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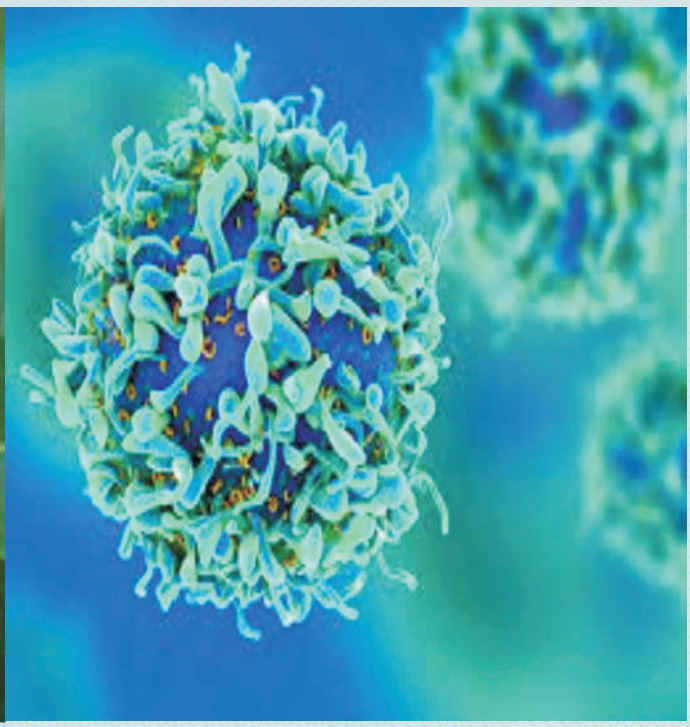
R&D NEWSLETTER

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

Rosy periwinkle plant



Carbon nanodots adhering to target cells

A novel, fluorescent agent has been developed froma plant source for simultaneous detection and destruction of cancer cells.Thesenano sized carbon materials have been synthesized from the leaves of the rosy periwinkle plant. The material has the potential to track cancer cells by an imaging system and can serve as an efficient diagnostic and therapeutic agent (theranostic) for cancer. This workhas been carried out by Prof. P. Gopinath and his research group at the Department of Biotechnology with funding support from SERB and DBT, Govt. of India.

Recently Registered Research Projects

Organotin (IV) Carboxylates and their Mixed Ligands Compounds as Potential Chemotherapeutics and Study of Mechanism of their Cytotoxicity

Sponsor: Department of Biotechnology, Govt. of India

Prof. Mala Nath

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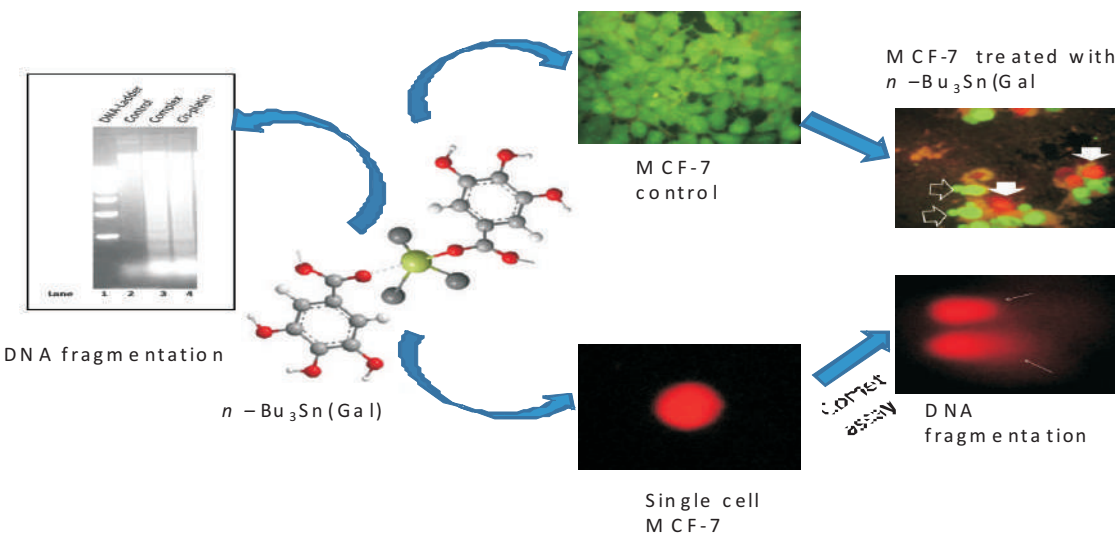
Abstract: Organotin(IV) carboxylates having very low IC50 values could be applied for the development of new anti-cancer drugs. However, the low solubility of organotin compounds poses an important difficulty, which may be partially addressed through the use of hydrophilic groups such as flouro and hydroxyl groups. Therefore, the main objective of this project is to synthesize new organotin carboxylates with more electronegative hydrophilic substituents and their mixed ligand complexes with heterocyclic N-donors such as *o*-phenanthroline and benzimidazole derivatives in order to individuate a balance between solubility and lipophilicity features to achieve better efficacy. Further, the mechanisms of action of organotins on biological targets are often different or not well known, so new biophysical techniques along with antioxidant enzymes, staining and DNA fragmentation assays need to be applied to understand where the organotin(IV) compounds exert their cytotoxicity.



