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CEFIPRA

Indo-French Scientific Collaboration for Sustainability & Innovation

Newsletter of the Indo-French Centre for the Promotion of Advanced Research

Editor's Note...

CEFIPRA continued to play a pivotal role by facilitating the Indo-French collaborative research & innovation through its programmes & activities. CEFIPRA participated actively in the 3rd edition of Knowledge Summit, an Indo-French bilateral forum through a panel discussion on "Indo- French Scientific Cooperation' held at the inaugural session & also by organizing two scientific workshops on Artificial Intelligence (AI): AI for Sustainable Agriculture and AI for Healthcare at this Summit during 24 - 26 Nov, 2021.

This newsletter features the recent achievements of CEFIPRA supported projects. In one of our projects, researchers deciphered molecular differences associated with the two most pathogenic Aspergillus species, A. fumigatus and A. flavus. The outcomes highlighted the differences between these two species and emphasized on the need for species-specific antifungal treatment. Another Industry-Academia project highlighted the development of energy-efficient bio-composites from bio-wool waste, that could also be utilized as excellent filler material in insulation panels for construction and building applications.

A joint project between Laboratoire de Chimie Coordination (LCC) Toulouse, France and IIT Kanpur, India enabled the understanding of reaction mechanisms and discovered a novel mechanism for redox-active metals in borrowing hydrogen chemistry. Under another interesting project in the domain of Materials Science, the Indo-French research team developed a novel absorber coating for reducing thermal emittance, increasing solar absorbance and thermal stability for a diverse range of applications.

The collaborative team from National Center For Biological Sciences (NCBS), India and École supérieure de physique et de chimie industrielles de la Ville de Paris (ESPCI), France has discovered the self-reproducing capability of frequently used RNA recombinase, which is also capable of shuffling other RNA fragments to generate completely new RNA sequences with potentially novel properties. The team is currently investigating this exciting capability to shuffle sequences under recombination and its wider implications for evolution.

While my exciting journey with CEFIPRA comes to an end with this issue, I'm sure CEFIPRA will continue to reach greater heights and keep serving the scientific communities of the two countries and beyond ! I take this opportunity to thank all of you for your valuable support and guidance and being a part of my motivating journey as Director CEFIPRA.

I would like to take this opportunity to wish you all a Merry Christmas & Happy, Healthy and Eventful New Year 2022!

Dr. Purnima Rupal
Director, CEFIPRA

Whats inside...

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Bienvenu, Dr. S. Chandrasekhar

(as the new Indian Co-Chair of Governing Body of CEFIPRA)

A very warm welcome to the new Indian Co-Chair of the Governing Body of CEFIPRA - Dr. Srivari Chandrasekhar, Secretary, Department of Science and Technology, Government of India.

Dr. Chandrasekhar was the Director of the Indian Institute of Chemical Technology (IICT) sine 2015. He is a renowned synthetic organic chemist and has made significant contributions in diverse areas of organic chemistry with special emphasis on chiral chemistry, total synthesis of biologically active natural products and pharmaceutical products. He introduced polyethylene glycol (PEG) as a novel, environmentally benign solvent medium. He has developed technologies for the synthesis of latest anti-tuberculosis drug, bedaquiline; anti-tumor and abortive drug, misoprostol; anti-platelet molecule, beraprost; antidepressive compound, sertralin and drug for treatment of schizophrenia, asenapine. His research efforts, with an impressive degree of innovation and enterprise, have led to the synthesis of complex and scarcely available natural products and new molecular entities for affordable healthcare. His endeavors have provided cost-effective technologies to the chemical industry through the identification of new reagents / solvents for specific transformations. He has received several accolades including Eminent Scientist Award for contributions in the field of Chemistry from for his contributions in synthetic organic chemistry with special focus on the synthesis of complex molecules from natural sources and innovative, practical approaches to pharmaceuticals of current interest to industry.

Dr. Srivari Chandrasekhar was the lead Principal Collaborator from Indian Institute of Chemical Technology (IICT), Hyderabad along with Ecole Nationale Supérieure de Rennes for the CEFIPRA supported project on 'Misoprostol' which was an orally active synthetic prostaglandin E1 (PGE1) analog essential medicine. The project developed innovative technology which successfully reduced the cost of production. Dr. Chandrasekhar also guided the activities of CEFIPRA as a member of the Governing Body. CEFIPRA also has the honour of having been associated with him for various other networking activities. CEFIPRA is looking forward to work under his able leadership and further enhance the Indo-French ST&I colloboration.

Adieu...

CEFIPRA bid farewell to Director, Dr. Purnima Rupal as she completed her tenure and joined back CSIR, headquarters. The event was graced by the presence of various dignitaries and officials from the Department of Science and Technology, Ministry of Science and Technology, French Embassy in India. Among the guests present were Dr. Ashutosh Sharma, Former. Secretary, Department of Science and Technology (DST) and Indian Co-Chair of CEFIPRA, Mr Sanjeev K Varshney, Head ICD, DST; Mr Emmanuel LEBRUN-DAMIENS, Counsellor for Education, Science & Culture, Dr Didier Radisson, Attaché for Scientific and Academic Cooperation, Delhi and founder Director of CEFIPRA, Mr. PGS Mony.

CEFIPRA family will forever cherish the leadership and guidance of Dr Purnima Rupal and wishes her success and happiness in both her professional & personal journey!

Women in S&T
Challenges and opportunities in emerging context

16 - 18 August 2021

Dr. Purnima Rupal, Director, CEFIPRA was invited as a panelist in a special session on 'Women in S&T: Challenges and opportunities in emerging context' chaired by Prof. Rohini Godbole, IISc Bangalore. She highlighted the need for networking, authenticity & communication of ideas for leadership roles. This session was a part of three day National Conference (virtual) on "Science and Technology in India: A Historical Introspection with a Contemporary Perspective" organized by CSIR-NIScPR during 16-18 August, 2021.

Visit of Director, IGSTC to CEFIPRA

CEFIPRA welcomed
Sh. Rajachandran Madhan

CEFIPRA welcomed Sh. Rajachandran Madhan, Director of the Indo-German Science & Technology Centre (IGSTC) to CEFIPRA 28 July 2021. He shared some glimpses of ongoing scientific activities and programmes of IGSTC with the Scientific Team of CEFIPRA.

