



Contents

Director's Message

Indian Nuclear Power Program

- Development of Inspection Systems **2**
- Recovery of Uranium **9**
- Environmental Monitoring **11**
- Nuclear Hydrogen **14**
- Advanced Reactors and Associated Materials **15**
- Fusion Reactor **18**
- Spent Fuel Reprocessing **19**
- Radioactive Waste Management **20**

Advanced Technologies, Radiation Technologies and Applications

- Research Reactors **24**
- High Flux Research Reactor **27**
- Accelerator, Laser and Plasma **27**
- Sensors, Detectors and Specialized Instruments **30**
- Energy Storage **32**
- Radiopharmaceuticals **32**
- Water Purification, Groundwater Management and Solid Waste Management **34**
- Agriculture and Food Technologies **37**
- Healthcare Technologies **39**
- Hydrogen Technologies **39**
- Specialized Technologies **41**
- COVID-19 Technologies **45**

Basic and Directed Research

- Astrophysical Sciences 48
- Synchrotron Beamline 49
- Lithium Batteries 51
- Mass Spectrometers and Spectroscopy 52
- Nuclear Physics 54
- Solid State Physics 55
- Technical Physics 56
- Chemical Sciences 58
- Reactor Water Chemistry 59
- Healthcare Materials 60
- Materials 63
- Environmental and Separation Science 66
- Bio-fouling Studies 69
- Advanced Studies 71
- Analytical Services 74
- Materials Science 75
- Computation and Modelling 78
- Radiochemistry 82
- Biology 88
- Advanced Radiopharmaceuticals 89
- Cancer Studies 90

Mega Science and Collaboration 96

Human Resources, Scientific Information Resources and Technology Management 100

Outreach 108

Infrastructure Development 112





Director's Message



Bhabha Atomic Research Centre is a multidisciplinary organisation, dedicated to Research and Development across the gamut of domains pertaining to the activities of nuclear fuel cycle and the use of radiation technology for societal applications. As the mother institute of DAE, right since its inception, as a foundational activity, BARC has also been involved in R&D in Physical, Chemical, Biological and Material Sciences etc. and has been instrumental in the seeding and growth of numerous research programmes, with direct applications to the nuclear sector, but also with spin-off benefits accruing to various other industries and sectors in the country and abroad.

In the implementation of its programmes, BARC has always been a symbol of success and self-reliance, epitomising the spirit of AtmaNirbhar Bharat and finding a strong resonance with the spirit of 'Azadi ka Amrit Mahotsav', being celebrated to showcase the achievements of the country over the 75 years since it attained independence.

Some of the noteworthy contributions during this period include the development and installation of linear accelerator for irradiation of industrial products, the development of an indigenous cargo scanner, a rapid CRISPR based Covid-19 detection kit and the commissioning of MACE, which is the largest gamma ray telescope in Asia. More than 70 new technologies have been transferred to entrepreneurs in addition to seventeen agreements signed with rural entrepreneurs for the transfer of technologies under the Advanced Knowledge and Rural Technology Implementation (AKRUTI) programme.

During this period, BARC continued to participate and contribute to multilateral programmes aimed towards extending the frontiers of knowledge as well as towards the development of new cutting-edge technologies. Development of human resources, knowledge management and knowledge transfer as well as propagation of a research culture, of equal importance in the growth and sustenance of an organisation, have also received appropriate attention and importance in the programmes of BARC.

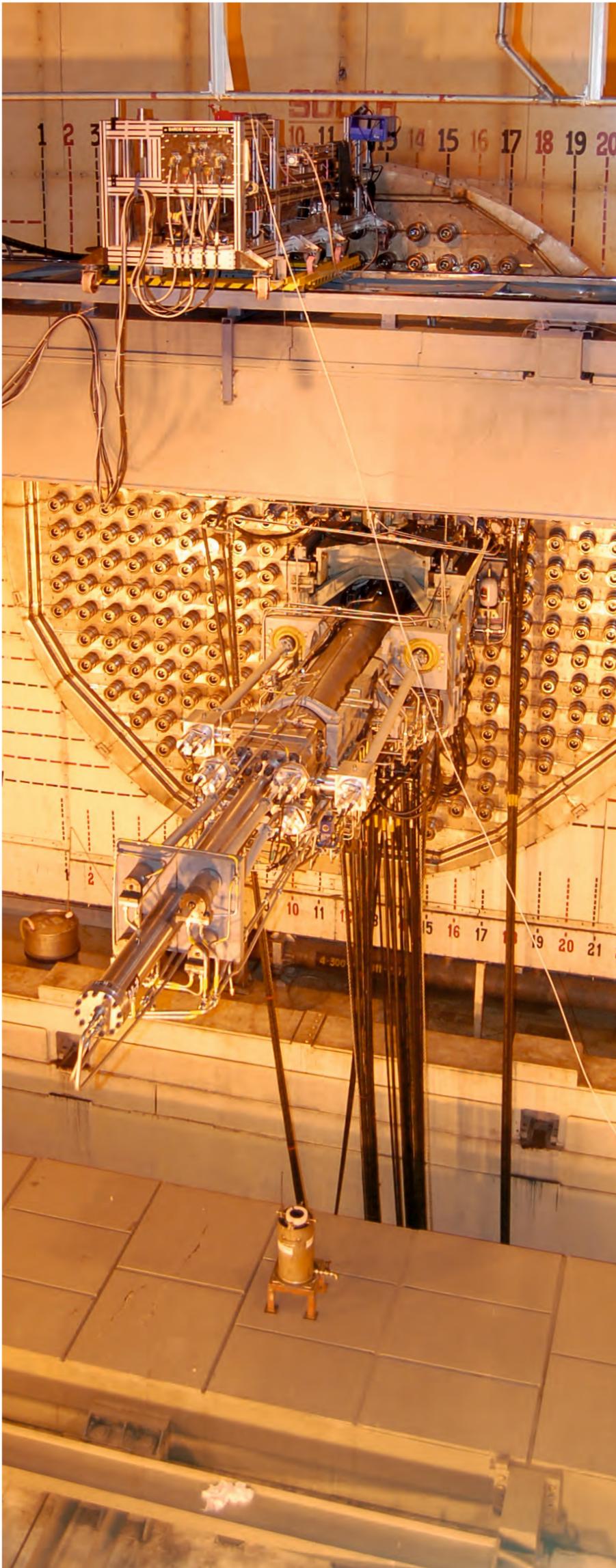
This Annual Report 2021 will provide comprehensive details of the entire range of BARC activities and has been appropriately named 'BARC VISTA'. For easy reference, the report has been divided into seven sections - Indian Nuclear Power Program; Advanced Technologies, Radiation Technologies and Applications; Basic and Directed Research; Mega Science and Collaboration; Human Resources, Scientific Information Resources & Technology Management; Outreach, and Infrastructure Development.

This document is not only an annual record of the activities, but would also serve as a point of ready reference for anyone seeking information about the ongoing activities in BARC on specific domains of the nuclear sector. I compliment SIRD for carrying out the task of creating this comprehensive document in a timely and systematic manner.

Dr. Ajit K Mohanty

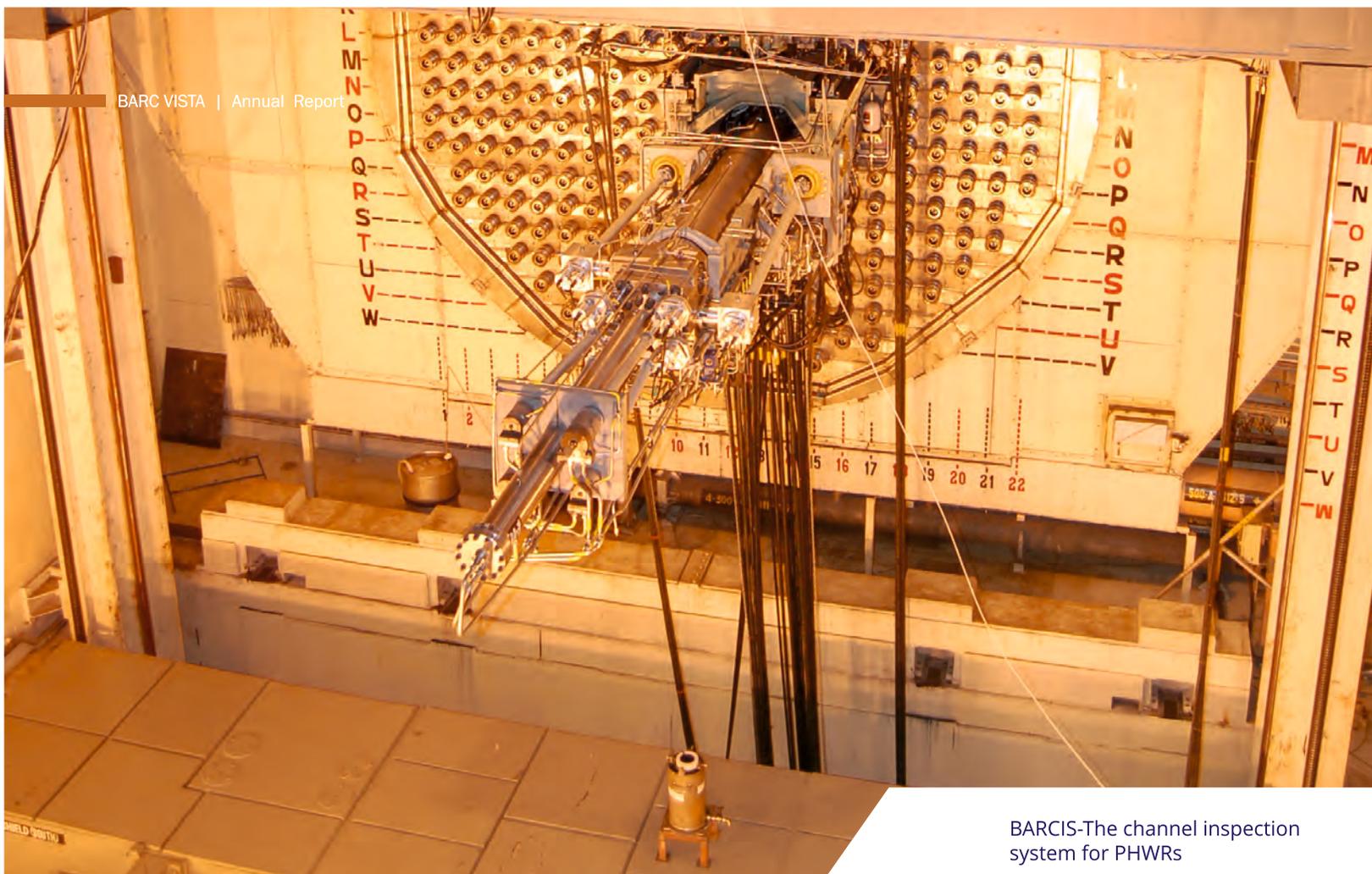


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INDIAN NUCLEAR POWER PROGRAM

The centre is engaged in multi-disciplinary and multi-scale activities towards the development of technologies related to nuclear power program of India. These include fuel fabrication, quality assurance (QA), In-Service Inspection (ISI), Post Irradiation Examination (PIE), Inspection tools for research reactors, Pressurized Heavy Water Reactors (PHWRs) and the first two Tarapur nuclear power plants. The technologies related to front and back end of the nuclear fuel cycle, which includes spent fuel reprocessing and nuclear waste disposal, are within the ambit of forefront research areas of this centre. The activities under these thrust areas cover the first three Vision programmes of BARC, the highlights of which are sketched in this section.



BARCIS-The channel inspection system for PHWRs

Indian Nuclear Power Program

Development of Inspection Systems

A number of sophisticated instruments were developed during 2021 for in-service as well as offline inspection of various components of nuclear reactors and fuel reprocessing facilities.

Fuel Pin Inspection System

Image Analysis based software modules were developed to analyze radiographic images of fuel pins for automated detection of local Dense Packing (DP) of fuel elements. It is intended to assist in inspecting the fabricated fuel pins for defects. A sudden and significant drop in image gray level is automatically detected by image analysis software to indicate a local Dense Packing in fuel pin.

Measurement of Gap between CT and PIU

A new ECT based tool for measurement of gap between CT and PIU was qualified and final clearance for deployment was granted by Atomic Energy Regulatory Board (AERB). The tool was deployed through BARCIS delivery mechanism and measurements were carried out at TAPS-4. The results were presented to EGCC, AERB.

A new UT ToF tool was qualified and deployed for characterization of flaws more than 4% at TAPS-4. The tool was deployed through BARCIS delivery mechanism.

Fission Counter for Pressurised Heavy Water Reactor

A new Fission Counter (FC), employing triple concentric cylindrical electrode geometry with 48 mm diameter, 380 mm length and 1S Al

construction has been developed indigenously. The design uses qualified large size friction welded Al-SS clad plates for obtaining leak tight weld between SS-Al, ceramic supports for electrodes and a specially developed PEEK insulated Al body HN connector pair with SS thread inserts. Owing to the increased area for special material coating, the FC gives ~ 0.5 cps/nv sensitivity.

The detector, by its inherent design, gives significantly higher n-γ discrimination and 1S Al construction results in low residual activity in high neutron flux. Amongst other applications, the developed FC fulfils the specific requirement for use in PHWRs as in-core detector in high dose rate ambience above 105 R/h for start-up after long shut down.

Pipe Mounted Online Boron Concentration Meter for Indian PWR

For control and safety of Pressurized Water Reactors, boron concentration in primary coolant water needs to be continuously monitored at various locations, using On-Line Boron Meters (OLBM). Two prototype units of pipe mounted boron concentration meters are developed using indigenous BF_3 neutron detectors. The OLBM comprises a pair of detectors and pulse processing electronics. The detector units have an external jacket to provide water cooling.