Activation of C-H bond and synthesis of organometallic ruthenium and palladium complexes: Applications in organic syntheses and a search for new directing group(s).

Sponsor: Council of Scientific and Industrial Research (CSIR, India)

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Abstract: Functionalization of non-activated C-H bond catalyzed by transition metal ion is an important area of chemical research. The selectivity of a particular type of C-H bond (phenyl hydrogen, alkyl, aryl or vinyl) is control by the relative strain of the constrain bond or by intra-molecular hydrogen abstraction. With the development of organometallic complexes a variety of methods have become available for site-selective C-H functionalization. Hence in the recent years there are many example of C-H activation via transition metal centre(s), often under remarkably mild conditions with high selectivity. Such studies are not only important in organometallic chemistry but also such studies give rise new methodologies for synthesis of important molecules like drugs molecule, natural products molecular material and polymers.

Antimicrobial resistance and pollutants: interactive studies and novel sensor technologies

Sponsor: Natural Environment Research Council-Department of Science and Technology

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Abstract : Antimicrobial resistance (AMR) represents a major threat to modern healthcare. In India, the high unsupervised consumption of antibiotics, ubiquitous presence of AMR, and high levels of pollutants that exacerbate the problem. This project aims to develop novel sensors to detect and monitor pollutants focusing on studying AMR co-selectors to improve the understanding of how these pollutants mediated and impact AMR with five integrated work-packages that will i) Identify novel polymers for pollutant pre-concentration (potentially removal at source) and integration into

sensors; ii) Develop novel sensors to detect and monitor heavy metals, antimicrobials and AMR genes; iii) Create low-cost paper-based sensors for pollutants; iv) Create easy-to-use, robust, low-cost integrated detection systems; v) Undertake case studies to identify the main AMR genes and levels of pollutant at test sites in India and the UK, and validate the performance of detection methods.

Chemical genetic approaches for discovery of novel antibacterials against antibiotic resistant gram- negative bacterial pathogens

Sponsor: Department of Science and Technology-Science and Engineering Research Board