Meeting with Co-Chairs of CEFIPRA
10 November, 2021

CEFIPRA welcomed **Dr. M. Ravichandran**, Co-Chair & Secretary DST (Additional Charge) & MoES and **Mr. Matthieu Peyraud**, French Co-Chair, Ministry for Europe & Foreign Affairs, Government of France on 10 November, 2021. Sh. Sanjeev K Varshney, Advisor & Head, International Cooperation Division, DST, GoI and Dr. Nicolas Gherardi, Deputy Counsellor for Education, Science and Culture, Embassy of France in India were also present. The other members of French delegation from Ministry for Europe & Foreign Affairs were Mr. Thibaut Dutruel, Officer at University and Scientifc partnership, Mr. Eric Chevreul, Advisor to the Asia Director and Mr. François-Xavier Mortreuil, Attaché for Scientific and, Academic Cooperation, Bangalore. A video showcasing CEFIPRA's journey of more than three decades was presented to the members.

Invited PIs of CSRP & IARDP praised the CEFIPRA team for their support. The members of the two sides addressed & noted the concerns/suggestions made by some PIs regarding the projects being funded.

Meetings at CEFIPRA

Expert Committee Meeting under DST-Inria Targeted Programme
6 December, 2021

The virtual meeting of the Expert Committee (Indian Side) of DST-Inria Targeted Programme under Indo-French Programme in Information and Communication Science & Technology (ICST) was held on 6 December, 2021. The Committee evaluated the proposals received under the 8th Call.

A total 07 proposals were received under the three domains -Artificial Intelligence, Cybersecurity and Signal Processing of ICT were received out of which three were recommended from experts.

All proposals were peer-reviewed and comments of reviewers are highlighted in agenda for consideration by experts. Jointly selected proposals will be funded in India by DST through CEFIPRA and in France by Inria (for Inria Research Team).

Kick off meeting on Project: 6304-1

CEFIPRA Scientific Staff participated and provided the clarifications on various project management related matters to the two collaborating teams, CSIR Central Mechanical Engineering Research Institute, Durgapur and CNRS-LIRMM, France under the Project No. 6304 - 1 on 30 November, 2021 at their kick off meeting. The collaborators deliberated on various objectives achieved in their project so far.

Knowledge Summit-3 (KS3), 24-26 November, 2021
Inauguration & Plenary Session

Knowledge Summit (KS) is a bilateral forum dedicated to scientific and academic cooperation between India and France. The 3rd Knowledge Summit focused on research and scientific activities. The main objective was to promote the tools and methods for better structuring our cooperation, and its alignment to the current reforms. It is an opportunity for our respective countries to underline the success of our scientific collaboration, to draw some new leads of joint research work and also to discuss and exchange ideas on global challenges that had to be tackled. The First edition was organized to identify the priority areas in research and innovation, whereas the second edition was an attempt to formulate concrete strategies for the execution of joint action involving both Academia and the Industry.

Inaugural Session

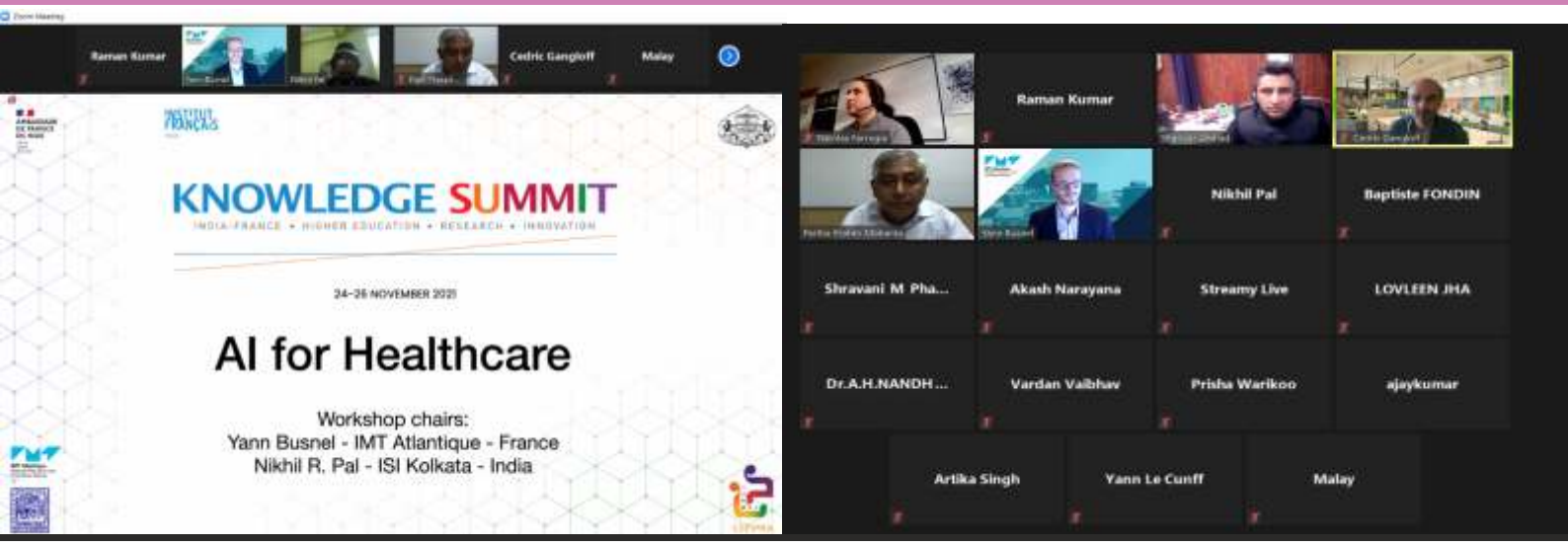
The 3 edition of Knowledge Summit was an online event inaugurated by Shri Dharmendra Pradhan, Hon'ble Minister of Education, Govt. of India, H.E. Mrs. Frédérique Vidal, Hon'ble Minister of Higher Education, Research and Innovation, Govt. of France, Dr M. Ravichandran, Secretary, Ministry of Earth Sciences and Department of Science & Technology, Govt. of India and Prof Nitin R Karmalkar, Vice Chancellor, Savitribai Phule Pune University, Pune, on 24 November 2021.