The pulse processing units are kept in the control room. A multicore cable feeds the operating supply for the detector unit and transmits back the neutron signal to the pulse processing system. The signal is converted into boron concentration using a specialized algorithm. The pulse processing unit also has alarm and error warnings. The prototype units were tested for B10 concentration from 0 to 1.6 gm/Kg in the DM water.

Remote Handling and Automation of Fuel Pin Welding using Magnetic Pulsed Welding

A 200 kJ capacitor bank with 45 kV CCPS along with automation system for Magnetic Pulsed Welding (MPW) of fuel pin tube to end-plug has been installed and commissioned at A3F, Tarapur.

Laser Spectroscopy based Heavy Water Detection and Analysis System in Air for Nuclear Reactor Environment

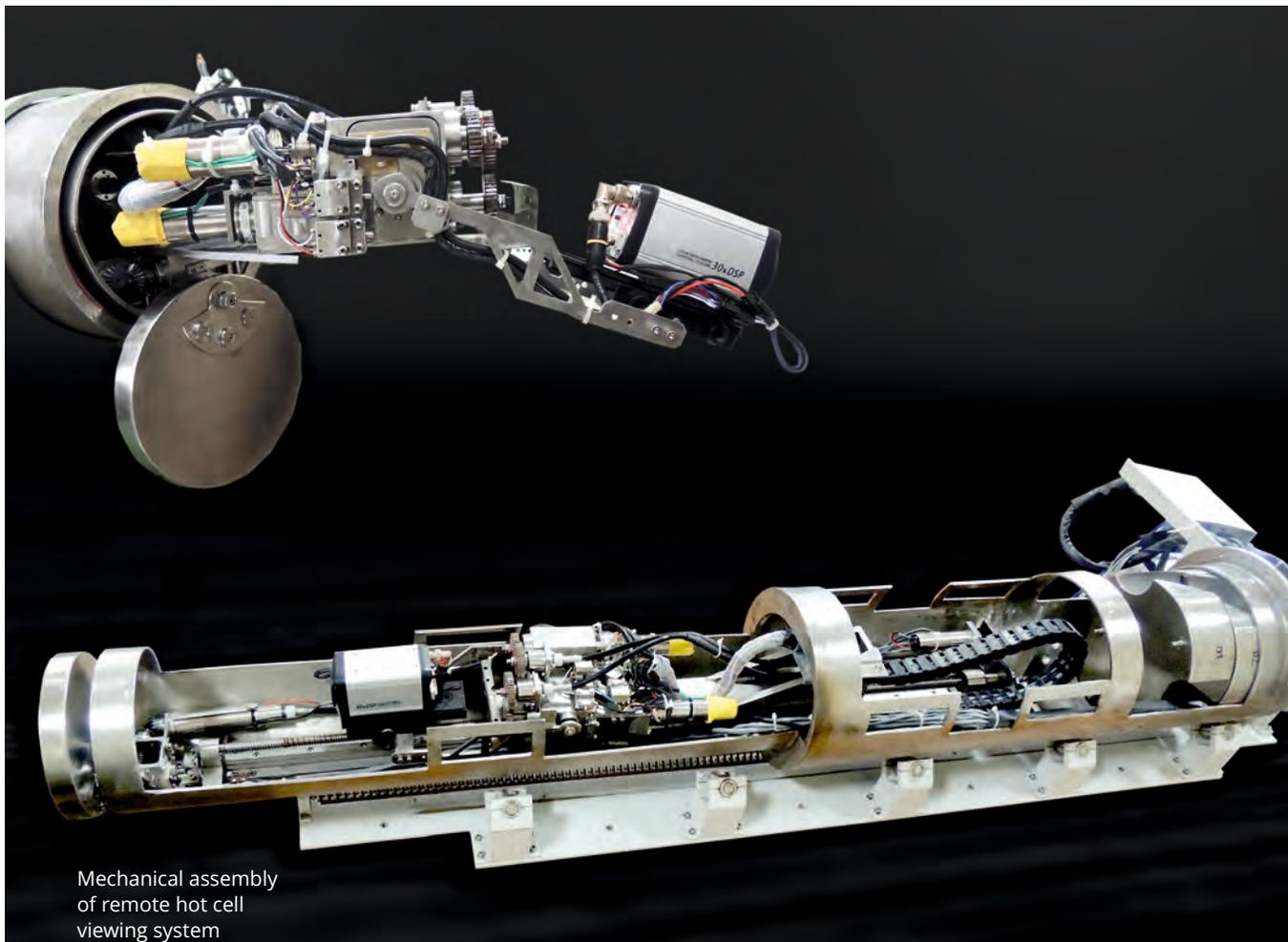
A laser spectroscopy based system has been developed indigenously for interference-free real time online monitoring of heavy water (coolant) leaks in pressurized heavy water reactors (PHWRs). An advanced laser absorption spectroscopic technique, "Off-Axis Integrated Cavity Output Spectroscopy (OA-ICOS)", has been used for a high sensitivity of detection and analysis. The HDO and H_2O absorption lines in 1390 nm wavelength range are used to estimate the concentration of water and semi-heavy water in the air using this system. Field testing of the instrument has been carried out in the research reactor Dhruva and the test has showed very good correlation with the traditionally used tritium activity measurements.



Heavy water analyzer

UT based Online Interface Tracking System for Liquid-Liquid Solvent Extraction Process

A Two Phase Interface Detection System (TPIDS v1.0) has been developed and installed. This system comprises an in-house designed and developed self-calibrating ultrasonic sensor, its associated hardware connected over 100m



Ethernet link and a User Interface with algorithms for real-time tracking of liquid-liquid interface within an accuracy of 1mm at an update rate of 2 seconds. The sensing system has been tested exhaustively with various liquid pairs, environmental conditions and in the presence of soluble/insoluble liquid/ particulate impurities. The performance of the system had been validated in situ by operating it continuously for 8 h.

UT based Online Pulsation Monitoring System

Online pulsation monitoring system has been developed for measurement of pulsing amplitude, frequency and waveform in pulsed columns. The system is developed with air coupled ultrasonic sensor, in-house developed FPGA based data acquisition system and a Python based signal processing and parameter estimation software. The system acquires signals from UT sensor, pressure transducer and valves. It is validated in

bench scale with multiple operating conditions, and installed in a pulse column.

Automated Remote Viewing System for Hot Cell

An automated remote hot cell viewing system has been developed for visual inspection through wall port of hot cells. A PC based GUI is used to remotely operate the system and the embedded controller executes real-time sequencing logic and safety interlocks for interactive & guarded system operation. Other major features of the system include provision for manual system recovery in case of motor failure, guided scissor lift platform to facilitate easier insertion/retrieval of system from the port and automatic vision based tracking of target object. A mock port facility has been setup at the laboratory to check the adherence of the system to the cell port and all the functionalities of the system have been tested and found to be working satisfactorily.



Alarm Annunciation System of FBTR upgraded with TPLC-32 Platform based Computerized System.

TPLC-32 Platform based Computerized Alarm Annunciation System for FBTR

Alarm Annunciation System of Fast Breeder Test Reactor (FBTR) is being upgraded with TPLC-32 Platform based Computerized Alarm Annunciation System (CAAS).

The CAAS is a distributed multi-nodal system with seven nodes, each node consisting of two subsystems which are hot-standby to each other. Hardware of CAAS has been manufactured at ECIL as per the design inputs from BARC. Hardware integration and environmental qualification testing of CAAS has been completed.

Development of Modules for NUCON PLC

NUCON-PLC is an indigenous Industrial Strength PLC with enhanced safety and security features to

meet diverse functional, performance, capacity and reliability needs of different applications. The module library of NUCON-PLC has been enhanced recently to meet specific user requirements.

A Fast Data Communication Module for fast data logging of parameters related to column pulsing required for Nuclear Reprocessing Plant was tested and implemented. As per requirements of INRP, a Modbus Gateway Module based on P1013 CPU has been designed for interfacing Remote I/O units of NUCON-PLC with third party devices that are distributed in the field and communicate on Modbus-TCP or Modbus-Serial RTU protocol. A high-performance Processor/ Communication Module based on T1014 CPU has been designed for use in computationally intensive high-end applications of NUCON-PLC Platform. Porting of Real Time Operating System ESOS on Next Gen

CPU board has been completed. Detailed testing of all RTOS API as per the test plan has been completed and test report has been prepared. Porting of in-house developed Secure TCP/IP stack on VME 8260 communication module has been completed.

Heat Treating Zr-2.5Nb Alloy Pressure Tube for 200 MWe PHWR

For heat treatment of pressure tube sections a vertical induction scanner has been designed and commissioned. Several trial runs were made to optimize the induction scanner parameter so as to get finer grain size with randomized crystallographic texture in the Zr-2.5% pressure tube (PT) for 200MWe PHWR. All trial runs were carried out with 200 mm length of PT.

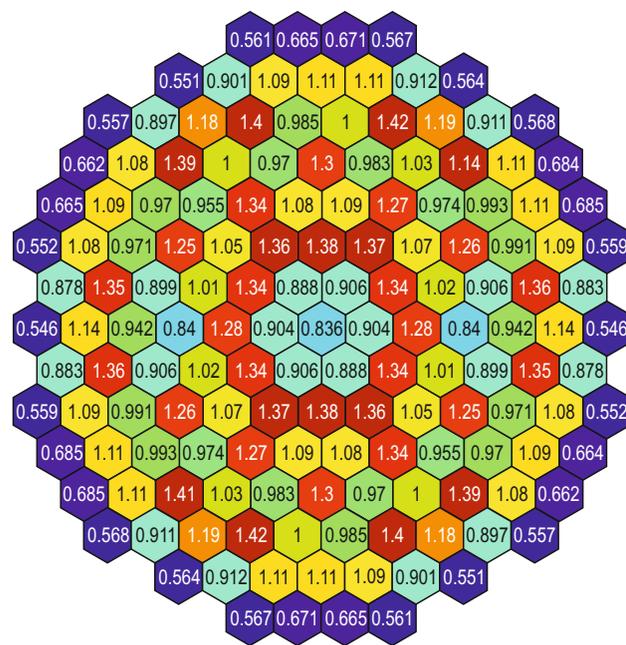
Metallography has been carried out to ensure uniform microstructure across the thickness and length. Electron Back Scattered Diffraction (EBSD) scanning was performed to compare crystallographic texture in as-received and after heat-treated condition. From the pole figures Kearn's factor for (0001) basal pole was also calculated, which shows a high degree of crystallographic randomization.

Delayed Hydride Cracking (DHC) Behaviour and Burst Testing of Zr-2.5Nb Pressure Tubes (PT)

Three types of experimental setups using 3-point bend, 4-point bend and cantilever beam geometry have been developed for determination of DHC velocity in radial direction of Zr-2.5Nb pressure tube material. Samples were charged with 100 wppm of hydrogen and loaded in the 3-point fixture. DHC test was carried out at 250°C at an applied load of 500 N.

An experimental facility has been fabricated to conduct burst testing of pressure tubes (length varying from 400 to 1500 mm) of IPHWR reactors under internal pressure up to 25 MPa at temperatures ranging from room temperature to 350°C.

The design assembly comprises an oil reservoir, heaters, oil circulation pumps, clamping fixtures,



Radial power distribution of Pressurised Water Reactor core simulated using a 3D space-time kinetics model.

and 12 thermocouples placed at different locations along the length and circumference of the tube, displacement measuring devices (LVDTs) to measure the diameter change, and control and monitoring units.

The pressure and temperature of the system is increased gradually by a PLC-based controller system. The experimental setup has been tested at various temperatures ranging from 100°C to 350°C with an interval of 50°C for pressures varying from 2 MPa to 25 MPa.

Radial Power Distribution of PWR Core

In the specialized domain of mathematical modeling, simulation and analysis of systems and components for nuclear, industrial and scientific applications, BARC has made significant achievements. Detailed steady state and transient thermal analysis of the SDCP level sensors have been carried out to optimize the design parameters.

A 3D space-time kinetics model for hexagonal core geometries has been developed and coupled with simplified mathematical models of fuel heat transfer, Reactor Coolant System thermal hydraulics, lumped steam generator and control devices.

Pressure Tube Rolled Joint Detachment System for 220 MWe PHWRs

A PTRJD system based on induction heating technique was designed for detachment of pressure tube from the end fitting without any cutting and potential radioactive dust production. Commissioning of the PTRJD tool of full length facility has been carried out with its induction heating system. An experimental trial simulating the entire length of end fitting and dimensional restriction as imposed by liner tube has been carried out successfully. Further trials were planned for optimization of process parameters.

Fatigue Cycling of 540 MWe Pressure Tube End Fitting Rolled Joint

A set up has been made for the study of fatigue cycling of 540 MWe Pressure Tube end fitting Rolled Joint. Around 9.54 lakh cycles were completed for a fatigue loading of 50 kg-m. The rolled joint has been tested for helium leak test and the results were quite satisfactory.



Facility for fatigue cycling test for 540 MWe Pressure Tube end fitting Rolled Joint

Calandria Tube Rolled Joint Detachment System for 540/700 MWe PHWRs

A Calandria Tube Rolled Joint Detachment System (CTRJD-540/700) is being developed to cater to the requirement of replacing the Calandria tube due to sagging of tubes and contact with horizontal

poison tubes and flux units in 540/700 MWe PHWRs. Fabrication of mechanical components of the system has been completed. Assembly and hydraulic pressure test of mechanical set up has been found to be satisfactory. Calandria tube spool pieces manufactured at NFC have been received. The inspection of six induction heating coil modules of CTRJD-540 tool at the manufacturer's site has been carried out and was found to be satisfactory.