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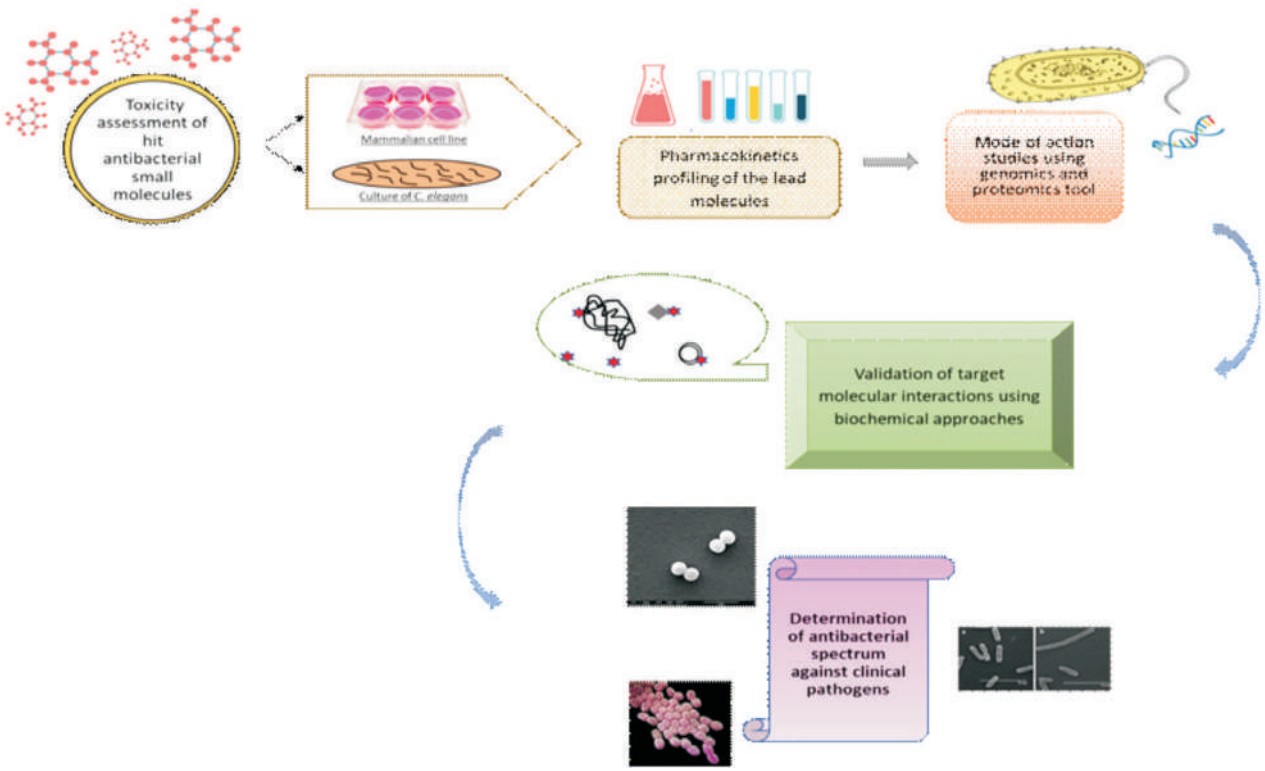
Abstract : Antibiotic resistance is a grave threat to the human health and needs immediate action. The drug discovery pipeline against multiple drug resistant pathogens is drying fast and needs multiple lead molecules that can be picked up by the Pharmaceutical companies for further clinical studies. Our team is using chemical genetic approaches for drug discovery against antibiotic resistant pathogens. Our efforts are targeted towards multiple pathways so that it is difficult for the pathogens to develop resistance against newly discovered lead molecules.



To achieve this, we will screen small molecule leads with demonstrated antibacterial potential (already characterized in a primary screen) for their toxicity in mammalian cell lines and *C. elegans* followed by their pharmacodynamics and pharmacokinetic studies.

Further, the targets of the lead molecules will be discovered in bacterial pathogens using genomic and proteomic tools. Antibacterial therapeutic potential will be assessed on clinical pathogens. This study is expected to discover novel and effective antibacterial molecules with clinical relevance and the lead molecules will have a potential to be taken up for clinical studies.

Study of thermospheric and mesospheric cooling by using Nitric Oxide radiative emissions

Sponsor: Department of Science and Technology- Science and Engineering Research Board