Plenary Session

A plenary session on "Indo- French Scientific Cooperation" had Prof K. Vijayaraghavan, Principal Scientific Advisor, Govt. of India, Dr Purnima Rupal, Director, CEFIPRA and Dr Nicolas Gherardi, Deputy Counsellor for Education, Science and Culture, Embassy of France in India as panelists.

During Knowledge Summit 3, CEFIPRA partnered with French Embassy & Institut Francais in India (IFI) and organized workshops on Artificial Intelligence (AI) for Sustainable Agriculture and Healthcare, 25-26 Nov 2021.

Workshops on Artificial Intelligence (AI) in Healthcare and Sustainable Agriculture



CEFIPRA organized **workshops on Artificial Intelligence (AI), 25-26 Nov 2021 at the Indo-French Knowledge Summit 3. These workshops envisioned specific fields of application of AI in Healthcare and Sustainable Agriculture**.

The two-day workshop on Artificial Intelligence for Healthcare (AIH) was moderated by, Prof. Yann Busnel, IMT Atlantique, IRISA, France and Prof. Nikhil Pal, ISI Kolkata, India during Nov 25-26, 2021 with a focus on diagnostic assistance for health workers in rural or peri-urban areas, and on the sensitive issue of collecting and protecting health data.

There were eight speakers including three medical doctors, scientists from startup companies and researchers from renowned University. The following points emerged from the discussion over the two days: Any successful AI system for healthcare demands a large volume of reliable and labeled (annotated) data, which most often are not available. The abundance of missing data, unstructured nature and heterogeneous characteristics of the data pose a real challenge to develop practically useful AI/ML based healthcare applications. All the talks were technically very rich. Some of the talks focused on development of AI systems to reduce the cost of diagnosis, some focused on reducing the hazards and / or use of invasive techniques associated with diagnosis, some talked about development of light-weight and less data-hungry AI/ML algorithms, several emphasized on how to address the issues with real-life healthcare data and design useful AI/ML system on that; while majority of the speakers directly and indirectly indicated the need for having better accuracy in diagnosis and comfort of the patients. Last but not least, the issue of trust in AI was raised: practitioners and patients do not trust AI. It is essential that they start believing in the decision support process via AI. One way to solve this is to bridge the gap between discipline and AI experts: It is emphasised on building AI solutions on what and how we do instead of blind methods applied to databases. Prospective thematic areas emerged for the future:

1. Less data hungry and light-weight AI/ML algorithms and architecture.
2. Affordable rural healthcare support with AI/ML
3. Explainable AI/ML for healthcare.
4. Interoperability between health data warehouses, which works in silo only.
5. Making Health Data a Reality: engineer point of view (stress feature selection, CNN architectures, deep and federated learning deployment, etc.)

Workshops on Artificial Intelligence (AI) in Healthcare and Sustainable Agriculture

The Workshop on the contributions of AI to Sustainable & Precision Agriculture, was coordinated by Prof Pascal Weil from France and Prof Utpal Garain from India. In total, thirteen speakers presented their research studies during the two workshop days. The speakers were from diverse fields like Agronomy, Plant Science, Computer Science, Mathematics, Statistics, and Social Science. Two were from start-up companies (one from an Indian spin off and the other one from a French start-up). Apart from the speakers several participants attended the workshop and joined the discussion in the focus area of irrigation management & chemical inputs, and strategies of farmers for transport and the marketing of their productions. Within the scope of AI for agriculture, the following are important thrust areas.

1. Solutions based on image or remote sensing analysis (e.g. plant, pest or crop identification, yield estimates, monitoring of the welfare of farm animals).

2. Solutions based on heterogeneous data, mixing e.g. image, video, weather patterns or forecast, water management data, market information.

3. Solutions based on robotic intervention, for monitoring or for labour-intensive tasks for which labour is hard to find.

4. Interdisciplinary studies evaluating the accessibility of proposed solutions for farmers (on different sorts of farms) and the impact of these solutions, both at the local level and at broader scales. The involvement of social scientists would be essential in such studies.

Biocomposites from Sheep Wool form Excellent Insulation Panels

Wool is a premier protein fiber with distinct properties. Being made of proteins (keratin), wool has excellent elasticity, high warmth retention, flame resistance, ability to absorb volatile organic compounds (VOCs) and is easily biodegradable. About 1.2 billion sheep produce approximately 1.0 to 1. 2 million tons of fibers every year which is about 1% of the global fiber production. Wool considered to be a niche fiber, is preferred for apparels, carpets and furnishings. India produces about 40 million kilograms of wool fibers annually with most of the fibers used for knitwear. Despite such desirable properties and relatively low availability, only a small proportion of wool fibers can be utilized for textile and other high value applications. Only wool fibers have specific properties (length, fineness) are suitable for apparel and other high value applications resulting in major proportion of wool being discarded as waste. Several countries have classified wool as an agricultural byproduct and do not offer any incentives for utilization or value addition to wool. In India, sheep rearing is focused for production of meat and the wool fibers obtained are mostly classified as coarse wool (diameter higher than 32.5 microns) and unsuitable for high value apparel applications. Hence, such coarse wool and wool discarded as waste during shearing and processing are available in large quantities without major applications. Also, conventional use of coarse wool for carpets and rugs is also declining due to the preference for synthetic fiber based products. Disposable of waste wool is also a major concern since burning or burying of wool is restricted or prohibited in many countries. All of these factors combined with the unique properties (Figure 1) make a compelling case to consider waste wool for developing bio based products.

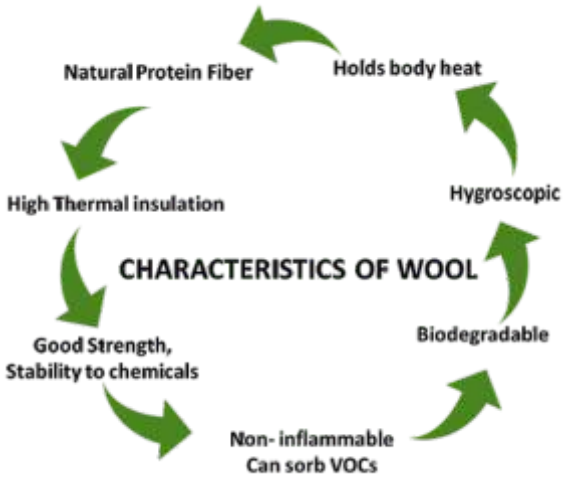


Figure 1: Properties of wool fibers

The ability of wool to absorb heat, noise and volatile organic compounds makes it an ideal fiber for developing insulation panels for building interiors. In this CEFIPRA funded project (project number 7134) with collaboration from researchers at **University of South Brittany** and **University of Montpellier**, we have attempted to develop biocomposites from waste wool for interior applications such as false ceilings, acoustic absorption panels in auditoriums and other civil constructions.