Measurement of Gap between Poison Injection Unit Tube and Calandria Tube in 540 Mwe PHWR

In 540 MWe PHWR, the gap between calandria tube and PIU tube is a critical parameter, which has to be monitored periodically for safe operation. Laboratory trials were carried out on a fabricated remote field Pulsed Eddy Current (PEC) tool head and the trials showed good repeatability of measurement on a simulated setup.

Measurement of Pressure pulsation at KAPP-3 Headers

Pressure pulsation at Reactor Inlet Headers (RIH) and Reactor Outlet Headers (ROH) of KAPP-3 was measured during the hot conditioning of the reactor. The overall pressure pulsation values in time domain (up to 500 Hz) and pressure pulsation value at specific frequencies have been estimated.

Data Processing Software of Pressure Tube Sag Measurement system

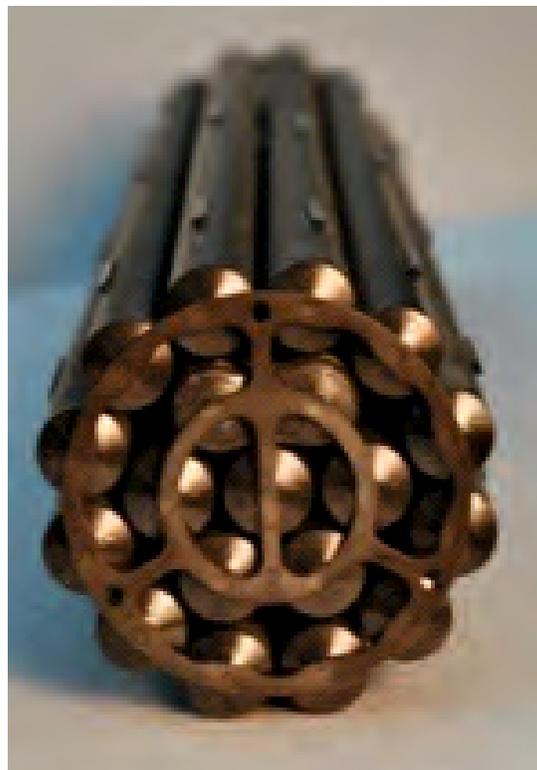
A dedicated data processing software has been used for processing of curvature data obtained from Pressure Tube Sag Measurement system (PRESAM) tool to channel the sag profile. The new version has been improvised to be more user-friendly. In addition, it has a dedicated module for calculation of LVDT calibration factor too. The new version has an extensive error control feature for avoiding user input or procedural errors. The user manuals for both PRESAM 540 and 220 versions have also been prepared.

PRESAM 220 Mark III Tool Head

Prototype PRESAM 220 Mark II tool heads were developed and deployed in field operations of PHWRs. The tool head design which is currently deployed as well as a new design made by ECIL known as LVDT were evaluated for over 100 reactor channel measurements, and their performance was found to be satisfactory. 10 PRESAM 220 Mark III tool heads along with LVDTs made by ECIL were manufactured and field deployed.

Capsule Carrier Bundle for PHWR

The capsule carrier bundle is typically used to generate irradiation data of pressure tube material. The bundle was tested for compression load of 1800 kg under shield plug and 1300 kg for side stop support. Helium leak testing of the bundle was done for varied gauges.



Capsule Carrier Bundle for PHWR

Maintaining the long run of PHWR

- ✧ Development of SS-Zircaloy binary alloy matrices for hull management.
- ✧ Studies to demonstrate the feasibility of joining SS 321 to Zr-2.5%Nb by diffusion bonding using suitable multiple interlayers.
- ✧ Stress corrosion cracking studies in martensitic stainless steels for characterization of oxide formation on SS.
- ✧ Oxidation behaviour of 304L SS exposed to high temperature, high pressure demineralised water.
- ✧ Niobium determination in Niobium doped gadolinium-Zirconate Microwave-assisted dissolution and spectrophotometry.
- ✧ Determination of phosphorous in nuclear matrices by using Ion-chromatography.
- ✧ Comparison of irradiation response of indigenous RPV steel forgings by using proton irradiation.
- ✧ Preparation of reactive and refractory metal borides, including NdB_6 , ZrB_2 , B_4C , NbB_2 for potential nuclear reactor control and high temperature applications.

Recovery of Uranium

New Process Flowsheet

A process flowsheet was developed for recovery of U values from the Chitrial ore (Telangana) analysing about 0.06% U_3O_8 . Due to the presence of U in refractory phase along with Zr, the overall recovery of U was limited to about 78% of U_3O_8 values as U-peroxide yellow cake product, without recirculation of any process streams.



Nuclear Grade Yellow Cake

Conversion of Crude Sodium Diuranate

Conversion of crude sodium diuranate (SDU) produced at Tummalapalle uranium mill into high purity high temperature uranium peroxide (HTUP) was carried out "on-site" on a large scale in scalable technological units, using a specially designed process scheme. The process yielded HTUP product with U_3O_8 assay of about 90% (purity about 95%), with quantitative recovery. Impurity elements like Zr, Mo, Si and C, which create process difficulties during uranium refining stages were substantially minimized.

The Kudada ore sample indicated the presence of uraninite as the main uranium phase and monazite as another atomic mineral by XRD studies. Molybdenite, Pyrite, Chalcopyrite, Nickeline and Fukuchilite are the other ore minerals identified. Antigorite, Magnesite and Talc are the rock forming

mineral phases. Partial chemical composition showed U_3O_8 and REEY assay of 0.027% and 0.26%, respectively. The other constituents are MgO 23.9%, SiO_2 43.8%, FeO 13%, P_2O_5 1.4% and LOI 6.9%. The 'S' (from sulphide minerals) is about 0.1%. The sample indicated the presence of other valuable metals in the following concentration (ppm) range: Cu 100; Ni 366; Mo 181; Co 51; Cr 1664 and V 117. Uranium leaching experiments under bench-mark process conditions indicated leachability of about 90% of U values with very low simultaneous solubilization of REE.

To circumvent the significant loss of U in different processing streams (raffinates of alamine & TBP circuits & Pb-Ba cake) at OSCOM plant of IREL, polymeric composite beads encapsulating extractants (D2EHPA, TBP, DHOA) have been developed and are being evaluated. A phosphate precipitation method was found to be effective in quantitative recovery (99.9%) of U from TBP solvent extraction circuit raffinate. In IREL's OSCOM plant uranium gets lost in raffinate of alamine and TBP circuit of NGADU production and in Pb-Ba cake. The D2EHPA solvent encapsulated polymeric composite beads and phosphate precipitation routes were found to be effective in recovery of >99.9% uranium from the raffinates (0.08 g/L - 1.9 g/LU).

Extraction and Stripping of Zirconium

Experiments were carried out in miniaturized pulsed stirred column (MPSC) for selective extraction of Zr from ZNCS (Zirconium Nitrate Concentrated Solution) containing 69.3 g/L Zr and 2.65 g/L Hf in nitrate medium using organic 0.3 M TAPO in 60:40 ID: DD mixture. Effect of residence time and stirring speed on extraction was studied. HETP for Zr extraction by 0.3 M APO in MPSC is found to be 0.83 m at 800 rpm and aqueous superficial velocity of 0.32 cm/s. The 1 m height in MPSC corresponds to 1.2 stages. The stripping of organic loaded with 12.4 g/L Zr with 0.7 M oxalic acid revealed that 100% stripping is achieved at 1000 rpm and O/A 0.75. The purity of product is 99.5% and Hf content is 46 ppm. The operation was trouble free with no formation of solid or emulsion.



Miniaturized Pulsed Stirred Column setup used for extraction and stripping of Zr from ZNCS

Direct Denitration Demonstration Plant at PREFRE-2, Tarapur

Direct thermal denitration of uranyl nitrate reduces the number of processing steps as compared to the conventional practice followed for production of uranium oxide from nuclear pure uranyl nitrate solution.

The direct denitration process avoids use of ammonia and permits recovery of nitric acid. In the plant being set up to demonstrate the process with the actual uranyl nitrate solution generated in spent fuel reprocessing, equipment installation, piping works, installation of enclosure and air monitors, commissioning of instrumentation control panel, pneumatic pressure testing of the entire plant, testing of metering pump and external mix type twin fluid nozzle were completed.

Thermal and Thermophysical Characterization of Dispersion Nuclear Fuels

Thermo-physical studies on cermet fuels have been initiated for the dispersion fuel development program. Three different cermet compositions (S1, S2, S3) containing varying content of surrogate ceramic phases were obtained. With increasing temperature, thermal diffusivity decreased while specific heat showed an increasing trend.

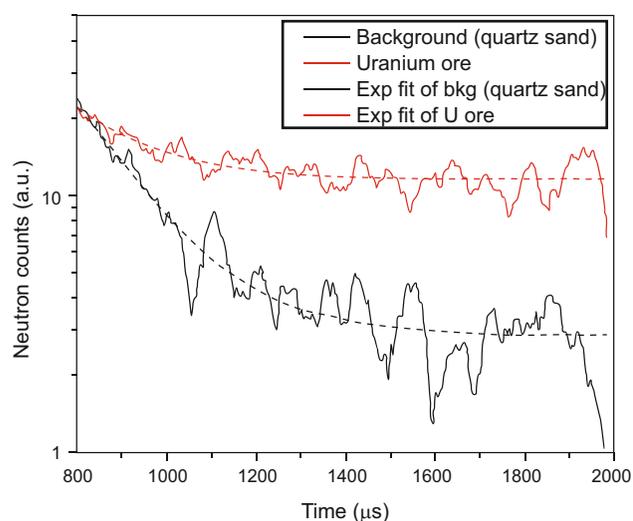
Bulk thermal expansion was measured over 298K to 873K under inert atmosphere. Average coefficients of thermal expansion (CTE in ppm/K); evaluated from isotropic dilation curves were found to be 16.9, 17.9 and 15.6 for S1, S2 and S3, respectively. Thermal conductivity of cermets varied from 70 W/m.K (at 298 K) to 35 W/m.K (823 K). These results are useful to delineate the phase behavior of dispersion fuels under thermal stress.

In-situ Uranium Ore Enrichment Characterization

In-situ uranium enrichment analysis is based on the differential die away method, which records the temporal spectrum of fast neutrons in a fissionable medium when an external pulse of fast neutron neutrons is injected in the interrogated volume.

Uranyl Nitrate Conversion Facility

In view of improving the processing capacity, morphology of uranium oxide product for its proposed re-utilisation and reducing manual intervention, upgradation of Uranyl Nitrate Conversion Facility has been taken up. The system is augmented with new equipment including notch filter, dryer, rotary calciner etc along with desired automation to meet the objective. Equipments are fabricated and received at site. Site readiness for installation of new equipment is completed. Ventilation system has been augmented. Installation of equipment is under progress.



Uranium ore detection using active neutron interrogation technique.

Environmental Monitoring

IERMON (Indian Environmental Radiation Monitoring Network) serves the purpose of countrywide monitoring of environmental radioactivity for background monitoring.

The Environmental Radiation Monitors installed under IERMON are standalone solar powered battery-operated system, having GSM based communication. IERMON has achieved many milestones, including the rare one as being the nationwide operational network of 500 or more unattended monitoring stations. Recently, the system has been upgraded with satellite based direct communication system, making it independent of mobile base stations to continue to provide data even in cases of extreme natural calamities.

The system known as ERMSAT is compact, rugged, is meant for open field deployment and has successfully withstood the varying environmental conditions across the country. In total 40 units of ERM-SAT have been installed at various locations in India.

The systems are currently operational and are sending data via two redundant modes, GSM and Satellite. The data is received at the Earth Station established at CTCRS, Anushaktinagar, Mumbai.