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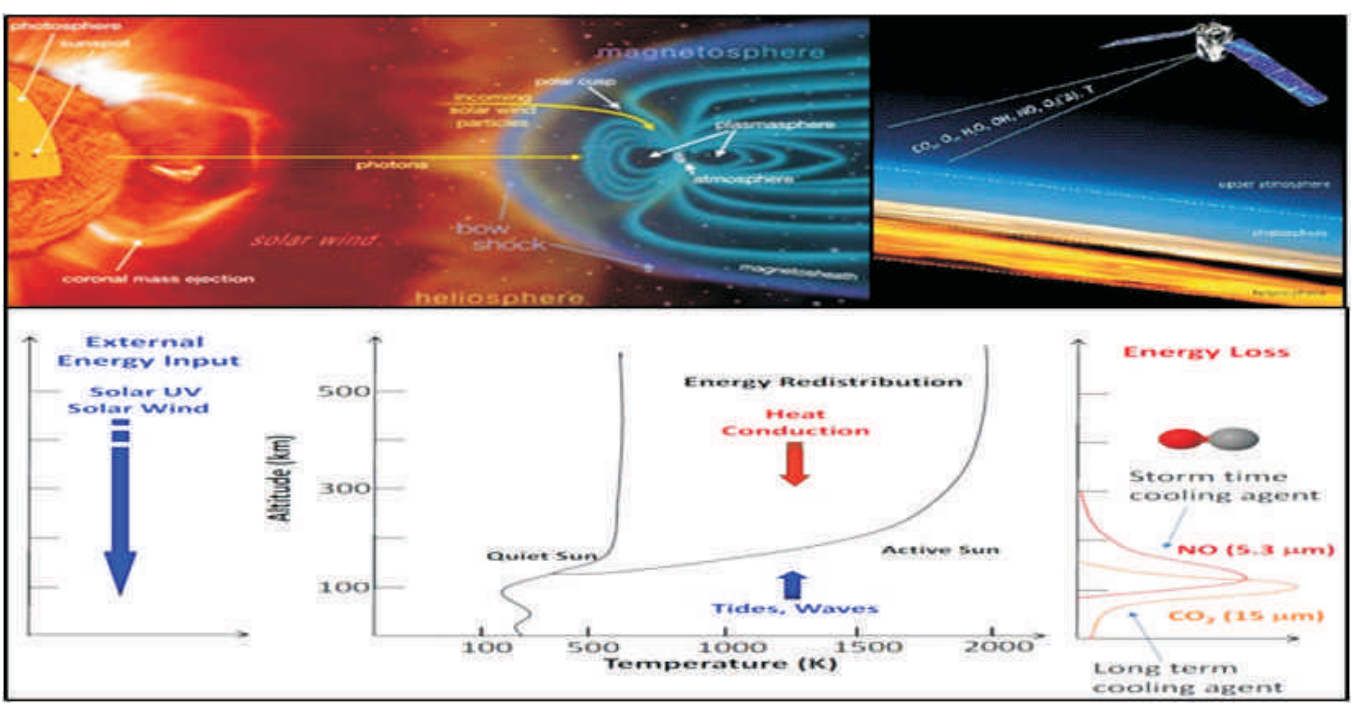
Abstract : The Sun is a variable star and solar prominences such as coronal mass ejections and flares are most frequent when the Sun is active. During these events highly energetic plasma outbursts reach the earth triggering large fluctuations in the Earth's magnetic field and cause a drastic change in the overall



Space weather modulation of geospace (T), excess energy loss during magnetic storms by radiative cooling mechanism (B)

heat budget. Nitric Oxide is a very important trace species in thermosphere which radiates this excess energy at 5.3 μm into space and is generally called as Earth's natural thermostat. In this project we plan to implement global atmospheric models such as WACCM-X and TIE-GCM in combination with physics based models and satellite data to understand the effect of extreme space weather events on the thermospheric and mesospheric heat budget. This study aims to uncover less understood effects of proton and HILDCAA events on the upper atmospheric processes.

Computational designing of stimuli responsive complexes basedon Carbon nanostructures

Sponsor: Department of Science and Technology-Science and Engineering Research Board

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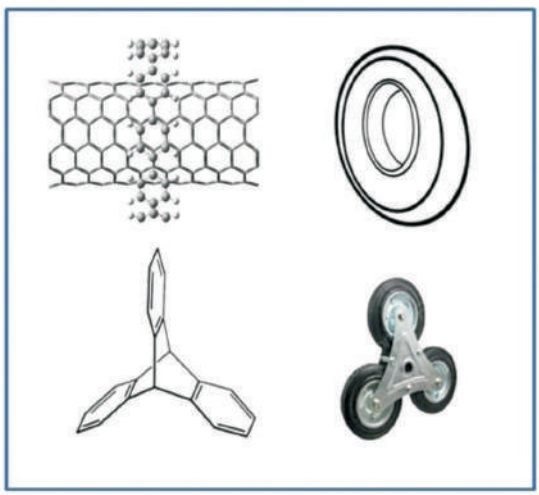
Abstract: Molecular motors, the microscopic analogues of large scale machines at the molecular level have received significant attention recently. With the advances in science and technology molecular structures that resemble macroscopic machines have been developed. However, such molecular architectures developed/proposed have a large number of flexible bonds (eg. Alkylchains) in their backbone leading to multiple configurations thereby limiting their applications.



Molecular analogues of bearings and wheels

The present project is an attempt in this direction. The project aims on the designing of stimuli responsive molecular structures based on different carbon nanostructures which impart structural rigidity along with multiple functionality.The individual and collective movements of various components of the systems in presence of external stimuli such as light, electric field and magnetic field will be investigated for their possible applications in the form of bearings, wheels, actuators, nanofluidic pump etc.