Figure 2: Process of developing biocomposites from discarded wool

The biocomposites have been developed using a simple compression molding technique. Two approaches have been used to develop the wool based biocomposites. In the first approach, wool fibers were used as reinforcement for gypsum and the changes in properties were studied. However, the amount of fibers that could be used was restricted to 30%. Coir fibers were also used with wool to improve strength and durability. The composites obtained had thermal conductivity between 0.17-0.30 W/mk and sound absorption coefficient between 0.15-0.35 (**Guna, et.al. Wool and coir fiber reinforced gypsum ceiling tiles with enhanced stability and acoustic and thermal resistance." Journal of Building Engineering 41 (2021): 102433**). Since gypsum is non-biodegradable and the amount of wool fibers used was low, the research team attempted to develop biocomposites using polypropylene as the matrix in the second approach. As shown in Figure 2, waste wool was combined with polypropylene and compression molded into composites of varying fiber proportion, density and thickness. Composites with 80% of sheep wool and only 20% of the binder could be developed. These composites have thermal conductivity of 0.194 W/mK and sound absorption co-efficient of 0.5.

Based on these studies, it is reasonable to consider discarded wool for developing insulation panels.

Similar to wool, poultry feathers are made up to proteins (keratin), are generated in large quantities and disposed as waste. Feathers have low density and excellent noise and thermal insulation properties. Hence, we have considered combining wool with poultry feathers in various proportions and developing insulation panels. Composites developed using the wool and feather blends (50/50%) have thermal conductivity of 0.397 W/mK and acoustic sorption of 0.56.

Studies conducted so far have been very encouraging in converting the waste wool into insulation panels. However, challenges such as the collecting, cleaning and washing wool without using excessive chemicals and water are being investigated. Various wool varieties are being collected and their influences on the properties of the composites are being analyzed. Being a natural fiber, wool is susceptible to attack by moths, microorganisms and moisture. The most effective and biological approaches to protect wool and the biocomposites from environmental degradation will be studied in the next part of this project. The Indian part of this collaborative project has been financially supported by **Agringenium Innovations Private Limited**, a start-up located in Bengaluru. The researchers estimate that that the biowool based ceiling tiles can be economically competitive to the gypsum based ceiling tiles and could also attract a premium based on the environmental, social and technical considerations of using discarded wool.

PROPERTIES OF BIOWOOL COMPOSITES COMPARED TO GYPSUM FALSE CEILING TILES OF SIMILAR DENSITY

Biocomposite Composition	Tensile Strength, MPa	Flexural Strength, MPa	Thermal Conductivity (W/mK)	Sound Absorption Coefficient
Wool-gypsum (%/%)	-	1.86	0.308	0.32
Wool-Polypropylene	10.3	55.6	0.194	0.52
Wool-coir-gypsum	-	3.78	0.305	0.35
Wool-feather-polypropylene	9.68	13.15	0.397	0.56
Commercial gypsum ceiling tiles	9.60	7.16	0.057	0.50

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Forthcoming Meetings...

1. **37th Industrial Research Committee (IRC) meeting,** 7-8 January, 2022
2. **67th Scientific Council (SC) meeting,** 10-13 January, 2022

Both the meetings will be held virtually.

Pathogenic Aspergillus
(Grant No. 5403-1)

Although fungal diseases do not convey the attribute epidemics, they are increasingly and rapidly becoming a significant medical problem. The high mortality rate due to invasive fungal infections (IFI) could be comparable to tuberculosis and malaria. Nevertheless, research on IFI is a disregarded field in many parts of the world. Among IFI causative agents, airborne pathogens play a crucial role and are responsible for diseases in both immunocompetent and immunocompromised individuals.

We were funded by CEFIPRA to work on pathogenic *Aspergillus* species, the major airborne fungal pathogens. Although belong to the genus *Aspergillus*, *A. fumigatus* is primarily involved in invasive pulmonary infection, whereas *A. flavus* is a common cause of superficial infections including fungal keratitis, an infection of the eye. The infective propagules of these two *Aspergillus* species are their asexual spores (conidia). We compared them to understand conidial predilection to different infection niches. Morphologically, *A. fumigatus* conidial sizes were uniform (2.6 ± 0.2 mm) with proteinaceous rodlet layer covering conidial surfaces, whereas *A. flavus* conidial size varied between 5.2±1.9 mm with a heterogenous surface architecture and exposed cell-wall polysaccharides. Owing to these features, conidia of *A. fumigatus* were hydrophobic, while that of *A. flavus* were hydrophilic. This could partially explain why the hydrophobic conidia of *A. fumigatus* can easily reach up to the lung alveoli while hydrophilic nature of *A. flavus* facilitates them to cause mostly superficial infection.

Intranasal administration (the natural route of conidial entry into human system) of both *A. fumigatus* and *A. flavus* conidia resulted in a proinflammatory immune response in immunocompetent mice. However, *A. flavus* conidia stimulated significantly higher secretion of cytokines compared to that of *A. fumigatus* conidia. This suggests that inhaled *A. flavus* conidia are better cleared by our immune system. On the other hand, conidia must germinate (forming mycelia) to establish an infection and the germinating conidia of these two *Aspergillus* species showed significant differences in their cell-walls, the first fungal component to interact with the host immune system. Chitin content in the *A. flavus* mycelial cell-wall was significantly higher than *A. fumigatus*; chitin, a homopolysaccharide composed of N-acetyl-glucosamine is responsible for the cell-wall rigidity. Galactosaminogalactan (GAG), a germination specific heteropolysaccharide composed of galactose, galactosamine and N-acetyl-galactosamine, was found associated with the rigid fibrillar structure of the cell-wall of *A. flavus* unlike in *A. fumigatus* where it does not contribute for the fibrillar structure. Further, b-1,3-glucan, a major polysaccharide in the cell-wall, had more ramification in *A. flavus* compared to *A. fumigatus*. Overall, the differential arrangement of polysaccharides explains higher rigidity of the *A. flavus* mycelial cell-wall compared to that of the of *A. fumigatus* mycelial cell-wall. Differential rigidity of the cell-walls of the two *Aspergillus* species contributed to the differences in antifungal susceptibility. Compared to *A. fumigatus*, *A. flavus* was