Stack Monitoring

A new stack monitoring system, which provides information about the release rate of I-131, FPNG, Ar-41, Xe-133 and particulates has been designed and developed for PRPD. The whole system was developed in-house, tested and calibrated. The system provides the total activity released and gives an alarm whenever the activity levels exceed the pre-set limits. This on-line monitoring system specific to PRPD will ensure compliance with the safety requirements in the operation of the facility. All radioactive releases from the facility are also properly monitored to ensure the releases to the environment are well within the approved discharge limits. The Gaseous Effluents Monitoring

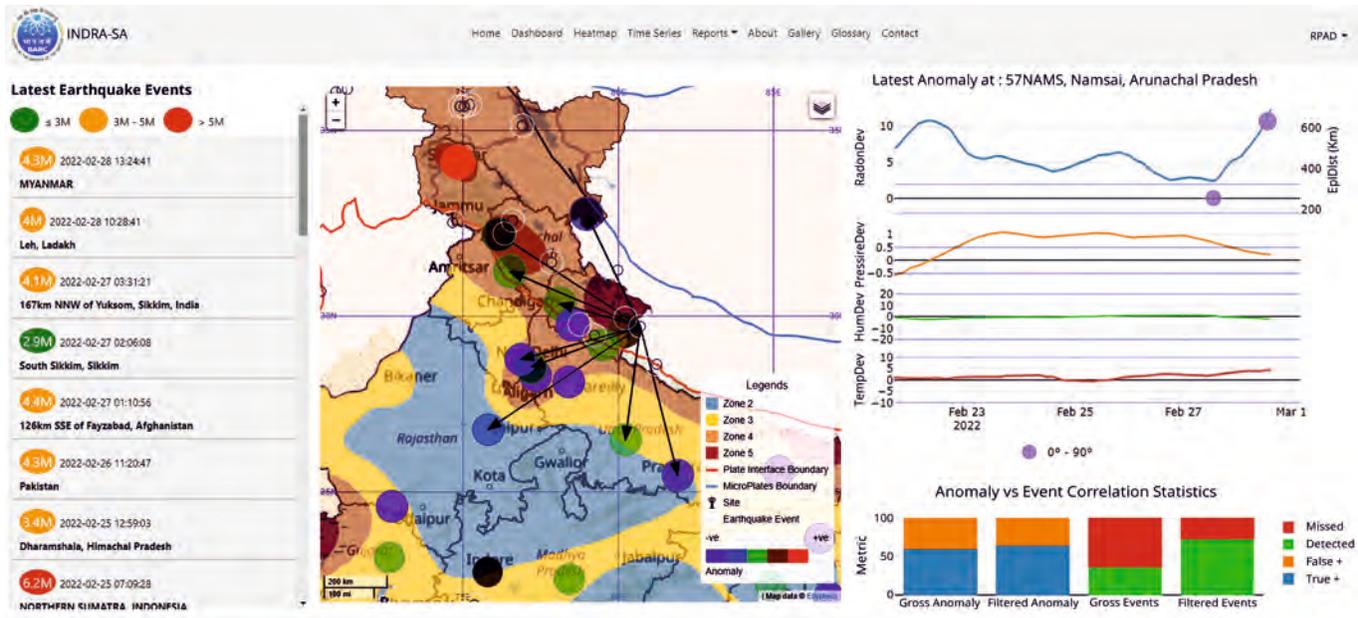


2 Stack Monitoring Systems of KARP-II

System (GEMS) contains an individual shielded chamber for collection of each type of sample and associated detector assembly within the chamber so that the natural background is reduced significantly. After making all three shielded chambers in-house, a radiometry test was conducted. A thorough study has been conducted to establish the efficiency, MDAs for each detector, capability of the detector and associated electronics to measure the maximum authorised release values and accuracy of the results for various range of isotopic activities. The efficiency calibration of Particulate and Iodine monitors was carried out as per standard procedure with the available sources in the facility. A portable chamber with the NaI(Tl) detector placed at the centre was fabricated and used for efficiency calibration of FPNG, Ar-41 and Xe-133. Energy and Efficiency calibration was carried out for Ar-41 and Xe-133. The newly developed system will provide a comprehensive quantification of radionuclides released through stack such as particulate activity, I-131, Ar-41 and Xe-133.

Indian Network for Detection of Radon Anomaly (INDRA) for Seismic Alert (100 Stations)

This project is aimed at setting up a country-wide network of 100 units of in-house developed solar powered Radon Geo Stations to investigate earthquake predictability using radon anomaly as an earthquake precursor. At present, 57 Radon



INDRA-SA Network for Seismic Alert

Geo Stations have been established along the Indian tectonic plate boundary with the central server stationed at CTCRS, Mumbai. About 3 million data points of radon and atmospheric parameters (Temperature, Humidity, Pressure) have been gathered at the central server to initiate a large scale machine learning analysis towards seismic predictability. New sites along and across the Indian tectonic plate boundary have been selected. The aim is to understand the correlation between radon anomaly and earthquake events using the acquired data. INDRA-SA Homepage has been designed and commissioned at Central Server for visualization of radon anomalies along with the earthquake events in a seismic map of India. Analysis of results indicates that true positive cases of detected radon anomaly is about 73% and prior detection of earthquake events falling within two times the strain radius is about 82%.

Deployment of Environmental Gamma Spectrometry System

Environmental Gamma Spectrometry System (EGSS) is an indigenously developed standalone, solar powered and battery operated unit for measurement of radionuclides in the atmosphere. It has a 2" diameter by 2" height NaI(Tl) scintillator based gamma spectrometer, coupled with GM tube based gross gamma detector. For optimised

power utilisation, the spectrometric analysis is triggered only when the GM tube detects gamma dose rate beyond a pre-set threshold value. The monitored data is communicated through GSM to a central receiving station. A methodology has been developed for restoration of the shift of spectrum due to change in ambient temperature, making the system fit for use in varying temperature conditions. Requirement of data logging computer for storing large sets of data has been eliminated by integrating an in-house developed low power multichannel analyser. A rugged hermetically sealed mechanical housing has been designed and fabricated in-house, making it suitable for deployment in extreme environmental conditions.



Environmental Gamma Spectrometry System (EGSS)

EGSS is a cost effective import substitute, developed for large scale deployment in a countrywide network for real-time identification of radionuclides in case of radiological/nuclear emergency. The system will provide the much needed isotopic composition data from the open field to estimate the time varying source term (release rates) in case of an accident at a nuclear power plant.

Development of Air Moisture Sample Collector for Tritium Analysis

Tritium is one of the important radionuclides monitored regularly around Nuclear Power Plant (NPP) sites. Tritium in air is estimated by collection of air moisture in the environment and analysis is carried out using Liquid Scintillation Analyzer. Presently, Environmental Survey Laboratories (ESLs) collect air moisture samples by conventional ice-cold condensation method at various identified locations in periodic intervals throughout the year. Using this method, random samples are collected for a short period of time as it is difficult to collect long time cumulative samples thereby limiting the amount of moisture being collected. To overcome these limitations, an automated air moisture sample collector, working on thermo electric cooling technology, is designed and developed for collecting air moisture for analysis of tritium in the environment around NPPs. This is an indigenous development and this type of sampler is not available in the international market. The sampler is standalone and doesn't need any manual intervention for operation. A standalone solar powered system with battery backup has been fabricated. The sampler will immensely support the surveillance programme of ESLs being carried out around NPP sites to demonstrate compliance of regulatory limits and protection of the environment and members of the public.

A Tritium-in-Air Monitor System (TIAM) equipped with a ultra-low current measurement system for measuring a range of 1 to 199 DAC. TIAM systems equipped with a 40L



Tritium-in-Air Monitor System (TIAM)

detector, pump, flow meter, Ion trap with pipes/hose and an electrometer unit connected to the detector and ion trap using cables and installed into a rack, have been installed and commissioned .

Silicon PIN-detector Based Smart Device for Detecting Gamma Radiation

ANUSUCHAK is a light weight, low power and smart device based on silicon PIN-detector which can detect elevated levels of gamma radiation. It is connected to a PC/smart phone through a USB port and displays the measured dose in a numerical and graphical format on the connected device.

The features provided in the software include audio and visual warning and alarm for dose exceeding threshold limit. The response of the dongle has been calibrated for 0.5 mR/hr - 2 R/hr, energy flattening within $\pm 15\%$ for Am-241, Cs-137 and Co-60.

New Approaches for a Vibrant Back-end Nuclear Fuel Cycle

- ✧ Pilot Plant for production of Zirconium and Hafnium Oxide
- ✧ Experimental studies on uranium extraction in Pulsed Disc and Doughnut Column (PDDC) setup
- ✧ Studies for determining the thermophysical and structural properties of ceramics as part of efforts to develop alternative matrices for waste immobilization
- ✧ Development of stable crystalline matrices for immobilization of radioactive Cesium
- ✧ Synthesis of photoluminescent nanoparticles for detection of actinides
- ✧ Synthesis of $\text{Na}_4\text{Ti}_9\text{O}_{20} \cdot x\text{H}_2\text{O}$ and its performance evaluation for Sr (II) extraction from nuclear waste
- ✧ Advanced Crown Ether Synthesis Plant (ACESP) for recovery of Strontium from synthetic nitrate solution
- ✧ Development of phosphate and phosphomolybdate-based polymeric gels for greater uptake of fission products

Nuclear Hydrogen

Electrolytic Hydrogen Production at Indian Nuclear Power Plants: Profitability Analysis

Indigenous production of green hydrogen is being strongly emphasized by the Government of India for deep decarbonization of sectors which currently consume hydrogen derived from mostly imported fossil fuel source. The business case for nuclear hydrogen was thoroughly analysed.

The techno-commercial analysis shows that India's existing water-cooled nuclear reactors can produce hydrogen by water electrolysis at annualized life cycle costs of US\$3.2 to 8.5 per kg of H_2 , depending on the scale of operation (1.25 to 5 MW(e) modular H_2 plants). Long-term hydrogen production cost targets of less than US\$2 per kg H_2 are also achievable at certain power with a lowered capital cost of the plant.

Hydrogen Preferential Pick-up by IPHWR Coolant Channels

For zirconium based structural materials at reactor operating conditions, the accepted mechanism is



The Passive Catalytic Hydrogen Recombiner (PCHR) with Platinum and Palladium wire gauge catalyst bearing panels

that the nascent hydrogen/deuterium generated due to reduction of H^+/D^+ at metal and metal oxide interface, is partially absorbed by the structural materials.

The nascent hydrogen/deuterium was generated on Zr-2.5%Nb metal surface employing electrochemical method. After H/D charged on Zr-2.5%Nb alloy piece, H & D content was determined employing HVE-QMS technique. After subtraction of initial hydrogen content from the observed H content, plot was constructed between H preferential uptake factor (ratio of $(X_{(H,M)}/X_{(D,M)})$ and $(X_{(H,S)}/X_{(D,S)})$) versus $(X_{(H,S)}/X_{(D,S)})$ (here M; material, S; solution). It was observed that, at all ratios of mole fractions of H_2O & D_2O in the solution, hydrogen was preferentially absorbed by Zr-2.5%Nb alloy by about 5 to 7 times compared to deuterium. These observations closely match with the observed results of some coolant channels of typical IPHWRs.

Indigenization of Passive Catalytic Hydrogen Recombiner

To mitigate the hydrogen risk and to ensure the containment integrity during accident conditions, passive catalytic hydrogen recombiners (PCHRs) are being developed (in collaboration with NPCIL) using in-house technology. A design basis report for an indigenized-PCHR was prepared, wherein Pt+Pd/SS wire gauze catalyst bearing panels (CBPs), used in the passive catalytic recombiner devices deployed in PHWRs, were reconfigured to fit into the PCHR dimensions while attaining the desired hydrogen removal rate of 0.56 kg h^{-1} at 4% H_2 in air. The reconfigured CBPs were fabricated through ECIL, Hyderabad and validated for their performance at the test-rig at KKNPP.

Based on the superior performance of indigenous CBPs, a prototype recombiner with dimensions and catalyst placement configuration similar to PCHR has been fabricated through ECIL and supplied to NPCIL for evaluation at HRTF, Tarapur. Necessary approval for evaluation has been received from the Standing Committee – Integrated Test Facility for Thermal Hydraulics Experiments (SC-ITFT), NPCIL.

Mitigation of Hydrogen in HLW Tanks

In order to mitigate hydrogen generated (by radiolysis of water) in high level waste tanks, the suitability of Pd+Pt/SS wire gauze based hydrogen mitigation catalyst was evaluated on samples exposed to nitric acid fumes for different duration. Samples exposed for a period up to four months were found to be active for hydrogen-oxygen recombination reaction.

Low Level Hydrogen Detection System in Liquid Sodium Coolant

H_2 Sensitivity range of 80 ppb to 2500 ppb achieved in vacuum and a sensitivity range of 400 ppb to 2000 ppm has been achieved in Helium. Ion Current output (4 – 20 mA) can be utilized to set Trip switches at different H_2 concentrations.

Advanced Reactors and Associated Materials

The critical power of AHWR fuel bundle has been demonstrated experimentally using a full scale simulated fuel rod bundle under reactor operating conditions. The data obtained from the experiments was used to estimate critical power correlation of AHWR bundle design as well as its thermal margin.

An improved prediction method has been proposed for evaluating load bearing capacity of cracked dissimilar metal pipe weld between the steam drum and the down comer piping of AHWR as part of the studies done routinely for safety assessment of weld joints with defect.

A numerical simulation approach was used for evaluating load carrying capacity of concrete frames under seismic simulated loading conditions in shake table testing. A significant reduction in load carrying capacity was observed in case of corroded frames in comparison with the uncorroded frame.

A unique experiment for measuring the reactivity under different voiding fractions of High Density Polyethylene (HDP) coolant was carried out in the AHWR Critical Facility at BARC. The experimental



The molten salt corrosion test facility in BARC

cluster consisted of seven pins of (Th, 1%Pu) MOX fuel whose dimensions were maintained same as that of AHWR type fuel pins. Experiments were performed with four different voiding conditions of 33%, 50%, 66 % and 100%. The maximum deviation in the predicted and measured critical heights for the various configurations came to about 0.23 mk in reactivity change. A very good agreement of this measurement with the modelling is another step in code validation exercise and validation of AHWR physics design.

Pre-experimental analysis with 5.8 kg of fuel salt (LiF-UF_4) to assess reactivity effects of introducing a Molten Salt Fuel Tube (MSFT) was carried out in the central and peripheral locations of the lattice arrangement at the AHWR Critical Facility. The levels of moderator were varied to achieve a definitive critical core with the fuel salt assembly. Efforts are in progress to estimate the quantum of tritium produced during the experiment.

A vertical single stage pump of Ni-Mo-Cr-Ti alloy make has been chosen as the Coolant Salt Circulating Pump (CSCP) for the experimental 5 MWth Indian Molten Salt Breeder Reactor. The set-up has been custom designed wherein the rotary assembly could be removed easily and can be subjected to inspection in a hot cell.

A Graphite Fuel Salt Interaction Facility (GFS-IF) for extensive study of interaction between graphite and molten fuel salt at the temperatures and pressure prescribed for the 5 MWth IMSBR

has been established at the Molten Salt Breeder Reactor Long Term Test Facility (MSBRDF-LTTF) based at Vizag. Due to extreme sensitivity of molten salts to moisture and oxides, the facility was installed inside a negative pressure glove box.

An oscillating cup viscometer of Mark 2 Version is being developed for measuring the viscosity of molten salt of interest for IMSBR. The viscosity of the salt is determined by measuring the change in damping of free oscillations of the cup suspended from a wire both in presence of the sample and also without it.

