to the root surface to identify genes implicated in the plant root entrance. Future construction of mutant strains will allow unravelling these genes' role in plant root entrance.

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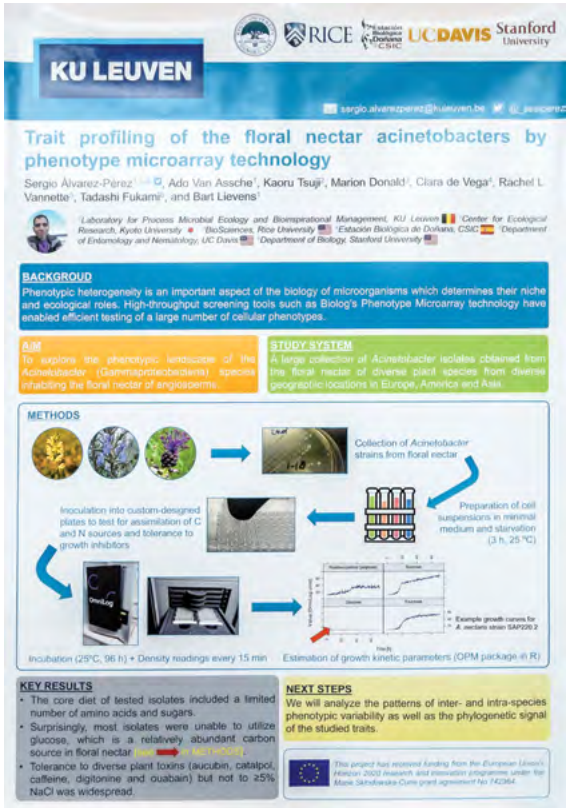
Trait profiling of the floral nectar acinetobacters by phenotype microarray technology

Phenotypic heterogeneity is an important aspect of the biology of microorganisms which determines their niche and ecological roles. High-throughput screening tools such as Biolog's Phenotype Microarray (PM) technology have enabled efficient testing of a large number of cellular phenotypes. Basically, this technology consists of 96-well microplates with pre-arrayed sets of phenotypic tests (e.g. assimilation of diverse nutrients and tolerance to inhibitors) and an accompanying automated OmniLog incubator/reader. Response to the test conditions is then assessed through reduction of a tetrazolium dye and/or biomass increase over a time course.

Our ongoing MSCA project [1] involves the phenotypic profiling of a large collection of Acinetobacter (Gammaproteobacteria) isolates obtained from the floral nectar of diverse angiosperms from different geographic locations. Custom-designed microplates were assembled using diverse carbon and nitrogen sources in relevant concentrations (1% and 0.06%, respectively, as previously used for nectar yeasts) and a selection of inhibitors. Cells were starved for the substrate category of interest prior to inoculation of PM plates, which were then incubated at 25°C for 96 h. Biomass increase in each well was registered every 15 min and the data collected over time was summarized and used to estimate different kinetic parameters using the OPM package in R. Our results showed that the core diet of tested isolates included a limited number of amino acids and sugars such as sucrose and fructose. Surprisingly, most Acinetobacter isolates were unable to utilize glucose, which is a relatively abundant carbon source in floral nectar. Tolerance to diverse plant toxins (aucubin, catalpol, caffeine, digitonine and ouabain) but not to ≥5% sodium chloride was widespread. Next steps in the project will involve the analysis of inter- and intra-species phenotypic variability as well as the study of the phylogenetic signal of the studied traits.