Development of a rapid and robust high throughput reporter cell based bioassay for detection of xenobiotics in milk

Sponsor: National Agricultural Science Fund (NASF), Indian Council of Agricultural Research, New Delhi

Prof.Partha Roy

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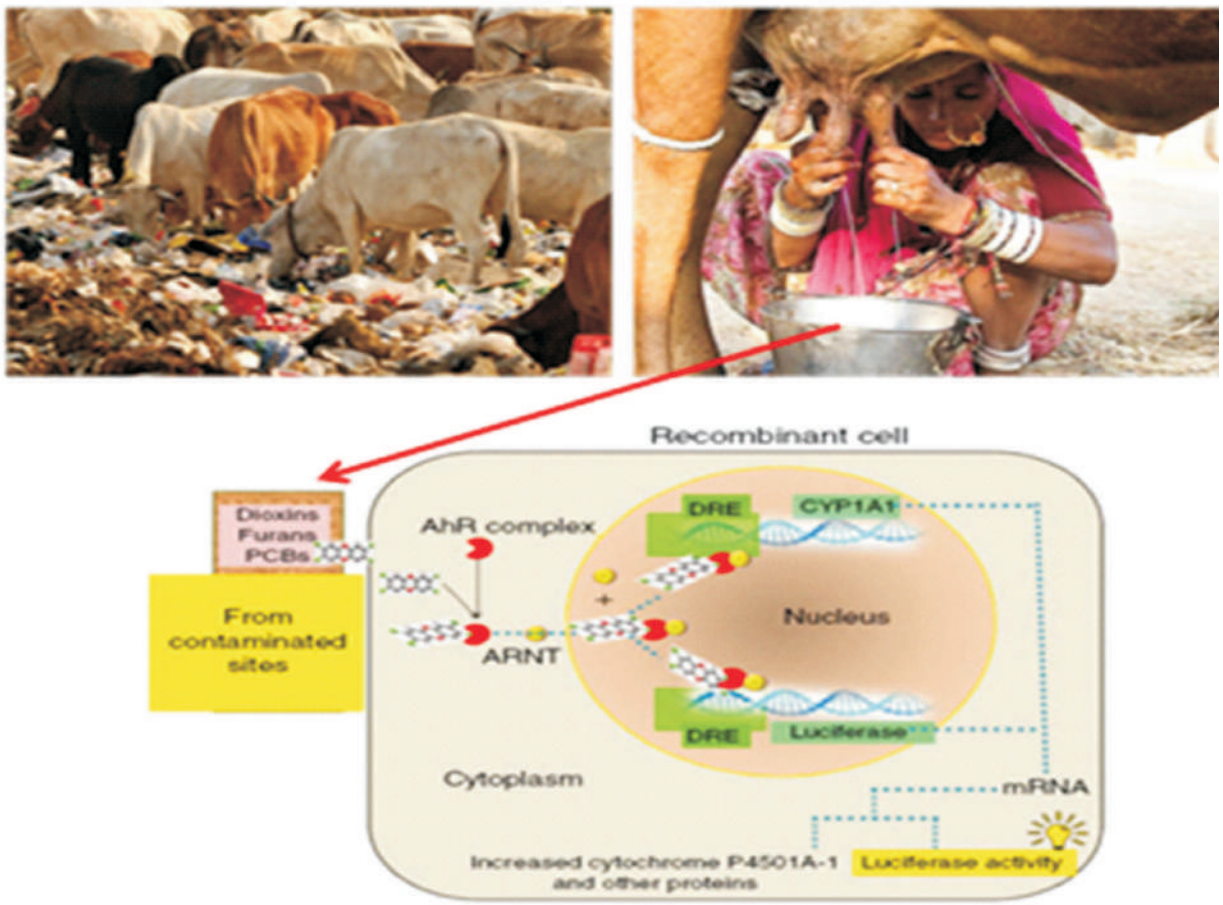
Abstract: Milk in its natural form has a high food value, since it is comprised of a wide variety of nutrients, which are essential for proper growth and maintenance of a healthy human body. In recent decades, there has been an upsurge in milk consumption worldwide, especially in developing countries, and it is now forming a significant part of the diet for a high proportion of the global population. Unfortunately, Indian milk was found to have traces of metabolic/endocrine disrupting chemicals (EDCs), which enter our body through dietary constituents. Such findings created a depraved propaganda by International media stating that Indian cows produce toxic milk as many of dairy animals in our country are fed on garbage, chemical enriched fodder including plastic bags, grazing lands contaminated with pesticides and industrial chemicals, especially in urban areas.