An electromagnet brake based oscillation damping system has been included to allow faster reset of the system during its operation, which also functions as an alternate oscillation initiator. For measuring the oscillation parameters, a system based on reflection of laser onto a microprocessor based photo-diode array has been developed. The Mark-1 version of the viscometer was successfully demonstrated earlier with surrogate samples.

A Forced Circulation Molten Salt Loop (FCMSL) has been commissioned for the study of thermal-hydraulics of molten salts for MSBR and the instruments and components such as molten salt pump, freeze flange designed for it. The design pressure and temperature of the loop are 5 bar and 565°C. The loop has been charged with 200 kg of Nitrate salt and successfully operated.

Two static high temperature systems - Auto dipping and Autoclave - have been commissioned in BARC for material testing and corrosion studies on high temperature systems, including Molten Salt Reactor.

Electro chemical corrosion studies for developing of REDOX control techniques relevant to molten salt at high temperature were done at the autoclave system.

The auto-dipping facility is designed to carry out corrosion studies in high temperature coolants by weight loss method. The maximum operating temperature and pressure will be 750°C and 0.5 bar.

Development, Preparation and Characterization of Refractory Metal based Alloys

Development of Mo-Ti-Si-B alloy: The search for the new high temperature structural materials, which have the temperature capability beyond the Ni and Co-based superalloys attract wide attention because of numerous emerging applications including high temperature nuclear reactors. BARC has developed high temperature oxidation resistant Mo-Ti-Si based alloy with and without B addition. Oxidation studies of Mo-10Si-(0-2)B-(25-35)Ti (wt.%) alloys were carried out in TGA system for 72 h at 800, 1050 and 1250°C in static air. The Mo-10Si-2B-35Ti alloy showed best stability against oxidation at high temperatures among the alloys studied. High speed nanoindentation mapping technique was used to determine the mechanical properties such as hardness and elastic modulus of individual phases. Tungsten heavy alloys are widely used as radiation shielding components in cancer therapy machines and other gamma radiation exposure devices. BARC has developed a processing scheme for preparation of different grades of tungsten heavy alloys – D-170 (W-7Ni-3Fe), D-176 (W-4.9Ni-2.1Fe), D-180 (W-3.5Ni-1.5Fe) and D-185 (W-2Ni-1Fe) by compaction followed by liquid phase sintering route. A WHA (W-2Ni-1Fe, D185) billet having a dimension of 15×20×200 mm (~2.5kg) was fabricated in-house. The density and hardness of the sintered alloys were found to be equivalent to the commercially available D185 manufactured by M/s Plansee.



FLiNaK salt prepared inside molten salt corrosion test facility (MSCTF)

Fluorophosphate Matrix - A Possible Waste Matrix for IMSBR

Halides containing radioactive wastes are generated during pyro-chemical reprocessing of spent nuclear fuel of advanced nuclear reactors like molten salt reactor, metallic fuel based reactor etc. Vitrifying halide wastes in alkali borosilicate glass is not suitable due to the low solubility of halide ions in such host matrices. Hence fluorapatite compounds of calcium and strontium; ($\text{Ca}_{10}(\text{PO}_4)_6\text{F}_2$ and $\text{Sr}_{10}(\text{PO}_4)_6\text{F}_2$), were explored as an alternative to borosilicate glass. Heat capacity and enthalpy increments of these compounds were measured using calorimetric technique. Variation of different bond lengths and polyhedral volumes against temperature were calculated by Rietveld refinement which confirmed that PO_4^{3-} group remains rigid while M-O bond is mainly responsible for thermal expansion. The radiation stability up to 1000kGy of both the matrices against electron beam induced radiation was investigated. It was observed that $\text{Ca}_{10}(\text{PO}_4)_6\text{F}_2$ is more resistant towards structural damage upon electron beam irradiation as compared to $\text{Sr}_{10}(\text{PO}_4)_6\text{F}_2$.

Thermal Studies for MSBR

The thermodynamic properties of $\text{NaCeF}_4(\text{s})$ have been studied and identified as an interaction product of pseudo binary NaF-CeF_3 system for MSBR chemistry. CeF_3 is one of the burnable waste fluorides and Ce^{3+} is also the surrogate of Pu^{3+} . $C_p^\circ[\text{NaCeF}_4(\text{s})]$ has been measured experimentally with DSC and the Gibbs energy of formation, $\Delta_f G_m^\circ$ of $\text{NaCeF}_4(\text{s})$ has been determined using Solid Electrolyte Galvanic Cell (SEGC) with $\text{CaF}_2(\text{s})$ as solid electrolyte.

The binary phase diagram of $\text{NaF}(\text{s})\text{-CeF}_3(\text{s})$ system has been calculated based on experimental thermodynamic data. To study the stability domain and coexisting phases of $\text{NaCeF}_4(\text{s})$, the chemical potential diagram of Na-Ce-F-O system and ternary phase diagram of Na-Ce-F₂ system has been calculated. In order to study the interactions between coolant salts and structural materials, thermodynamic properties of LiF-NiF₂ system has been carried out. The $\Delta_f G_m^\circ$ of $\text{Li}_2\text{NiF}_4(\text{s})$ has been

measured with SEGC technique. The ternary phase diagram of Li-Ni-F₂ system and chemical potential diagram of Li-Ni-F-O system has been calculated in order to study stable coexisting phases of Li₂NiF₄(s) at the reactor operating temperature (600°C/873 K). In order to understand the thermodynamic behaviour of fuel-coolant system, the pseudo binary phase diagram of NaF-UF₄ system was determined over full range of composition ($X_{UF_4} = 0$ to 1) by DTA measurements. C_p of Na₂UF₆, Na₇U₆F₃₁ and NaU₂F₉ were measured. Thermodynamic (activity and activity coefficients) and kinetic (diffusion coefficients, activation energies, parameters of UF₄ and ThF₄ in UF₄-ThF₄-FLiNaK mixture were determined by various electrochemical techniques (CV, CP, and SWV in temperature range 823 to 873 K for different compositions of UF₄ and ThF₄. These kinetic parameters are important for efficient electrochemical pyroprocessing of MSBR spent fuel.

Reactor Antineutrino Studies

A large area plastic scintillator (PS) detector setup ISMRAN (Indian Scintillator Matrix for Reactor Anti-Neutrinos) has been fabricated and installed at Dhruva research reactor. The setup consists of PS bars arranged in a 9 x 10 matrix with an active volume of 1ton, enveloped inside a passive shielding of Lead and Boronated Polyethylene staged on a base structure with a total weight of 19.4 ton. Through the measurement of antineutrino, ISMRAN seeks to obtain answers for several outstanding problems of fundamental importance such as the existence of sterile neutrinos, reason for excess of antineutrino spectral yield. and reactor power monitoring in a non-intrusive way. Using this setup, measurements have been carried out for the decay products of cosmic muons which are stopped inside the detector matrix and cosmic muons passing through the full geometry. The ISMRAN setup is now continuously acquiring data both in the Reactor "ON" and "OFF" mode. As data with more statistics will be acquired, the measurements are expected to provide answers to several outstanding problems of fundamental importance.

Fusion Reactor

Lead-Lithium (Pb-Li) Extractor Loop

A test loop has been developed and installed for Hydrogen Isotope extraction studies from Lead Lithium (Pb-Li) eutectic at 450°C. The study will help in understanding hydrogen isotope behavior in molten metal, which will be useful for future coolant and breeder for Test Blanket Module (TBM) in fusion reactor. The system consists of a recirculation loop with melting tank, electromagnetic pump, electromagnetic flow meter, structured packed column and gas extraction system.



Pb-Li Extractor Loop showing high temperature electromagnetic pump

Iron Aluminide Coating for Test Blanket Module

Pack aluminizing technique was employed to develop iron aluminide coating on P91 steel. This type of coating is required for test blanket modules (TBM) of fusion reactors. Iron aluminides have superior oxidation and corrosion resistance properties which make this type of coating



Aluminized (inner surfaces) SS 316 storage modules

essential for thermal power plant applications also. Pack aluminizing process parameters were varied in order to arrive at optimized coating parameters. Single phase Fe_2Al_5 coating with varying thickness (15-130 μm) was found to form in the temperature ranging from 600-700 $^{\circ}C$. Heat treatments of as-coated samples were performed at their application temperature range 600-750 $^{\circ}C$ by varying time. FeAl layer of varying thickness (5-25 μm) has been observed in the temperature ranging from 550-750 $^{\circ}C$ for time (8-40 h). Oxidation test of as-coated and bare samples have been done between 700-1100 $^{\circ}C$ under different environments revealed the benefits of coating as it leads to protective alumina scale formation.

The Aluminide coating over low alloy steel showed a single layered coating comprising of Fe_2Al_5 phase having a thickness of 60 μm that was prepared at 600 $^{\circ}C$, while multi-layer coating comprising of $Fe_2Al_5/FeAl/FeAl$ of 120 μm thickness was formed at 900 $^{\circ}C$. Halide activated pack cementation process was developed to enrich the surface of SS 316 components with aluminium for developing permeation barrier coating. Pack aluminizing coating was conducted at about 525 $^{\circ}C$ for 16h. The required coating was prepared on the inner surfaces of the modules. The thickness of the aluminide coating obtained is about 25-30 μm .

Spent Fuel Reprocessing

Recovery of Special Nuclear Material

Plutonium Plant (PP) operation has been continued leading to recovery of Special Nuclear Material (SNM). Sustained and continuous operation of PP for the recovery of SNM with Dhruva spent fuel has resulted in NIL inventory of spent fuel for reprocessing at reactor-end presently.

The spent fuel of Dhruva reactor was transported to Plutonium Plant, Trombay after ensuring the desire cooling period. The spent fuel was decladded by chemical dissolution and processed to recover SNM using PUREX based reprocessing flowsheet. Plutonium Plant, Trombay was operated successfully for reprocessing of spent fuel of the research reactor and recovery of SNM ensuring no back log of reprocessible spent fuel.

Subsequent to the last batch charging, initiation of plant shutdown activities has been taken up. Decontamination of process cells is under way to bring down the radiation field inside the hot cell to facilitate the planned modification/refurbishment work, with minimal personal exposure, aiming towards the life enhancement of facility.

Deployment of Advanced System for Spent Fuel Storage Pool

Ion exchange based system is utilised for cleaning of water of Spent fuel storage pool to maintain the desire visibility and limit the radiation field on the pool. Replacement of cation resin is required at regular intervals. In view of reducing personal exposure and enabling adequate conditioning of spent resin while replacement of resin, Resin Hopper Cask Trolley system is being augmented near spent fuel storage pool of Fuel Reprocessing facility. The fabrication and commissioning of RHCT was completed.

The system was delivered at the site after satisfactory load trial, Interlock checking and emergency operation evaluation.

Spent Fuel Charging System

In view of enabling Dissolver-2 system of Fuel Reprocessing facility, an operable, spent fuel charging system is being augmented at Fuel Handling Area (FHA) of the facility. The system consists of charging cask transfer trolley along with cross travel transfer system for charging of spent fuel to dissolver system. Charging cask transfer trolley has been fabricated, tested and delivered at site. The same is being installed at Plutonium Plant.

Radioactive Waste Management

A Remotely Replaceable IP camera on crane was developed in hot cell at WIP and the same was installed on in-cell crane. EP Mounted Retractable IP Camera has been developed and tested outside hot cell. As a part of advancement of work station at WIP-Trombay for remote viewing and control with improvised hot-cell viewing capability, work stations have been commissioned with PLC based system, networking rack and cables were installed. Most of the cameras have been hooked up with networking rack, video wall has been commissioned, relay based system has been kept as backup of PLC and commissioned.

Face Recognition Cameras have been installed and commissioned for strengthening surveillance of high security zone. Installation and Commissioning of APFC panel was carried out for power factor improvisation.

Management of High Level Liquid Waste and Value Recovery

The High-Level Liquid Wastes (HLLW) emanated during reprocessing of spent fuel at Trombay showed the presence of problematic components like sulphates along with high inactive salt load. An innovative method based on partitioning of the radio-elements from the inactive salt constituents by deploying indigenously developed solvents has proved to be very successful in management of radioactive waste with multi-fold advantage. By adopting this scheme, the strategy of waste management on minimising the volume of waste and concept of recover & recycle of waste

components has been implemented. The HLLW is subjected to a three-step separation process involving TBP for U-separation, Calyx crown solvent for Cs-137 separation and TEHDGA solvent for Sr and actinide separation. 41000 L of U lean HLLW has been managed by this scheme enabling recovery Cs-137 product stream and Sr-An-Ln rich product stream. Cs-137 product stream, containing 143000 Ci of Cs-137, was concentrated and is being vitrified to produce Cs specific glass for making Cs glass pencils for blood irradiator. The Sr-An-Ln product stream was concentrated and vitrified using induction heated metallic melter to produce 3 numbers of vitrified canisters. The HLLW management process was operated successfully to reduce the waste volume for final repository by multiple fold, to attain overall decontamination factor of more than 1E9 resulting in near zero discharge of radioactivity and to enable recovery of valuable fission products such as Cs-137, Sr-90, Ru-106 for societal applications.

Management of Low Level Liquid Waste

Un-interrupted services of collection, treatment and disposal of low level radioactive liquid waste generated from various plants and laboratories in Trombay were ensured at Effluent Treatment Plant, Trombay. 44,593 m³ of low level radioactive waste was received. The waste was safely managed by employing Chemical Treatment Flow sheet. The low-level effluents were disposed after monitoring.