[1] http://cordis.europa.eu/project/rcn/208553_en.html



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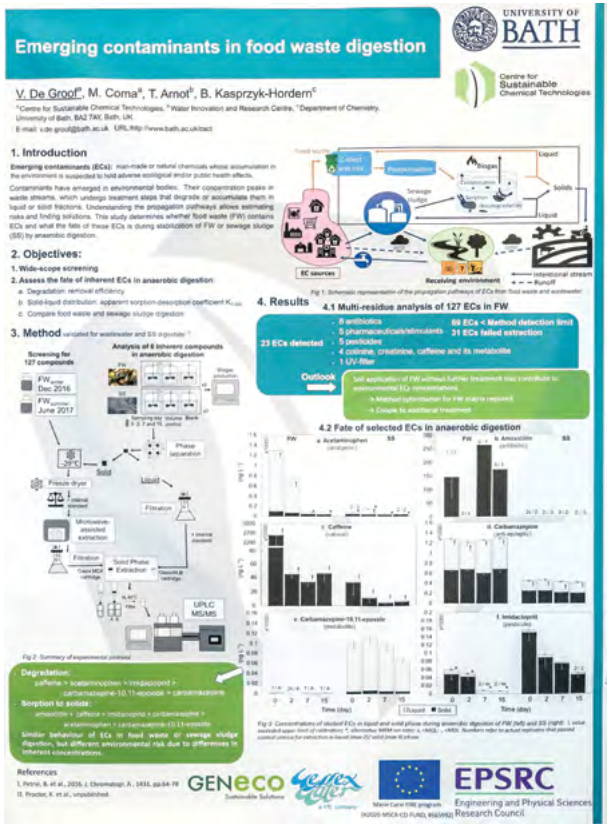
Emerging contaminants in food waste digestion

Over the past decades diverse contaminants emerged in environmental water bodies with identified propagation pathways including wastewater treatment effluent, run-off from agricultural land from pesticide or wastewater-derived applications and leaching from diffuse sources. The current study identifies another possible source that is currently unaccounted for: biowaste-derived digestate applied as soil amendment. Food waste from an industrial-scale treatment plant was subjected to a multi-residue screening for 127 emerging contaminants. Six detected contaminants (acetaminophen, amoxicillin, caffeine, carbamazepine, carbamazepine-10,11-epoxide and imidacloprid) were selected to follow their degradation and sorption during anaerobic digestion of food waste and sewage sludge as a control. In the food waste a total of 23 micropollutants were detected, comprising pharmacologically active compounds, pesticides, a sunscreen agent and natural compounds, some in concentrations higher than reported for in wastewater. Initial concentrations varied for food waste or sludge digestion, however, micropollutant behaviour did not significantly differ. Removal efficiencies decreased in the order of caffeine > acetaminophen > imidacloprid > carbamazepine. The carbamazepine metabolite, carbamazepine-10,11-epoxide, was only present for sewage sludge digestate. Compounds were mainly found in the solid phase after digestion, with exception of carbamazepine and carbamazepine-10,11-epoxide showing equal and predominant presence in the liquid phase, respectively. According to the author's knowledge, this is the first study that screened and detected multiple micropollutants in food waste, indicating possible incorrect disposal, or persistence of applied pesticides and veterinary drugs. Understanding in which phase the micropollutant resides allows to asses bio-availability and evaluate the requirement of additional treatment methods for the digestate such as aerobic composting for the solid fraction or tertiary wastewater treatment for the liquid phase. Further optimisation of multi-residue analysis to matrices such as food waste or digestate will allow more accurate identification and quantification of ECs leading to more comprehensive risk assessments for food and agro-wastes.



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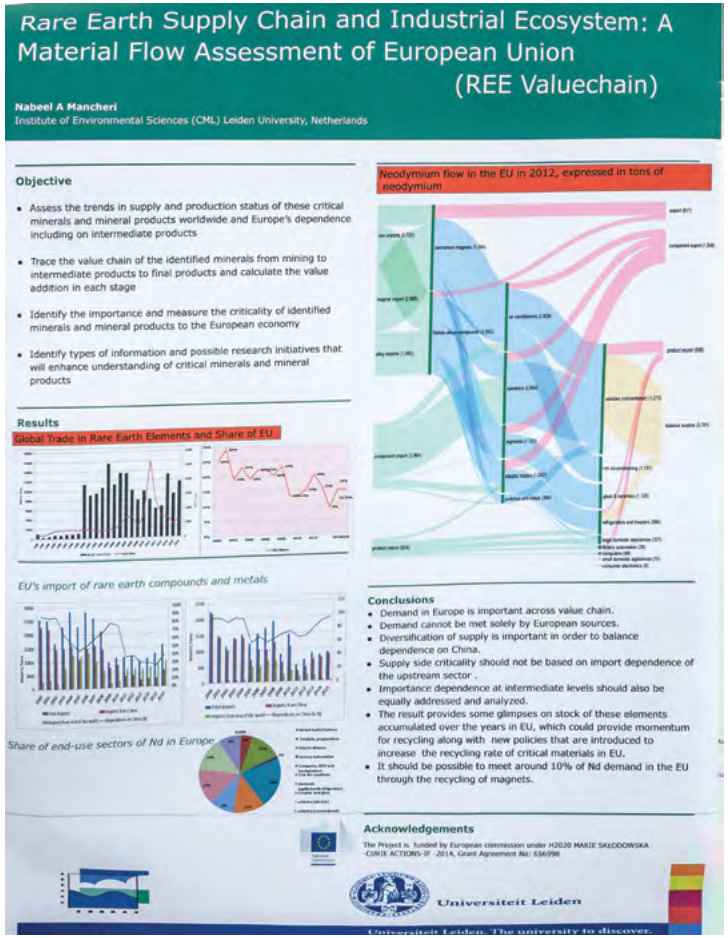
Rare earth supply chain and industrial eco system: a material flow assesment of EU