French partners visited the organization of the Indian partners

less susceptible to the cell-wall targeting antifungals, caspofungin and nikkomycin, the inhibitors of b-1,3-glucan, and chitin biosynthesis, respectively. Differences between *A. fumigatus* and *A. flavus* was not only restricted to the polysaccharides in the cell wall but reflected in the conidial surface proteome as well as germinating conidial exoproteome. In both these proteomes, although the two *Aspergillus* species shared a core common proteome, each of them possessed a species-specific signature proteome that could help them adapt to the different infection niches, namely the lung and the cornea. Translationally, these species- specific proteome profile could be of interest in the diagnosis of their infections.

In essence, we have deciphered the molecular differences associated with the two most pathogenic *Aspergillus* species, *A. fumigatus* and *A. flavus* (Wong SSW et al., 2021). Our study highlights the differences between the two Aspergillus species, thereby emphasizes the need for species-specific antifungal treatment. This is essential while undertaking antifungal regimen for invasive pulmonary aspergillosis (IPA) patients, as, although *A. fumigatus* is the major species responsible for the fatal IPA, owing to the abundance in the environment and the ability to survive in humid environment, *A. flavus* is the predominant species causing IPA in Africa, Asia and in the Middle East countries.

On the other hand, *Aspergillus* conidia being airborne, interact first with alveolar environment or the ocular surface. However, most of the in vitro studies on conidial interaction with the host immune system make use of human/fetal calf serum in the culture medium. Moreover, the alveolar immune system is comprised of both cellular and humoral immunity; nevertheless, the role played by humoral immunity has been understudied in the context of airborne fungal pathogens. When we opsonized *A. fumigatus* conidia with pooled human serum or bronchoalveolar lavage from control individuals, followed by extracting conidial surface bound proteins and subjecting them the proteomic analyses, we could observe that at least 22-25 different humoral immune components interacting with the conidial surface, suggesting that they may play a crucial role, as most of them are pattern-recognition receptors. While humoral immune components identified upon conidial opsonization with serum or bronchoalveolar lavage showed significant differences, which further impacted their interaction with human macrophages, the major innate immune cells in the alveolar environment (Wong SSW et al., 2020). We extended this work to *A. flavus* conidial opsonization with the bronchoalveolar lavage and identified that there were substantial differences in the interaction of humoral immune components in the lavage with *A. fumigatus* and *A. flavus*. Thus, it is essential to select experimental conditions almost mimicking the natural niche of a pathogen to study their pathobiology.

Human fungal pathogens, including *Aspergillus* species, are the hidden killer. In healthy indivuduals they are eliminated without altering host system, but in vulnerable hosts they become opportunists leading to infection. The best example in the current pandemic situation is the COVID19 associated pulmonary aspergillosis (CAPA), where IPA is an emerging complication among patients in intensive care unit (ICU) with acute respiratory distress syndrome (ARDS) receiving corticosteroids treatment. Moreover, unlike bacterial and viral pathogens, highly adaptative nature and occurrence in different morphotypes bring in additional complication associated with fungal infection. Therefore, focused pathobiological study is needed to understand fungal infections, to develop appropriate therapeutic strategy. In this regard, we are grateful to CEFIPRA for funding our project, through which we could demonstrate the molecular mechanisms associated with two most important pathogenic species of Aspergillus worldwide while establishing their pathogenicity.

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Pre-evolutionary processes inautocatalytic RNA networks (CEFIPRA Project 5904-G)

Overview

The emergence of life on earth is one of the most fundamental questions driving scientific enquiry and exploration. One such interdisciplinary approach employed by Sandeep Krishna from the Simons Centre at NCBS and Philippe Nghe from ESPCI Paris uses 'RNA-based autocatalytic systems' to further our understanding of the mechanisms of the origin of life.

Autocatalytic systems are basically collections of components such as biomolecules and chemical reactions capable of information storage as well as catalysis of their own replication, thus allowing them to be self-sustaining systems. Such autocatalytic systems can be composed of biomolecules like RNA and/or proteins that act as catalysts - molecules that increase the rate of chemical reactions without directly being consumed in these biochemical reactions.

As part of a CEFIPRA-funded grant, the scientific teams of Sandeep and Philippe are collectively employing such self-reproducing RNAs as a starting point to develop RNA networks with evolutionary properties. Such RNA-based autocatalytic networks can be used to eventually implement Darwinian evolution from chemicals for the first time ever.

In this regard, the Indo-French team of researchers have developed a technology for screening a large diversity of autocatalytic networks using methods like microfluidic droplets, molecular bar-coding, and Next-Generation Sequencing. This has allowed them to characterize the growth rate of networks, study the network determinants of heredity, model the perturbation laws within such networks, and understand the conditions for their evolution. They have also studied the topological determinants of compositional memory, which is a necessary condition for heredity and the only remaining pre-requisite for Darwinian evolution, apart from variation and selection.