Augmentation of Ion Exchange System at ETP for Treatment of Low Level Liquid Waste

In order to realize "zero discharge concept", a selective sorbent-based ion exchange facility was planned at ETP after substantive trials of LLW in pilot scale facility. The facility is provided with four columns of 500 litre bed volume complete with shielding and column handling equipment. The facility is designed for remote operation. Installation of the facility was completed during the current period. Testing of various components of the facility like pumps, valves and columns was completed. Cold commissioning of the system was

carried out. Safety clearances were obtained for hot commissioning and trial operations. Around 275 m³ of LLW was processed through Zeolite – based ion exchange facility.

Construction of Multi-tier Reinforced Concrete Disposal Module (MRDM)

MRDM construction was completed. After obtaining clearance from OPSRC, the module is being utilized for disposal of Category-I waste. A Gantry Crane, of 10/02 ton capacity and 26 metre span, was fabricated and installed at site for enabling smooth material handling operations for MRDM.

Development of Alpha Drum Assaying System

Passive gamma assay technique based on the measurement of known gamma-ray energies is used for alpha waste monitoring. HPGe detectors are employed for high resolution spectroscopy with a relatively low detection efficiency, whereas NaI(Tl) crystals are used for low resolution spectrometry with relatively high efficiency.

Gamma assaying system based on NaI(Tl) for alpha waste monitoring was installed at Laboratory 210B, WIP. It consists of drum manipulator, detectors for segmented counting of drum, MCA & data acquisition system.

The drum manipulator is a mechanical system to facilitate vertical and rotational movement of the



Alpha Drum Assaying System

drum during assaying. It is provided with rotating SS roller platform and is supported on vertical sliding guides to provide up & down movement to the drum. Electrical & electronics gadgets are also provided to the drum manipulator to achieve automated movements with desired accuracy. Drum manipulator system was commissioned after placing four detectors vertically, 200 mm apart, using 10 mm lead as collimator to scan entire drum of 800 mm height. All four detectors were individually calibrated using standard Cs-137 and Co-60 sources. Three point calibrations with similar slope and intercept confirmed linear behaviour of count vs energy curve for all the detectors. Total counts vs Pu quantity was plotted using Pu standards in the range of 40 to 950 mg. Location of Pu standards was shuffled to confirm the reproducibility of the counts for a given combination of total Pu. More than 100 trials were carried out to generate this curve based on best average counts. A drum with known quantity of Pu was scanned in the developed system and the error in Pu estimation was found to be ~18%.

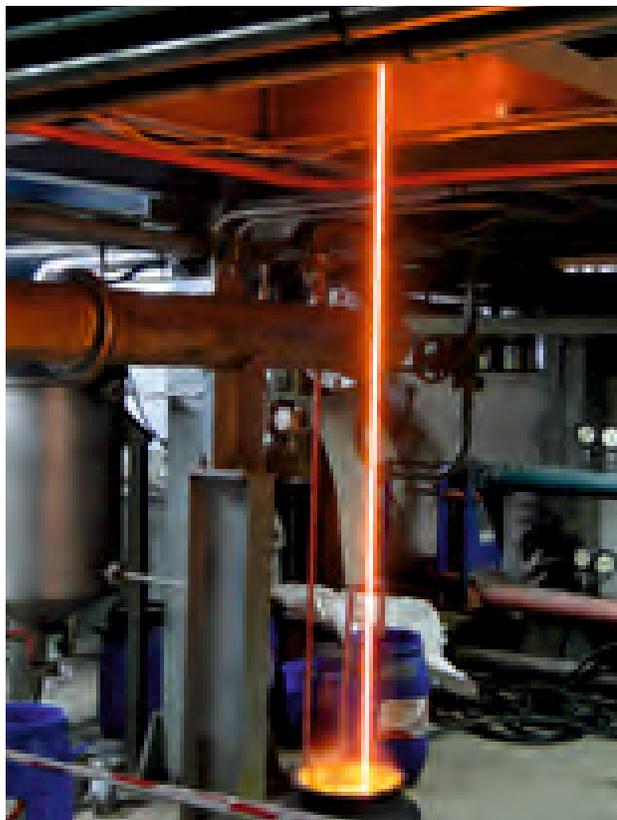
Development of Process for Simultaneous Removal of Hazardous Isotopes from Acidic ILW

¹⁰⁶Ru and ¹²⁵Sb constitute a significant hazard in ILW/LLW management, as they are radiotoxic and cytotoxic.

A process for simultaneous removal of Ru & Sb from acidic ILW was developed. The process utilizes precipitation of Zr-hydroxide to augment the removal of Ru and Sb upon an increase in pH of the acidic ILW to near neutral by addition of NaOH.

The process was demonstrated with actual acidic ILW generated from partitioning of HLW. During the demonstration trials, ¹⁰⁶Ru and ¹²⁵Sb activity was reduced to background level from 2.6 mCi.l⁻¹ and 6.2 mCi.l⁻¹ respectively.

The process development for simultaneous removal of Ru and Sb from acidic ILW has been completed. Based on the research outcome, a patent application has been filed for "A Process for Simultaneous Removal of Ru and Sb from Acidic Intermediate Level Waste (ILW)" in Europe & USA.



Cesium glass pouring under operation

Development of Plant-worthy Cold Crucible Induction Melter

The design of plant adaptable CCIM was arrived at after incorporating feedback obtained from various taskforce which were constituted for reviewing and also to provide feedback on the operational aspects of the plant. Various new features were introduced in the equipment to meet operating plant requirements, which include a secondary metallic containment to allay any fear of HLW waste leakage to the cell, alumina coated cooling tubes to prevent any accidental arcing by

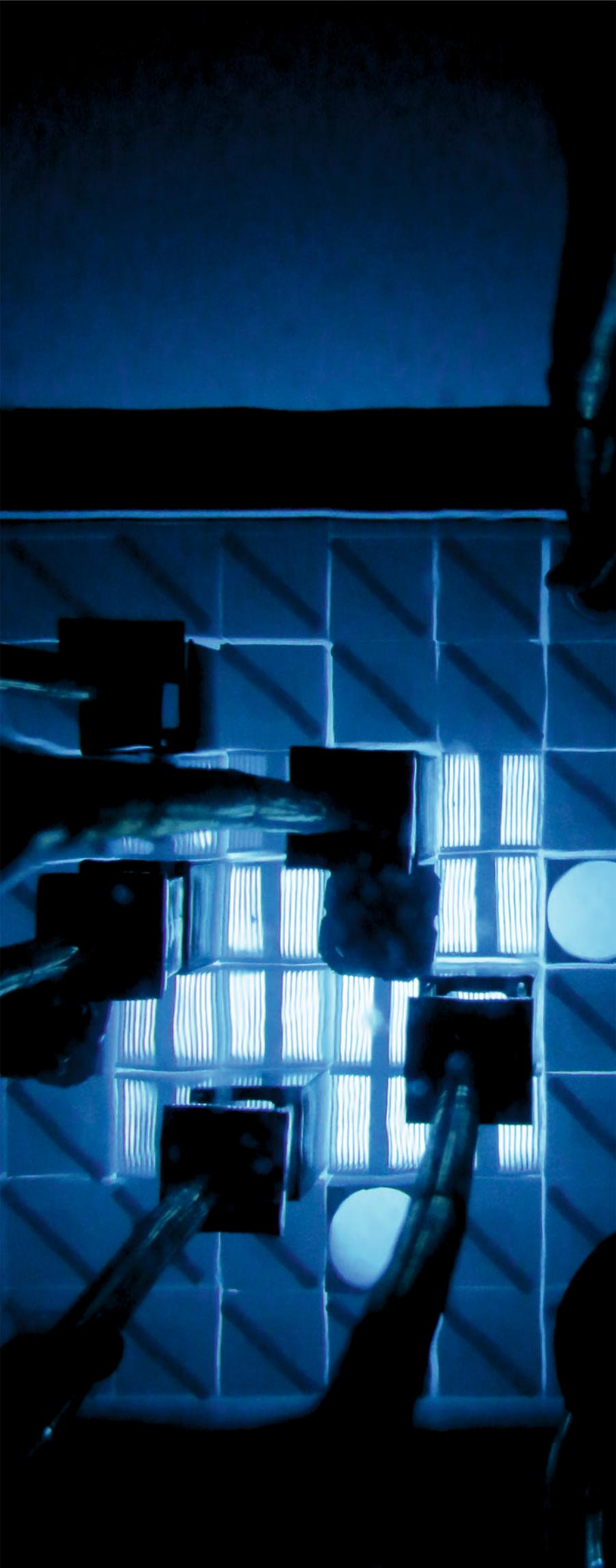
graphite ring introduced for start-up, additional pouring port for redundancy, remotely operable and maintainable pouring plug actuator, remotely operable quick coupling for all cooling water lines and customized connectors like block connector and three jaw connector for large sized cooling water line. The plant worthy cold crucible induction melter was fabricated with SS 304 L material following requisite QA plan and procedures needed for cell worthy equipment. The equipment was installed, tested and commissioned. Subsequently a proposal was put up for the transfer of plant adaptable cold crucible induction melter to Nuclear Recycle Board for implementation in Waste Immobilization Plant, Tarapur.

Construction of Alpha Solid Waste Treatment Facility

Alpha Solid Waste Treatment Facility (ASWTF), Trombay is being constructed for management of alpha solid waste. Construction of ground floor of Block II has been completed. Construction of Stair cases, RCC walls, columns, roof slab at Ground Floor was completed in Block II.

Construction of Tile Holes Disposal Module

Construction of Tile Hole battery comprising 94 Tile Holes (TH) at RSMS was completed. This includes construction of TH, Precast covers of TH, RCC Top slab and its water proofing from top. These disposal modules will be used for disposal of Category-III solid waste having surface dose 50R/hr.



ADVANCED TECHNOLOGIES, RADIATION TECHNOLOGIES AND THEIR APPLICATIONS

Research and Development program in BARC is focused on achieving self-reliance. Over the years, this approach has resulted in development of advanced technologies indigenously in the areas of Research Reactors, Accelerators and Lasers, Sensors and Detectors, Radiopharmaceuticals, Materials for Energy Storage, Management of Surface Water and Groundwater Resources, Solid Waste Management, Agriculture, Food, Healthcare and various niche domains.



Cherenkov Radiation seen in Apsara-U

Advanced Technologies, Radiation Technologies and their Applications

Research Reactors

Apsara-U Operation at 1.8 MW

After obtaining regulatory clearance, the 10th Standard Fuel Assembly (SFA) was loaded in the core and reactor power was raised in stages, with due surveillance on radiological parameters. Power level of 1.8 MW was achieved on 26th February, 2021. Subsequently, the reactor was satisfactorily operated at this power continuously. The pool water activity and radiation fields on PCW system were found to be steady at this power level.

Apsara-U Operation at 2.0 MW

After installation of 11th SFA in core, the reactor power was raised gradually after obtaining

regulatory clearance for operation at a rated power of 2MW. The Reactor power was raised to full power of 2 MW at 10:42 hrs on 8th October 2021.

The Reactor was operated continuously at rated power at core Position-B for 60 days. All the radiological and process parameters were found to be within stipulated limits.

Experimental Irradiation of NTD Silicon

A Tray Rod was designed to hold a 2 inch silicon ingot at central elevation. Irradiations of the ingot were conducted in the core region & reflector region. A cylindrical aluminium container was designed to hold the 2 inch silicon ingot in reactor irradiation position. A Small size silicon ingot and a silicon wafer were irradiated as part of the feasibility study for producing Neutron

Transmutation Doped Silicon (NTD-Si) in the Apsara-U reactor. Initially, sample irradiation with a 2 inch sample was carried out for characterisation of the irradiation positions, with manual rotation. Based on the thermal to fast neutron flux ratio, a suitable location for regular production of NTD silicon was identified. A relation was evolved between the time of irradiation and resistivity of the ingot. Protocol for ingot decontamination and annealing was also evolved.

In Apsara-U reactor, the thermal and fast flux monitors like gold and nickel were irradiated. Measured thermal and fast flux (>1MeV) at incident face of polythene block was found to be $8.74E+06$ and $2.87E+05$ n/cm²-s, respectively.

Design and Stability Checking of Apsara-U Beamlines

The design and stability checks of BT-6 and BT-8 beam lines of Apsara-U Reactor under the earthquake simulated load have been performed. The setup was found to be structurally safe and stable under recommended earthquake loads. The Shielding Hutch for Neutron Imaging Setup at BT-7 of Apsara-U has also been subjected to earthquake load and the setup was found to be structurally safe and stable under prescribed earthquake loads.

Measurement of N-16 Activity at Coolant Outlet Header

A spare Gamma Ion Chamber was installed on the coolant outlet header in the Delay Tank Room for measurement of N-16 activity, in a bid to co-relate it with the thermal power of the reactor. The Output current of GIC was measured at various power levels by electrometer and was seen to be following the reactor power closely.

Single Comparator Neutron Activation Analysis

Irradiation position (G4) at Apsara-U for implementation of single comparator (k_0 -based) Neutron Activation Analysis (NAA) method was characterized and validated by Python programming method using an iterative procedure for evaluating sub cadmium to epithermal neutron flux ratio (f) and epithermal neutron flux shape parameter (α). This method was used for the analysis of sodalime glass standard reference materials (SRMs) and automobile glasses for QA/QC towards forensic applications. The deviations in certified values and corresponding Z-scores were found to be within $\pm 5\%$ and ± 1 , respectively, which validate the accuracy of the method. The % RSD from the five replicates of automobile glass samples was found to be within $\pm 7\%$ showing the adequate precision of the method.