Rare earths are a critical component of many high and green technologies such energy efficient lights, wind turbines, hybrid and full electric vehicles (electro motors and batteries) and solar panels and are important ingredients in hard disks, lasers and superconducting magnets. The concentration of rare earth elements (REEs) and other critical metals in countries like China and Russia raises the vital issue of security of supply as Europe is the leading importer and consumer of these minerals both in mineral and applied forms. The criticality of these minerals were highlighted in the reports of the European Commission's Ad hoc Working Group on defining critical raw materials. These raw materials are fundamental to Europe's economy, growth and jobs. The importance of these minerals to the European economy has never been studied thoroughly, though more recently securing reliable, sustainable and undistorted access to crucial non-energy raw materials has been of growing concern. In the EU, responses have been initiated in different nations, economic areas and companies, with the European Commission launching the "Raw Materials Initiative (RMI)".

The European Commission has identified criticality of raw materials along with addressing the entire raw materials value chain in the raw materials part of the Societal Challenge 5 of Horizon 2020. Therefore an empirical study on rare earth elements and its importance to the European economy become an important issue to study. This study aims to identify the mineral sources, mineral production and recycling technologies, as well as key applications within European economies by combining the input-output matrix.The study will calculate the value addition at each stage of the life cycle of rare earths.



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Research Program: Studies on Intermediality and Intercultural Mediation

SIIM is a Research Group of Excellence based at Universidad Complutense Madrid (Spain).

Its Mission/Values are: The study of artistic forms as metacognitive tools; Strategic Storytelling and Creative Writing for Social Innovation (i.e. empowerment of marginal groups); International Cooperation and Intercultural Mediation; Sociological impact of World Literature(s); Research on multimodal social semiotics and intersubjective cognition; Intermedial studies, translation, re-mediation, adaptation; cross-cultural aspects attached to Social Sciences and Humanities; Teaching Innovation (i.e. practice in academic publishing).

SIIM has carried a number of research projects with the help of national and international funds.
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The group is also interested in international cooperation.
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Emotion regulation as a transdiagnostic factor in children and adolescence psychopathology

Most mental health disorders, including depression, substance abuse, eating disorders and anxiety have their onset during adolescence (Kessler et al., 2007). It has been argued that this peak in psychopathological symptoms is a result of developmental changes, which hamper adequate emotion regulation (Dahl, 2004). Cross-sectional studies have indicated that emotion regulation deficits precede the emergence of psychopathology, however, longitudinal evidence is missing.

My PhD will investigate the role of emotion regulation difficulties in the development of adolescence psychopathology in a large sample of children. More specifically, I will look at a) emotion regulation as a predictor of later psychopathology, b) factors influencing multifinality (i.e., similar emotion regulation habits resulting in different symptom exhibition) and c) heterotypic continuity (i.e., emotion regulation difficulties at different times in the development resulting in different outcomes).

Data will be derived from the Millennium Cohort Study, which examines various mental health and environmental correlates of 12,347 children living in the UK, starting in 2000.