Analysis of milk contaminants by recombinant cell based reporter bioassay

There is an excessive release of different pesticides, herbicides, insecticides, plasticizers etc. in our surroundings which are commonly used in agriculture practices and product storage. Being mostly lipophilic in nature, these EDCs are able to cross the cell membrane and also get stored in fatty tissues or adipocytes. This in the long run may lead to bio-magnifications, the impact of which is yet to be analyzed for many such xenobiotics. In this context, milk is reported to serve as a reservoir of EDCs thus warrants its estimation in various samples.

Several expensive, time-consuming and less sensitive detection methods are available for detection of xenobiotics in food materials like, 7ethoxyresorufin-O-deethylase (EROD) bioassay and GCMS based analytical approach. The current project aims to develop a cell based chemical-activated luciferase gene expression (CALUX) assay to detect the contaminating xenobiotics in the milk samples. This assay not only indicates the presence of these contaminants in the milk samples but also indicates its biological activity at cellular level and their potential hazards. The response would be estimated by the emission of light in presence of luciferin substrate. The developed assay will be sensitive and user friendly with high commercial impacts in terms of toxicity profiling of various chemical entities and environmental and food samples.

Design and development of a proof-of-concept model of a packaging methodology &rigidization for Gossamer Space Antenna structures

Sponsor: Space Application Centre (SAC), Indian Space Research Organization

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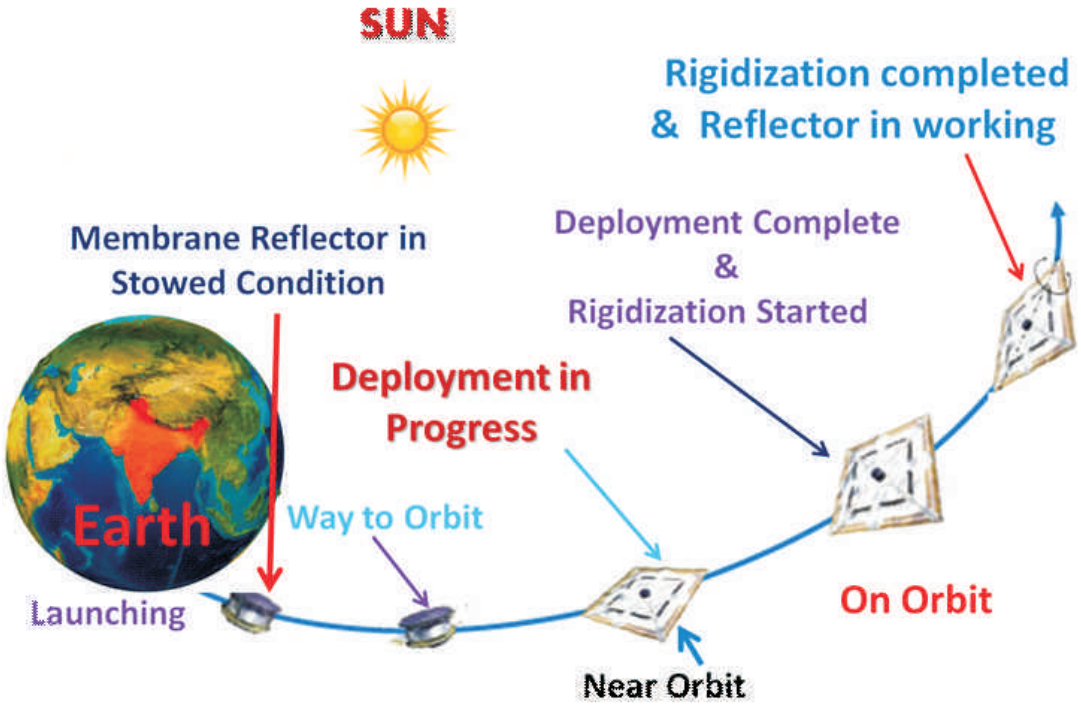
Abstract : The idea of Gossamer space structures dates back to the year 1960. In 1996 NASA sent first IAE in space to study the behavior of deployment of inflatable antenna and to predict its behavior, though deployment was successful but not controlled. The lack of understanding of dynamics of on-orbit deployment through inflation and rigidization and also no reliability in predicting the deployment &rigidization behavior has been a constant problem in this field. A common approach is to recourse structural finite element analysis, which ignores some potential important phenomenon, such as dynamics of the pressure, rate of gas flow, rigidization and its couple interaction with inflatable structure.