Relation of Chlorine Concentration in Pool Water and its Pick up by Aluminium Clad

To investigate the possible Chloride (Cl⁻) ion pickup by Aluminium (Al) from the pool water of APSARA-U reactor, 2 mm thick Al pieces (1 cm X 1 cm) were kept in contact with solutions of varying chloride concentrations at room temperature and at 50°C. The chloride remaining in the solution after different time intervals (up to 3 months) were analyzed. It was observed that the percentage of Cl⁻ ion uptake by the Al pieces were dependent on the chloride ion concentration and the temperature. Higher the chloride ion concentration in the aqueous phase higher is the uptake by Al. The uptake of Cl⁻ at a given chloride concentration increases with rise in temperature. At 150 ppb chloride concentration, the uptake was up to 80% whereas for the initial concentration of 15 ppb the uptake was found to be less than 20% for the contact period of three months. Thus, the water having chloride ions below 15ppb show significantly lower chloride pickup.

Remote Visual Inspection at Dhruva

As a part of ageing studies of reactor components, Remote Visual Inspection (RVI) of 100mm diameter horizontal beam hole HS-1019 re-entrant can and its rolled joint was inspected for the first time since Dhruva commissioning, after developing appropriate tooling to manage 1000 R/hr of radiation field. Helium sniffing and tritium leak checking of one beam tube rolled joint with Reactor Vessel was carried out. Rolled joint and its seal weld were found to be in healthy condition without any evidence of water leakage.



Inspection set-up at Dhruva beam tube

Dispersion Fuel Assembly - 4/3 Irradiation

The Experimental irradiation of newly developed 61 pin dispersion fuel assembly (DFA-04) at Dhruva was completed. The assembly was removed from the pile and the performance of the fuel was found to be satisfactory.

DHRUVA Reactor Cut End Rod Remote Handling, Mechanization and Automation System

Heavy Engineering Decontamination (HED) Area of Effluent Treatment Plant (ETP) receives used Cut-End Aluminium Rods of Dhruva reactor on regular basis. These rods are stored on interim basis and subsequently de-contaminated and recycled. In the existing system, most of the material handling operations are carried out manually. Therefore, the existing semi-automatic system has been completely re-designed by incorporating new

automation features for operational ease, safe handling, reducing man-rem expenditure & optimizing manpower requirement. The newly commissioned Fuel Rod Handling Mechanization & Automation System (FRHMAS) has successfully processed around 13.3 Te of Cut-end Rods.

Process Optimization for Fission Moly Production (FMP)

Process development for the production of medical grade ^{99}Mo was carried out initially with simulated solution (spiked with ^{99}Mo tracer) with regard to optimization of the FMP flowsheet using Indian resins and development of a new flow sheet. Subsequently, attempts were made to demonstrate indigenous production of medical-grade ^{99}Mo through irradiation of 5g of natural UAl_2 powder in Apsara-U. The product purity was verified and was found to be of medical grade.

Neutron Irradiation of Natural Cerium Sulphate Targets

Neutron irradiation of natural cerium sulphate targets was carried out and post processing 4 consignments consisting of 248 mCi of ^{141}Ce along with one indigenously fabricated perspex phantom were supplied to RMC for quality assurance of gamma camera used in nuclear diagnostic procedures.

Up to 5mg of natural cerium metal powder duly sealed in a quartz ampule was irradiated in DHRUVA reactor and subsequently was encased in a specially designed source holder. Three such sources in the range of about 100 μCi each were supplied to RMC for supplementing SPECT imaging procedures.

Installation of "Indian Scintillator Matrix for Reactor Anti-Neutrino" Detection

A full scale ISMRAN set-up having a 9 x 10 matrix of active detectors consisting of Gd wrapped Plastic Scintillator Bars was installed in the Dhruva Reactor Hall. The anti-neutrinos from the reactor would interact with the detectors to produce positrons and neutrons.

The detectors were surrounded by a shielding to reduce interference with the background reactor gammas and neutrons, as well as deeply penetrating cosmic muons. The set up was installed on a base trolley having side walls of 10 cm thick Lead inside Stainless Steel Containers and 10 cm thick Borated Polyethylene.

High Flux Research Reactor Prototype Assembly for Fuel Transfer System (FTS) of HFRR

A 3-D model of the prototype assembly for Fuel Transfer System of HFRR has been prepared. Detail drawings of sub-assemblies of prototype assembly such as gripper assembly, pulley housing assembly and hoisting mechanism assembly have been completed.

Seal Plug Assembly and Tooling for Fuel Test Loop of HFRR

A seal plug has been conceptualized and designed which can effectively close the terminal end of the fuel test loop to prevent the escape of test loop fluid. A 3-D model of full length tooling for plug operation has been prepared.



ISMARAN (Indian Scintillator Matrix for Reactor Anti-Neutrinos) detector setup at Dhruva Reactor

Accelerator, Laser and Plasma

6/4 MeV Dual Energy Linac

Dual energy experiments as per ANSI and IEC standards for material discrimination have been carried out at 200 Hz PRF in dual energy mode. 11 sets of material discrimination scans were taken

Up-keep and Upgrade

- ✧ Fabrication of new absorber assemblies for Dhruva shut off rod
- ✧ Testing of Prototype Shut down cooling System Channel (P-ECS) of Dhruva
- ✧ Process Water/Sea Water Heat exchanger of Dhruva was disassembled and serviced
- ✧ Upgradation of Low Isotopic Purity Heavy Water from Dhruva
- ✧ New Drive Mechanisms for Dhruva Shut off Rods
- ✧ Modification of sea water pumps
- ✧ Upgradation, Refurbishment and Automation Systems for Remote Surveillance
- ✧ Installation and commissioning of new Portal Monitors (PM) for Dhruva
- ✧ Preparations for Fission Moly irradiation at Dhruva & Apsara-U reactors

(IEC 62523 standard) at 100 Hz and 200 Hz PRF in dual energy mode. The penetration test was successfully demonstrated at 300mm steel with a 60mm kite behind it. Automatic frequency control (AFC) was implemented using feedback signal of output dose level, by varying the tuner position of the magnetron. In automation mode, the Linac has been tested successfully for all its technical specifications with material discrimination test for Aluminium and Acrylic.

Indian Cargo Scanner

After the successful testing, the whole 6/4 MeV Dual Energy Linac system has been dismantled in EBC and shifted to Gamma field, BARC for integration with the Indian Cargo Scanner. Presently the dual energy Linac is installed at Gamma field, BARC and characterized as per ANSI and IEC standards.



Indian cargo scanner developed in BARC

10 MeV, 5kW RF Linac

The subsystems of 10 MeV, 5kW RF Linac (horizontal type) have been fabricated and individually tested. The pre-buncher was tested with a cathode-based electron gun & LEBT system. Beam transmission of 99% was achieved through the pre-buncher by optimizing the focusing magnet. Integration of the Electron gun to the linac and leak testing of the whole assembly has been completed. Fabrication, testing and installation of all subsystems and alignments for the 10 MeV laser photocathode based accelerator have been completed.

10 kW Electron Beam Melting Machine

Electron gun characterization experiments were conducted to confirm the design data. Melt trials were completed. The machine is ready for commissioning at the user's site.



10 MeV, 5kW RF Linac



10kW Electron Beam Melting Machine

Testing of Pulsed Plasma based Underwater Shockwave Generator for Enhanced Oil Recovery

Two pulsed plasma-based underwater-controlled-shockwave generators developed by BARC were demonstrated at an ONGC facility in Ahmedabad for field experiments inside an oil well. During this process, shots were taken at depths of 350m, 550m, 750m and 850m. To test the structural integrity and smooth operation of the shock wave generator inside the oil well, a hydro test facility for testing up to 200 bar pressure has also been developed and installed.

Railgun Project

In phase-I trials of the Railgun project, a 1780 μ F/200kJ capacitor bank was directly discharged into the 1m long barrel assembly (8mm \times 8mm) and the injected current profile was



200kj capacitor bank of Railgun developed in BARC

of under-damped sinusoid. In the preliminary experiments at 10kV/220kA, a C-shaped projectile weighing ~6.6gm was accelerated to ~348m/s and it had punctured a 2mm thick Aluminum-6061 sheet that was placed at distance of ~1.2m from the muzzle end.

In phase II Railgun trials, experiments were conducted by injecting ~290kA peak sinusoidal damped discharge current at 14kV in to 1m long barrel assembly having a bore size of 13mm×13mm. In this setup aluminium projectiles of 5.5gm, 6.5gm and 8.5gm were accelerated to maximum velocities of 789 m/s, 670 m/s and 560 m/s, respectively. Indigenously made 5 compact B-dot sensors (BD) have also been integrated in the setup for in-situ measurement of projectile velocity inside the barrel.

Servo Control System for Indian Deep Space Network -18m Antenna

ISTRAC has setup an 18m indigenous deep space network (18M IDSN) antenna facility equipped with S and X band Tracking and Receiving capability to support ISRO's futuristic deep space programs. BARC, in association with ECIL, has designed the servo control system required to steer the Antenna in Azimuth ($\pm 270^\circ$) and Elevation (-2 to 92°) with pointing and tracking accuracies better than 20 mdeg (1 sigma) and 14 mdeg (1 sigma) respectively, at 60 Km/h wind speeds. Installation and Commissioning of the system at the IDSN campus, Byalalu Village, Bangalore has been completed after successful System Acceptance Test.



IDSN-18 Antenna

Design & Development of Pulsed Laser LiDAR

LiDAR (Light Detection and Ranging) uses pulsed laser light to measure range, altitude, direction and speed in a similar way as the RADAR. The LiDAR ranging system was mounted on a two-axis scanner to evaluate the range and direction correlation and also desired volume coverage. A large number of closely packed data points, called "point clouds" were generated and processed as a 3D visualization rendering as object displays.

Development of Nuclear Battery

Experimental studies were carried out using different beta sources such as Tritium, Nickel-63, Ruthenium-106 and Strontium-90 to evaluate their performance in a nuclear battery. Electric power production per mCi of beta source using pin diodes having low dark current was measured experimentally. Based on this, a radiation resistant nuclear battery was developed using Ru-106 as a high beta energy source (~1.6 MeV). An optimized device consisting of Ru-106 source of strength 3 mCi followed by Ce doped GGAG single crystal

Futuristic Technologies

- ✧ HPM source with tracking mode on trailer/truck of BHAIKAV-1 system
- ✧ Field Testing of Truck mounted X-band BWO system
- ✧ Characterisation of low impedance Marx Generator based FXR source has been completed
- ✧ A five stage, 250 kV Marx generator has been designed and developed as a pulse power system for Mesoband Wideband System
- ✧ A four-channel cable-fed FXR system was installed, tested and commissioned at ISRO's VSSC in association with ECIL, Hyderabad
- ✧ Development of Radioisotope Thermoelectric Generator for space applications

scintillator ($Gd_3Ga_3Al_2O_{12}:Ce$) and Si based p-i-n diode produced a short circuit current of 490nA, open circuit voltage of 0.18 V and power density of 18 nW/mCi. The radiation stability of scintillator crystal was checked for harsh radiation dose level of 5 MGy with 10 MeV electron beam. The optical properties of the crystal were found to be mildly degraded by 4%.

Sensors, Detectors, and Specialized Instruments

High Sensitivity ^{10}B Lined Proportional Counters

High Sensitivity in-core ^{10}B lined proportional counters with a small diameter of ~18.8 mm and



n-type HPGe detector fabricated in BARC

high sensitivity of 4.5 cps/nv with gamma tolerance up to 200 R/hr have been developed.

Indigenous development and testing of five ^{10}B lined proportional counters with integral super screened peek insulated cable has been completed. The performance of the detectors has been tested with pulse processing electronics from 10 nv to 25×10^3 nv range. The signal linearity was within 5% and remained stable for one hour at 100 KCPS ~ 2%.

Prototype Integrated HPGe Detector Readout Unit

A compact, low noise, standalone, Integrated HPGe readout system comprising of Spectroscopy amplifier (Shaper), Multichannel Analyzer (MCA), +/- 5 kV High Voltage (HV) Supply and LV in a single unit has been developed. The system accepts inputs from cryogenic charge amplifier of HPGe detector. The unit is interfaced with ANUSPECT spectrum analysis software package through Ethernet.

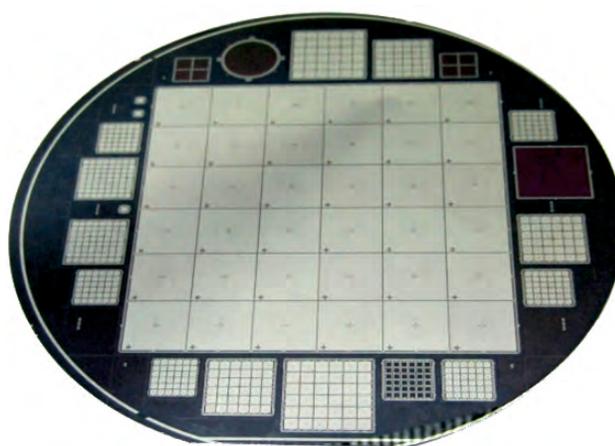
The system has been tested and characterized with a cooled HPGe detector. The pulse height spectrum has been obtained using Cs-137, Co-60, Ba-133 having photo-peaks over the whole detector energy range (40 keV-3 MeV). The 1.8 keV FWHM resolution has been achieved at 1332.5 keV peak of Co-60. The FWTM/FWHM ratio and FWFH/FWHM ratio are measured to be 1.88 and 2.53, respectively.