Following this, I will investigate how emotion regulation difficulties can be improved as means to treat and prevent mental illness in youth. As part of this a mobile app will be co-produced with young people, to assess and assist young people's emotion regulation in their daily life.

Mobile apps present promising means to effectively administer mental health interventions to young people and to collect longitudinal, context specific data, which will add significant insights to current mental health research. The project is expected to elucidate emotion regulation processes within a developmental psychopathology framework and to inform the development of a digital, youth -adequate mental health intervention.

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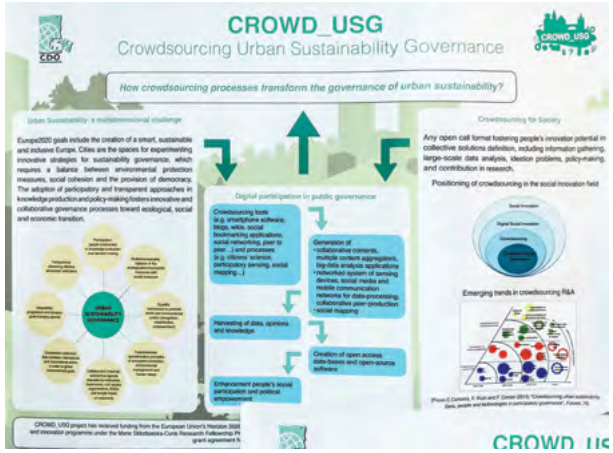
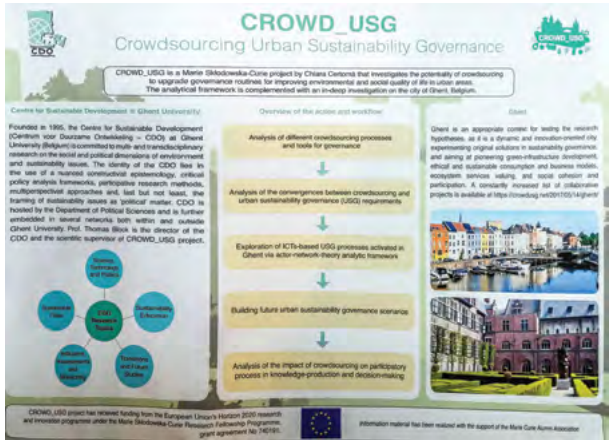
CROWD_USG Crowdsourcing Urban Sustainability Governance

How crowdsourcing processes can advance real participatory knowledge and policy-making processes in the governance of urban sustainability?

This is the key question investigated in the CROWD_USG project, a Marie Skłodowska-Curie research project by Chiara Certomà exploring how increasing ICT-people interactions are transforming the way in which citizens take part in the production of information, sharing of knowledge and decision making about the planning and management of environmental issues in their city.

In the recent decades cities attracted scholars and practitioners' interest as the appropriate space for experimenting innovative strategies for urban sustainability governance, which requires a balance between environmental protection measures, social cohesion and the provision of democracy. Special attention is now devoted to the adoption of participatory approaches, and the web 2.0 architecture for data collection &sharing through peer-to-peer and wiki-technologies has been exactly welcomed as a shortcut toward the democratisation of governance processes. Particularly crowdsourcing can impact on governance model by fuelling the integration of environmental, social and economic priorities in the urban governance agenda; and by reviewing the mode of interaction between governing bodies, research institutions, business and social actors. This can lead to the attainment of sustainability goals, by generating citywide technological leap-frogging and community-based decentralised knowledge and policy production systems.