Sandeep Krishna

Collaborative Journey

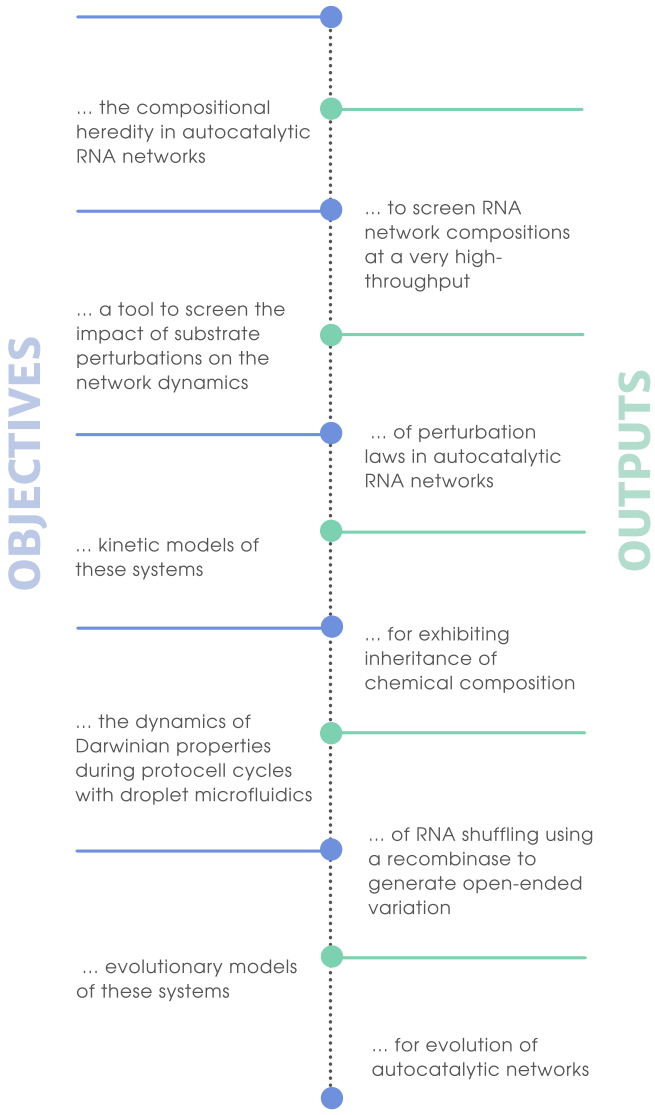
The COVID-19 pandemic caused some major road blocks to the project, especially given the team was split across three different geographical locations. In particular, we had to cancel several exchange visits planned for the scientific staff working on this project, which would have greatly helped advance the different strands of the project, such as a closer integration of theoretical and experimental aspects.

Nevertheless, we have managed to keep the project active and running by relying on measures such as virtual meetings and continued generating scientific outputs such as scientific publications, conference papers, talks and posters, as well as external grant awards.

So far, we have published three major papers and have a couple more in the pipeline. I'm particularly proud of the paper where we used a combination of models and experiments to show how the Azoarcus ribozyme system is capable of generating a diversity of molecules in an open-ended way - a crucial element in the exploration of chemical space that must have happened around the origin of life.

Preliminary findings of these researchers found heredity to be limited by the presence of self-assembled catalysts that form spontaneously. They are now exploring mutated sequences of RNAs that can still self-reproduce but do not form a self-assembled catalyst.

The researchers have also discovered that the RNA recombinase frequently used by them as a self-reproducing system, is also capable of shuffling other RNA fragments to generate completely new RNA sequences with potentially novel properties. This is an exciting and unexpected finding and the team is currently investigating (both theoretically and experimentally) this exciting capability to shuffle sequences under recombination and its wider implications for evolution.



ACHEIVEMENTS

- **3** Publications
- **7** Conference papers
- **3** Presented posters
- **7** Exchange visits
- **9** Personnel trained
- **1** Knowledge product
- **1** HSFP Grant awarded
- **1** ERC Grant awarded

Role of CEFIPRA

The CEFIPRA grant has been extremely stimulating for the collaboration between ESPCI Paris and NCBS Bangalore, and greatly strengthened the bonds between the two institutions. In particular, it has allowed both partners to expand the group of people working on this system, broaden the scope of scientific questions being addressed, and served as acritical catalyst to push for other sources of funding such as the ERC and HSFP grants.

Philippe Nghe

Sandeep Krishna
NCBS
Bangalore

Philippe Nghe
ESPCI
Paris

Novel chiral first-row transition metal complexes for asymmetric catalysis via activation of inert c-h and c-heteroatom bonds

ABSTRACT. Enantioselective homogeneous catalysis, which is a cornerstone of sustainable development, commonly employs rare and expensive heavy transition metals. Efficient catalysts based on more abundant elements are investigated within this Indo-French collaborative project.

The ambitious initial objectives of this project were to develop new efficient asymmetric transformations of unreactive substrates catalyzed by inexpensive first row transition metals (cobalt, iron and manganese) for via the so-called "borrowing hydrogen" methodology, which consists of the substrate activation by dehydrogenation, followed by transformation of the more reactive intermediate and final rehydrogenation of the unsaturated product. The Indian team is expert in borrowing hydrogen chemistry catalyzed by base metals but had previously used only achiral catalysts, whereas the French team is specialized in the synthesis and catalytic application of chiral ligands, particularly those that take advantage of the planar chirality of 1,2-disubstituted ferrocene. In addition, the French team is well-versed in the application of the computational approach to the mechanistic investigation of catalyzed processes.

In this regard, the French team has developed hitherto unknown hetero di- and trifunctional pincer ligands based on the ferrocene platform in multi-step syntheses, containing various combinations of phosphorus-, sulfur- and nitrogen-donor functions (PSP, PNN, PNP). All these ligands could be efficiently synthesized in either racemic or enantiomerically pure form for each enantiomer. A few unexpected results obtained during these ligand synthesis studies have also opened the access to new efficient transformations of potential used in other areas, for instance a two-step thioacetylization/reductive alkylation, which results in an efficient transformation of an alcohol to a thioether when other known strategy (e.g. via carbocation or by alcohol/mercaptan activation by a combination of phosphine and a diazadicarboxylate ester, the so-called Mitsunobu conditions) are unsuccessful or require the use of toxic and not easily handled volatile mercaptans. Delays related to the COVID pandemics (laboratory shut-downs, travel restrictions, compound shipment delays) have not allowed the ligands to be transferred to the Indian partner and tested in catalysis prior to the end of the project, but the collaboration will continue.