On top of that the orbital and launch condition make it even critical to deal with.The main objective of this research is to concentrate on the study of different folding methods and their deployment behavior considering rigidization with help of 2-D planar membrane. Modelling and simulate the configuration of the 2-D planar membrane by using as Oasys PRIMER and LS-Dyna software. Optimize the best among them. Experimental result will give the deployment &rigidization control mechanism. The analytical model interpreted from experiment will predict the deployment &rigidization behavior, which intern modelled to apply orbital and launch conditions.

An assessment of health systems responsiveness and availability of medical care for emergency treatment of RTI of the select States of India

Sponsor: Indian Council of Medical Research, New Delhi

Prof. M. K. Rao

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Abstract : Severe road traffic injury (RTI) and subsequent delay in hospital admission for more than 24 hours result in death, disability and outpatient care respectively. The present research aims to conduct

a comprehensive study with respect to the health systems' responsiveness and the timely availability of the medical care during the 'Golden Hour' of the road traffic injury. To fulfil the said objectives, the study would include some large, medium and small sized hospitals, Police records and indoor patients who are/ were the victims of the RTI. The study espouses to be a part of a larger enquiry into the social determinants of health inequities associated with road traffic injuries.

Multiscale simulation framework for defect formation studies in electronic materials and devices

Sponsor: Department of Science and Technology, ICT and Future Planning, Republic of Korea

Prof.IndraVir Singh

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Abstract : This project is being executed through a Joint Network Centre:***Computational Materials Science & Engineering*** with participants from Indian and Korean Institutes. JNCASR Bangalore, IIT Kharagpur, IIT Roorkee, IISc Bangalore and INST Mohali are participants from India and from Korean side: University of Ulsan, Kookmin University, Advanced Institute of Convergence Technology, Hanbat National University and University of Seoul are the collaborating Institutes.The issue of defect reduction required for the performance enhancement in various optoelectronic devices is of major concern for the electronics industry. This requires the understanding of the defect formation mechanisms in these devices, which can lead to the prediction of device performance in the presence of defects. This project involves the development of defect mechanics-based multiscale computational models to understand the defect formation mechanisms in electronic devices. A new finite element model that embeds edge and screw dislocations in piezoelectric solid will be developed. A theoretical model to predict dislocation density will be developed for piezoelectric multilayer applicable to quantum wells. A molecular dynamics (MD) model will also be developed based on quantum dot with lattices of different sizes. The developed continuum FE/XFEM model will be coupled with MD model.

Numerical Crack Growth Studies in Hybrided Pressure Tube of PHWR

Sponsor: Atomic Energy Regulatory Board, Government of India

Prof.IndraVir Singh

Abstract: Pressure tube (PT) is a critical component of the Pressurised Heavy Water Reactors and plays a vital role in its operation and safety. In the past, several long shut down of nuclear reactor have been caused due to the fracture failure of the PTs like Pickering Generating Station (2056 MW) of Canada being out of service for many months because of small cracks in 17 of the 390 pressure tubes. The main mechanism of failure was delayed hydride cracking. Due to high internal pressure, elevated temperature and corrosive environment in the pressure tube, delayed hydride cracking is actually accelerated. Therefore, in this project, the fracture behaviour of Zr-2.5 % Nb alloy tubes subjected to internal pressure at 300°C will be numerically computed. Crack growth behaviour of part through wall and through wall flaw will be investigated. Such crack growth studies will be investigated in the presence of residual tensile stresses. Stress intensity factors (SIFs) are used for assessing the safety of the tubes. These SIFs are based on the equations given in the standards used for design. It may be noted that complete range of crack depth and length are not covered in the standards. Therefore, the SIFs will be evaluated for the flaw covering the full range.