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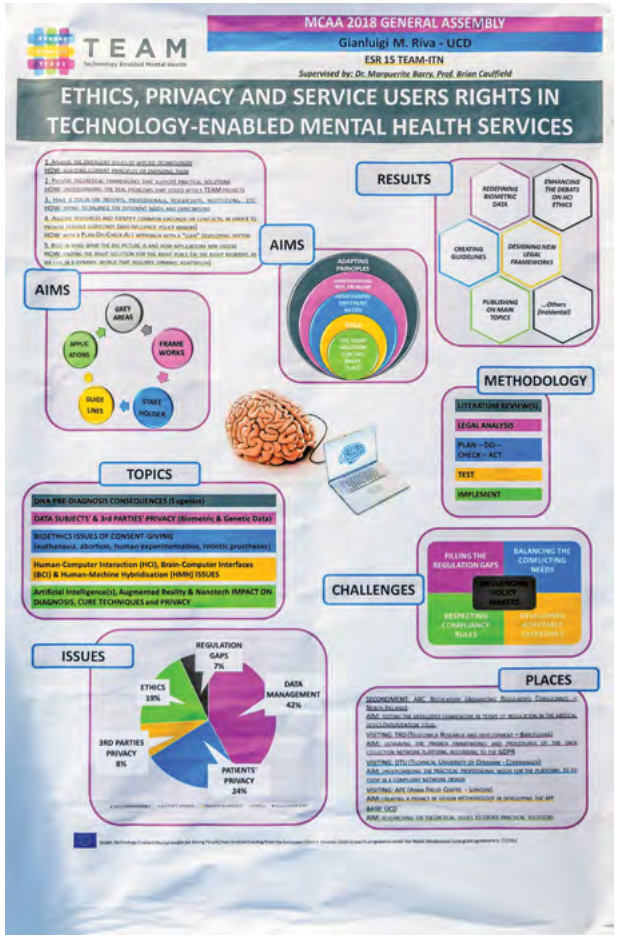
Ethics, privacy and service users rights in technology-enabled mental health services

Mental healthcare involves a broad spectrum of ethical and legal issues. When it concerns young people, there is a further ethical impact. The activities involved in assessing and treating mental health are then transversally crossed by privacy issues. This project aims overall to individuate ethical and legal principles applicable to each field involved in the TEAM Project and to outline gaps and grey areas in current regulations, towards both theoretical and practical solutions. This research is conducted to adapt ethical and legal principles to the practical needs of evolving assessment and treatment solutions in support of the development of new applied technologies for mental health. Specifically, this research will outline how ethical, privacy and fundamental rights principles are affected by new technologies in the field of free will/consent giving and how they have to be applied (and adapted) in the health environment, in order to preserve patient and other stakeholders' needs. The focus will be on consent giving process related Human-Computer Interaction (HCI) and Brain-Computer Interfaces (BCI) issues and the related ethical consequences of the increasing human-machine socio-legal interactions and relationships. This research will also pay attention to the issues related to the development and future exploitation of technologies such as A.I., nanotech, A.R. and BCI and the consequent (and plausible) future hybridisation between human and machines. Thus, the goal is to design a legal framework to support practical ethics and privacy guidelines, that could be adaptable to future change in technology and society.



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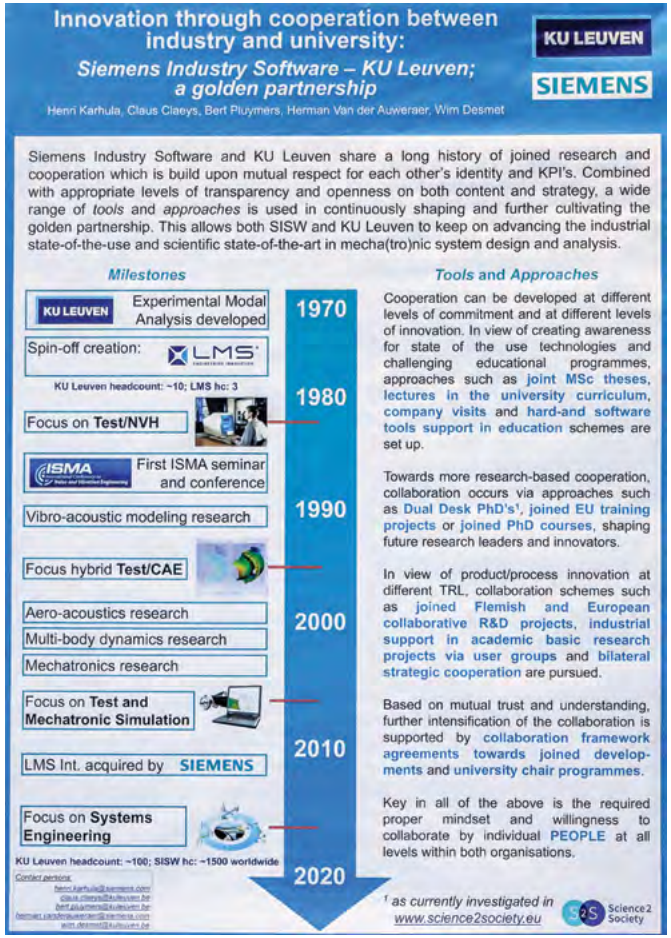
Innovation through cooperation between industry and university