In parallel, the Indian partner has pursued the exploration of an efficient catalytic system based on cobalt(III), in conjunction with mechanistic investigations by the French team. This work has resulted in the extension of the borrowing hydrogen strategy with the use of Cp*Co(III) molecules (Cp* = pentamethylcyclopentadienyl) to secondary alcohols (ROH) as alkylating agents for the alkylation of variety of primary aniline derivatives and amides ($ArNH_2$ and $R'CONH_2$, with C-N bond formation to yield the corresponding secondary aniline derivatives ArNHR and amides R'CONHR) [1], bulky aromatic methyl ketones ($ArCOCH_3$, with C-C bond formation to yield $ArCOCH_2R$) [2], carbonucleophiles such as oxindoles, benzyl nitrile and barbituric acid with C-C bond formation to yield the corresponding C-alkylated products at the position relative to the carbonyl carbon, e.g. 3-R-alkylated oxindoles [3]. A high impact of this work is the possibility to accomplish a large scope of useful transformations with a much less expensive and abundant metal (cobalt) than those developed until now (iridium, ruthenium).

An additional relevant achievement concerns the mechanistic understanding of these Cp*Co(III)-catalyzed reactions. Certain experimental observations could not be rationalized based on all known borrowing hydrogen mechanistic paradigms, notably the first key step of secondary alcohol dehydrogenation. The extensive computational work by the French team, complemented by key experiments involving the synthesis of model systems and kinetics investigations by the Indian team, led to the unveiling of a new paradigm. While for all previous transformations the substrate dehydrogenation was proven (or assumed) to involve transfer of the two H atoms either as two H- (hydrides) to the metal catalyst with concomitant metal oxidation or as one hydride and one proton with oxidation state invariance, the present system is shown to borrow the two H atoms as two protons with concomitant two electron reduction of the catalytic system. The two protons are stored on the ligand system and/or on an external base [4]. This new pathway may also be relevant for other potentially reduceable catalysts hitherto believed to operate via one of the other two previously established dogmas.

1. B. Emayavaramban, P. Chakraborty, E. Manoury, R. Poli, B. Sundararaju, "Cp*Co(III)-Catalyzed Direct Amination of Secondary Alcohols", Organic Chemistry Frontiers 2019, 6, 852-857. DOI: 10.1039/c8qo01389f.

2. P. Chakraborty, M. K. Gangwar, B. Emayavaramban, E. Manoury, R. Poli, B. Sundararaju, "Well-defined Cp*Co(III)-Catalyzed α-Alkylation of Ketones with Secondary Alcohols", ChemSusChem 2019, 12, 3463-3467. DOI: 10.1002/cssc.201900990.

3. P. Chakraborty, N. Garg, E. Manoury, R. Poli, B. Sundararaju, "C-Alkylation of Various Carbonucleophiles with Secondary Alcohols Under CoIII-Catalysis" ACS Catal. 2020, 10, 8023–8031. DOI: 10.1021/acscatal.0c01728.

4. P. Chakraborty, B. Sundararaju, E. Manoury, R. Poli, "A new borrowing hydrogen mechanism for redox-active metals" ACS Catal., 2021, in press. DOI: 10.1021/acscatal.1c02616.

International workshop organized at the end of the project

The international workshop "Virtual Symposium on organometallic chemistry and catalysis", co-organized by the two teams and featuring 12 distinguished speakers from India, France, Spain and Germany over three days (8-10/12/2020) attracted over 850 registrations from > 100 different institutions worldwide.

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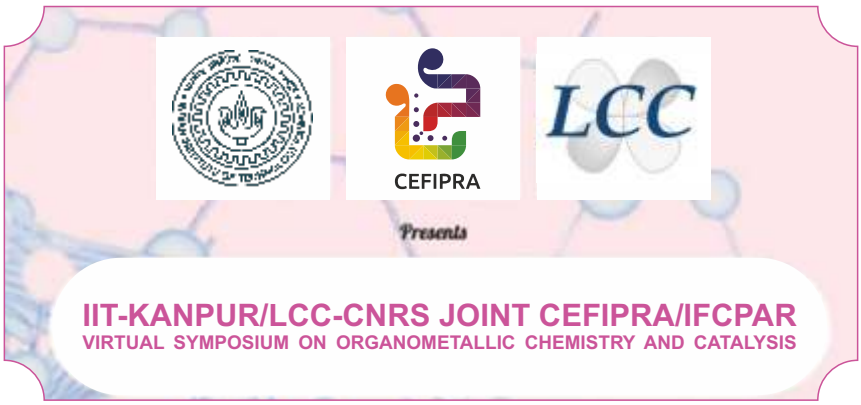
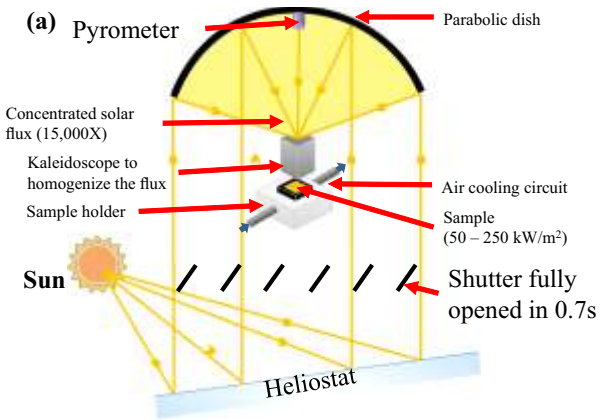


A novel high temperature selective coating on superalloy substrates stable up to 600°C in air for solar thermal electricity receivers: Studies on improved efficiency and accelerated aging tests

Summary

A novel high temperature stable tandem absorber of WAlN/WAlSiN/SiON/SiO_2 has been developed on various substrates with very high absorptance (0.955) and low thermal emittance (0.10). Complete characterization of the developed coating has been done using FESEM, AFM, SAD, HRTEM, XPS, FTIR, UV-Vis-NIR, scratch tester, etc. to understand the microstructure and optical properties. The thermal stability studies were carried out till 700°C in air and vacuum. Further, solar accelerated aging tests of the developed coatings were carried out in a solar furnace (SAAF) along with high temperature measurements of optical properties up to 500°C.

Performance Evaluation of the Solar Absorber Coating: Testing Under Solar Accelerated Ageing Flux



The coating exhibits superior mechanical properties. In addition, thermal shock tests at high temperatures and solar accelerated ageing measurements are investigated in-depth to analyze the performance of the solar absorber coating. The thermal shock tests of the samples at various temperatures in the range of 500 - 600°C depict the excellent thermophysical resistance of the as-deposited samples. To test the thermal durability of the solar absorber coating, we applied 200 cycles of solar accelerated ageing on the samples using a solar accelerated ageing facility with concentrated flux density varying from 50 to 300 kW/m2. These cycles have been defined to replicate real high solar flux and temperature on the front side of the samples along with high cooling and heating rates, reproducing the abrupt variations of solar irradiation due to cloudy weather and subsequent thermal shocks for a given receiver. Overall, the durability tests of the solar absorber carried out under various conditions indicate an insignificant change in optical properties, thus, making it a potential candidate for high-temperature solar thermal applications.