End-to-end Emotional Speech Synthesis

Sponsor : Samsung R&D, Delhi, India

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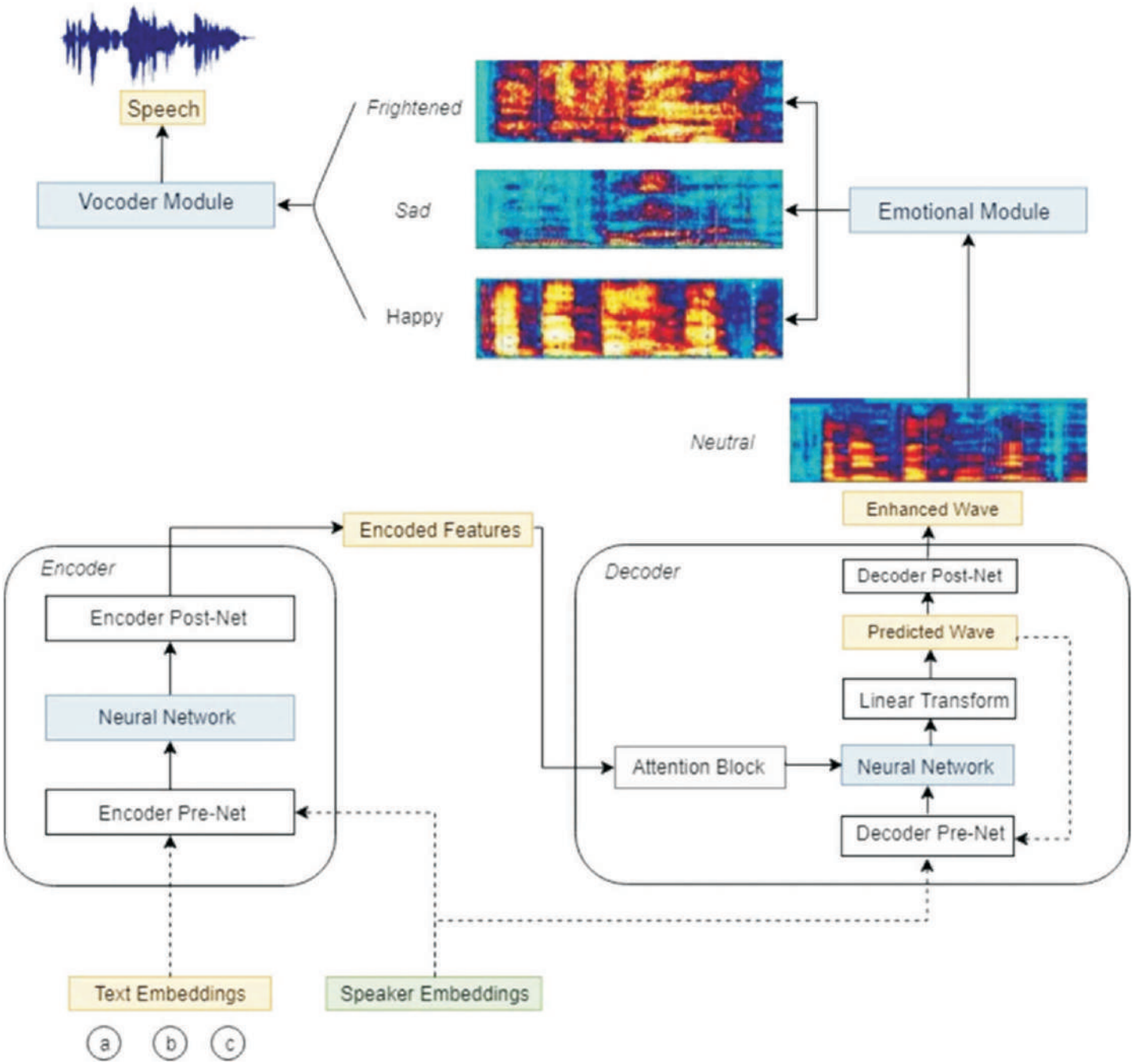
Abstract : The need to develop computational systems that can generate human-like speech directly from the plain text is increasing rapidly. Such systems are known as End-to-end Speech Synthesis Systems. They find their usage in a wide range of applications such as - telephonic inquiry systems, human-machine-interaction, aid to blind and vocally-handicapped people, *etc*. Various text-to-speech systems such as - Rule Based Systems, Statistical Speech Models, Concatenative Speech Systems, *etc*. have been used for speech synthesis. However, most of them require human intervention for acoustic-

feature engineering. Neural speech synthesis systems have emerged out as a viable end-to-end speech generationalternative. This project aims to build an efficient neural speech synthesis system that can accommodate human-like emotional affects and, can be deployed for real-time applications.



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