Siemens Industry Software and KU Leuven share a long history of joined research and cooperation which is build upon mutual respect for each other's identity and KPI's. Combined with appropriate levels of transparency and openness on both content and strategy, a wide range of tools and approaches is used in continuously shaping and further cultivating the golden partnership. This allows both SISW and KU Leuven to keep on advancing the industrial state-of-the-use and scientific state-of-the-art in mecha(tro)nic system design and analysis.



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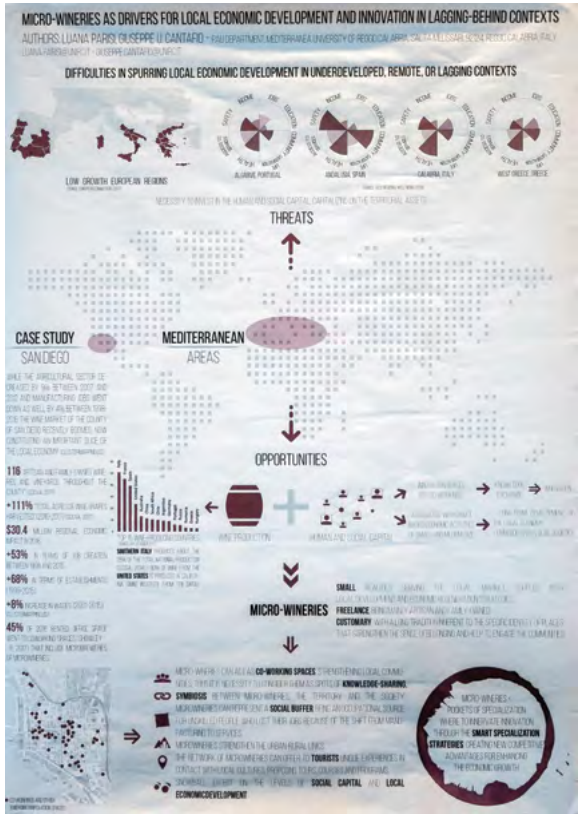
Micro-Wineries as Drivers for Local Economic Development and Innovation in lagging-behind contexts

Today, there is increasing awareness of the role that social capital can play in spurring Local Economic Development especially in underdeveloped, remote, or lagging contexts. It encompasses different aspects, such as relationship networks, allowing knowledge exchange and innovation boost, and is associated mainly with craft-based economic activities of small and medium-size, entrusted with the long-term development of the local economy and embedded into local societies. Micro-wineries represent a good example, being small realities that serve especially the local market, acting also as co-working spaces that strengthen local communities. Mediterranean regions have commonly been connected with these sectors; nevertheless, only recently, wine and oenological tourism have been coupled with local development and economic regeneration strategies. This study aims at pushing the body of knowledge in the development of micro-wineries in Southern Italy and, more generally, in lagging-behind contexts of Southern Europe, trying to regenerate the existing realities, creating spots of knowledge-sharing where also tourists can live experiences in contact with local cultures. Micro-wineries can constitute the pockets of specialization where to innervate innovation through the Smart Specialization Strategies framework, that helps creating new competitive advantages for enhancing the economic growth. In order to support the discussion, the San Diego wine cluster will be deepened as a case study, since its wine market recently boomed, challenging the historic worldwide producers and constituting an important slice of the local market. Findings from the research highlight the micro-wineries symbiosis with the territory and the society itself. Positive relations between them and the broad regional innovation strategy emerge as well, showing the snowball effect on the levels of social capital and Local Economic Development in lagging contexts. Useful lessons are drawn for encouraging policy makers and planners in undertaking actions towards strengthening the potential of micro-wineries and building networks among them.



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