Dr. Audrey delivering a lecture on "Materials and coatings for concentrated solar energy applications" at CSIR-NAL, January 21, 2020

Achievements

1. Development of a novel high temperature stable tandem absorber of WAlN/WAlSiN/SiON/SiO_2 on various substrates with very high absorptance and low thermal emittance.

2. Complete characterization of the developed coating using FESEM, AFM, SAD, HRTEM, XPS, FTIR and UV-Vis-NIR spectrophotometry, scratch tester, etc. to understand the microstructure and optical properties.

3. Thermal stability studies carried out till 700°C in air and vacuum. Coating stable up to 700°C in vacuum for longer durations (200 hrs).

4. Solar accelerated cyclic thermal ageing tests of the developed materials in a solar furnace with concentrated solar irradiance typical of aimed CSP applications (SAAF). Coating stable in such conditions up to 450°C.

5. High temperature measurements of optical properties, up to 500°C, for better representativity of performance assessment.

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No. of publications in SCI journals where IFCPAR/CEFIPRA has been acknowledged (for the whole duration):

1. Temperature and angle-dependent emissivity and thermal shock resistance of W/WAlN/WAlON/Al2O3-based spectrally selective absorber, Atasi. Dan, A. Soum-Glaude, A. Carling-Plaza, Clifford Ho, K. C. Chattopadhyay, H. C. Barshilia, Bikramjit Basu, ACS Applied Energy Materials 2 (2019) 5557.
2. Optimization of W/WAlSiN/SiON/SiO2 tandem absorber consisting of double layer anti-reflection coating with broadband absorption in the solar spectrum region, K. Niranjan, P. Kondaiah, G. Srinivas, H. C. Barshilia, Applied Surface Science 496 (2019) 143651.
3. Extremely high temperature stable nanometric scale multilayer spectrally selective absorber coating: Emissivity measurements at elevated temperatures and a comprehensive study on ageing mechanism, K. Niranjan, Audrey Soum-Glaude, Alex Carling-Plaza, Sandip Bysakh, Siju John, Harish C. Barshilia, Solar Energy Materials and Solar Cells 221 (2021) 11095.
4. Performance evaluation and durability studies of W/WAlSiN/SiON/SiO2 based spectrally selective solar absorber coating for high-temperature applications: A comprehensive study on thermal and solar accelerated ageing, K. Niranjan, Alex Carling Plaza, Théo Grifo, Martin Bordas, Audrey Soum-Glaude, H. C. Barshilia (submitted to Solar Energy).

No. of papers presented in conference:

High temperature emissivity and thermal stability of W/WAlSiN/ SiON/SiO2 solar selective tandem absorber coatings, K. Niranjan, Alex Carling Plaza, Théo Grifo, Paruchuri Kondaiah, Audrey Soum-Glaude, H. C. Barshilia, presented at 26th SolarPACES Conference 2020, September 29 – October 2, 2020, online event.

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CALL FOR PROPOSALS

under CSRP - Thematic Research

(Deadline for submission of Proposals 15 Jan, 2022)

CEFIPRA considers and supports research groups through high quality collaborative research projects in advanced areas of basic and applied science to nurture scientific competency in India and France. For upcoming cycle the thematic research specifically aims at contributing to solving important societal challenges. The four areas research themes covering cross-disciplinary (or interdisciplinary) issues.

Eligibility to apply

Principal Collaborators and Joint Collaborators (Indian & French) should have permanent position in an Indian or French University/R&D Institution. They should meet national level eligibility criteria with respect to the operation of grants and age of retirement.

Funding support for the proposals

- Manpower (PhD/Post-doctoral/Master students positions for French Partners; JRF/SRF/RA/Master students for Indian Partners)
- Purchase of consumables
- Travel (International & domestic)
- Equipment (only to Indian Partners : Minor equipment and accessories which are essential for the project with a limit of max. of 10% of total approved budget of the project (max. 20.000Euros))

The four thematic areas are:

Topic 1 : AI & Big Data

The aim of the thematic is to promote new research on the use of Artificial Intelligence (AI) and Big Data. The thematic will be structured around (but not limited to) the following areas:

- Applied Artificial Intelligence and real-life applications of AI
- Cyber-Physical Systems (CPS)
- Internet of things (IoT)
- Machine Learning / Deep Learning Applications
- Cloud / Edge Internet of Things
- Distributed Big Data Analytics
- Intelligent Agent Applications
- Data and Model reduction

There should be significant novelty in the computer science aspect of the proposal.

Topic 2 : Science for Sustainability

It includes, but not limited to, fundamental research on

- Better practices for the preservation of water resources
- Zero or low carbon emission technologies for an increased climate action
- The preservation of ecosystems and biodiversity
- Minerals resources and recycling technologies
- Science and policy for sustainability

Topic 3 : Quantum Materials

Quantum materials are materials where the quantum mechanical effects underline their physical properties, being dominated by quantum fluctuations, quantum entanglement, quantum coherence, topological behavior. The research in this interdisciplinary area which may include theory/modeling, advanced instrumentation, materials synthesis, knowledge of nano- and meso-scale science is at the intersection of physics, material science and engineering.

Key-words: Novel phenomena in topological materials like Topological Insulators. Dirac and Weyl semimetals, Quantum Spin Liquids, superconductors and their hybrids with possible applications such as ultra-sensitive sensors, Heterostructures of 2D materials, Discovery and growth of novel high-quality quantum materials by different methods, Quantum Materials Theory

Topic 4 : Addressing Biological Questions Using or Developing Mathematical, Computational or Physical Approaches

Elaboration of concepts, development of novel approaches or use/adaptation of innovative methods of physics, mathematics and computational sciences for addressing biological questions. A particular attention will be paid to the following fields (not limited): Data acquisition, treatment and analysis, interoperability; Predictive analysis; Simulation; Quantitative biology; Mechano biology; Single molecule studies.

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