Dual-use Technologies

- ⊗ A handheld H₂S sensor with an input voltage of 10V was developed for potential applications in oil and gas industry
- ⊗ Motorized Valve Actuator to enable fine and precise tuning of the flow of the process fluid
- ⊗ Process Sensors for measuring reactor zonal temperature
- ⊗ Diamond Detectors that can function at 300°C-400°C for fast neutron spectroscopy

High Purity Single Crystal Silicon Wafers for Fabrication of Strip-type (PAD) Detector

Silicon pixel detectors of various configurations were designed from 4-inch high purity Silicon wafers using in-house grown float-zone grown single crystal silicon. Initial electrical characterization results proved to be quite promising quality-wise. The characterization data of most of the detectors fabricated in the indigenously grown silicon wafer, was found to be comparable with similar kind of detectors fabricated using imported wafers, which are scarcely available.



Strip detector fabricated based on BARC expertise

Sensors for Healthcare Monitoring

A sandwich electrochemical biosensor was constructed using carboxylic acid functionalized polyaniline as an antibody immobilization matrix and used for the detection of the liver cancer biomarker, α -fetoprotein (AFP). The sensor displayed a sensitivity of $15.24 \mu\text{A} (\text{ng mL}^{-1})^{-1} \text{cm}^{-2}$, with good specificity, reproducibility (RSD 3.4%), wide linear range ($0.25\text{-}40 \text{ ng mL}^{-1}$) and a low detection limit of 2 pg mL^{-1} . The sensor was validated by detecting AFP in human blood serum samples where the AFP concentration obtained was consistent with the values estimated using ELISA. Polyaniline was covalently modified by thiol-ene click chemistry route to obtain carboxylic acid tethered polyaniline (PCOOH). Utilization of PCOOH for construction of an enzymatic biosensor was demonstrated by covalent immobilization of glucose oxidase, uricase and horse radish peroxidase for the detection of the corresponding

substrate glucose (G), uric acid (UA) and H₂O₂, respectively. The biosensor displayed excellent sensitivity with a detection limit of 0.01, 0.001, 0.008 mM for G, UA and H₂O₂, respectively.

Development of Sensor for Heparin

An unsymmetrical cyanine-based probe molecule, TO-PRO-3, was used for the naked-eye detection of Heparin in aqueous and in complex human blood serum samples. The demonstration of naked eye Heparin sensing is based on a huge blue shift ($\sim 115 \text{ nm}$) observed in the absorption maximum, and which is one of the highest reported shift for any Heparin sensing system. The shift in the absorption spectra has been attributed to the formation of H-aggregate of the dye molecules in the presence of Heparin. In addition to this, a tetracationic probe, tetrapyrrolium-tetraphenylethylene (TPy-TPE), was identified for sensing of Heparin by fluorescence method.

CeO₂ Thin Film based Sensor for NO₂ Gas

Nanostructured CeO₂ thin film was developed by Langmuir-Blodgett (LB) technique for highly sensitive and specific detection of NO₂ gas. These nanostructured CeO₂ thin film sensors showed sensitivity with NO₂ gas from 10 ppb to 12 ppm with fast response time (2 mins) and recovery time (40-50 mins). To understand the specificity of the sensor for NO₂ gas, several interfering gases were injected and it is observed that there is hardly any response with the same concentration of other gases thereby suggesting a highly selective and sensitive NO₂ sensor.

Thin films of Co doped (0, 2, 5, 10 and 20 at%) NiO nanoparticles were prepared by spray coating at room temperature on glass substrates using a syringe pump. Deposition parameters were optimized to get uniform, homogeneous films. Gas sensors were fabricated by thermal evaporation of gold interdigitated electrodes. Spray coated films exhibited good reproducibility compared to drop-cast films. While all the sensors showed good sensitivity and high selectivity for NO₂ at 200°C, undoped NiO samples exhibited the highest sensitivity (six times conductance change for 10 ppm NO₂).

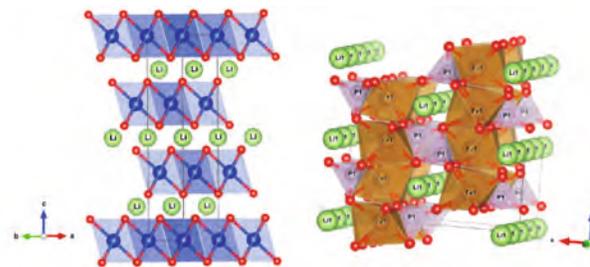
Energy Storage

Lithium Recovery from Used Lithium Ion Battery (LIB)

Cathode materials of used LIB was separated by modified pre-treatment method followed by dissolution in HCl. The cathode material consisted of Mn (20.68%), Li (5.38%), Co (1.17%) and Ni (0.0065%). Recovery of lithium from the dissolved solution was >90% under NaOH treatment. This method might be used for value recovery of lithium from used LIBs.

Development of Materials Relevant for Na and Li ion Battery

Research efforts have been made to develop materials for high energy, high power density and



Layered structure of LiCoO₂ and Li⁺ channels of LiFePO₄

economical lithium and sodium ion battery (LIB and SIB). Mo₂C nanoparticles dispersed over rGO electrode have been prepared and evaluated for use in SIB. The unique design of Mo₂C/rGO nanosheets exhibits specific capacity of 498 mAh/g at 50 mA/g current density against sodium electrode.

Carbonation in Lithium Recovery Plant

About 2.5 Ton lithium carbonate (Li₂CO₃) was produced from aqueous lithium hydroxide solution. Li₂CO₃ was precipitated by carbonation, filtered, dried, ground using air jet mill to particle size less than 10 micron. Around 2 tons of lithium carbonate produced from the plant was supplied to various private sector industrial units in the country.

Radiopharmaceuticals

Radioisotopes and Radiopharmaceuticals for Human Healthcare and Industrial Applications

A total of 2102 Ci (77.8 TBq) of radioisotopes were produced and chemically converted into radiochemical formulations for use in human healthcare, including ¹³¹I (866 Ci), ¹⁷⁷Lu (830 Ci), ⁹⁹Mo (272 Ci), ¹⁵³Sm (118 Ci), ⁶⁴Cu (8.2 Ci) and ¹²⁵I (8.0 Ci). These radiochemicals were supplied to various hospitals through BRIT for the detection and treatment of various types of human ailments, predominantly cancer.

35 DEDC kits were sent to All India Institute of Medical Sciences (AIIMS), New Delhi for the preparation of rhenium-188-nitrido-DEDC/lipiodol, used for the treatment of patients suffering from hepatocellular carcinoma. Till now, 38 patients with

inoperable liver cancer have been treated in AIIMS with ^{188}Re -DEDCL/lipiodol, prepared using DEDC kits supplied from BARC.

Radiotracer for SLN Detection

A kit for Human Serum Albumin (HSA) nanocolloid (particle size range 50-200nm), which can be used as a $^{99\text{m}}\text{Tc}$ -labeled radiotracer for SLN detection in the clinic, had been previously developed in-house, based on an IAEA documented protocol. To meet the continuous demand, regular batches of the product continue to be prepared and supplied to nuclear medicine centres through BRIT as an alternative to imported kits. During 2021, materials for production of up to 600 kits of HSA nanocolloid were prepared and dispatched to BRIT for supply to nuclear medicine centres across the country.

Fabrication of ^{125}I -brachytherapy Sources

Fabrication of ^{125}I -brachytherapy sources was carried out by adsorption of ^{125}I on palladium coated silver rods followed by their encapsulation in titanium capsules with the help of Nd: YAG laser. During the year 2021, 136 and 50 numbers of seeds were supplied for the treatment of eye and prostate cancer, respectively.

$^{64}\text{CuCl}_2$ for PET Imaging Prostate Cancer

Human clinical evaluation of no-carrier-added (NCA) $^{64}\text{CuCl}_2$ formulation produced in research reactor was carried out for the first time. No-carrier-added (NCA) ^{64}Cu was radiochemically separated from the irradiated target. Formulation of the product has been sent to RMC, BARC for clinical evaluation in prostate cancer patients using in-vivo PET (Positron Emission Tomography) imaging.

^{90}Y -glass Microsphere (BhabhaSphere) for Liver Cancer Therapy

Intrinsically ^{90}Y -labeled glass microsphere is the most widely used radiotherapeutic agent used for Selective Internal Radiation Therapy (SIRT). The indigenously developed ^{90}Y -labeled glass

microsphere (BhabhaSphere) has specifications which are very similar to commercially available and highly expensive TheraSphere™. Subsequent to the approval from DAE-Radio Pharmaceutical Committee, formulation of the product for human clinical use has commenced. Several customized doses of the formulation were prepared and supplied to Tata Memorial Hospital (TMH), Mumbai for the treatment of patients suffering from liver carcinoma.

^{177}Lu -Radiopharmaceuticals

Trastuzumab is a US-FDA approved monoclonal antibody for immunotherapy of breast cancer. Methodology for the formulation of ^{177}Lu -trastuzumab, for the radioimmunotherapy (RIT) of breast cancer was standardized in BARC. A proposal for manufacture and supply of ^{177}Lu -labeled trastuzumab for RIT of breast cancer was prepared and submitted to DAE-RPC.

DAE-RPC reviewed the proposal and accorded approval for the manufacture and supply of ready-to-use patient dose of ^{177}Lu -trastuzumab (up to 20 mCi) for the treatment of HER2-positive breast cancer patients.

^{177}Lu -DOTMP is a DAE-RPC approved radiopharmaceutical used for the treatment of palliative care of cancer patients suffering from debilitating pain arising due to cancer metastases. Ready-to-use patient dose of ^{177}Lu -DOTMP was prepared utilizing in-house formulated freeze-dried DOTMP kit was developed in BARC and supplied to Tata Memorial Hospital (TMH), Mumbai for cancer treatment.



Ruthenium-106 plaques for treating eye cancers

Development of Ru-Simulator and Ru-106 Plaques for Treating eye Cancers

Ruthenium-106 plaques are deployed in treatment of eye cancers. High Level Liquid Waste, arising from reprocessing of spent fuel, is a good source of Ru-106. A process methodology was developed indigenously for recovering Ru-106 of purified form and electroplating on Silver disk to produce Ru-106 plaque, in the form of sealed source, for eye cancer treatment. The work on the design and development of eye plaque of notched configuration has been completed successfully. The notched plaque is developed for the treatment of eye cancers located adjacent to optical nerve. During the first phase of development, 20 units of inactive plaques were fabricated and used for type approval tests.

A computer simulation software has been developed for dose rate distribution calculation for the planning of eye cancer treatment using Ru-106 plaques developed by BARC. The simulation software can run on Windows and Linux platforms and is provided with user interfaces for feeding details of tumor and Ru-106 plaque. Each plaque can be calibrated against the corresponding measured dose depth data before carrying out the simulation to obtain the treatment time and dose received by other nearby organs including the optic nerve. The development is an important milestone in providing affordable treatment of eye cancer as an import substitute.

Production of Cesium Glass Pencils for Blood Irradiator Applications

High Level Liquid Waste obtained from reprocessing spent fuel is a good source of Cs-137, which is recovered through solvent extraction

based pre-treatment process. The recovered Cs-137 product solution is vitrified in specially designed glass matrix to produce the Cs rich glass for gamma irradiation application. The Cs glass is melted in SS pencils using dedicated Cs glass remelting furnace. Each Cs glass pencil is sealed, overpacked inside another SS tube (outer pencil), externally decontaminated and subjected to stringent quality assurance tests to ensure leak tightness. Non-dispersive glass form of Cesium-137 adds to safety and security. About 20 Cs glass pencils were successfully produced and dispatched to BRIT after assuring the quality of sealed Cs glass source.

Super Bright Red Upconversion Nanoparticles for Bio-imaging Applications

Nanocrystalline materials emitting a single band red light under Near Infrared excitation has advantages in terms of cellular imaging in biological windows, as agents for photodynamic and photothermal therapy. Highly monodispersed upconversion nanocrystals functionalised with folic acid for targeting tumor cells, were prepared and tested for cellular imaging under UV light and NIR excitation.

Water Purification, Groundwater Management and Solid Waste Management

Freeze Desalination

Freeze Desalination experiments were performed on Scrapped Surface Cooling Crystalliser (SSCC) with diluted sea water with varying recirculation

Exploring Affordable Healthcare

- ⊗ Enrichment of isotope of samarium for bone palliation and preparation of ¹⁵²Sm EDTMP
- ⊗ ⁶⁸Ga-NODAGA-JR11 for imaging of neuroendocrine tumors
- ⊗ Microparticle carriers for Trans-Arterial Radio-Embolization (TARE) therapy of liver cancer
- ⊗ Image Processing based Advanced Fast Neutron Dosimetry System for Personnel Monitoring

flow rate, scrapping frequency and chilled liquid temperature, salinity to optimize the operating condition and cycle time. Ice production @ 2 kg/hr & salt rejection ~ 86% were obtained for feed salinity up to 15,000 ppm. The dynamic simulation of Scrapped Surface Cooling Crystallizer (SSCC) unit is completed for freeze desalination process to predict the performance under different operating conditions. The effect of duty cycle, coolant temperature and coolant flow on the performance of SSCC is studied. The model predicts the optimum duty cycle for the operation of SSCC unit. Design of Sea Water Flake Ice Machine with direct refrigeration cycle was made, along with technical specifications and drawings.



Community level purifier system for decontamination of Arsenic based impurities in water



Water filters for domestic use, developed in BARC, being distributed to villagers of Samastipur district in Bihar

Mitigation of Arsenic and Fluoride from Drinking Water

Under the DAE Project on “Deployment of water purification technologies in 50 villages in India”, 400 numbers of point-of-use arsenic decontamination devices of 24 LPD capacity were deployed in Village Harail, Dist. Samstipur, Bihar. The units provide arsenic free safe drinking water as per Indian Standard, BIS 10500 from the tube-well water contaminated with up to 400 ppb of arsenic.

A 2000 LPH capacity fluoride removal plant was installed, commissioned and handed over to the Sagargaon Gram Panchayat, Dist. Khordha, Odisha. The plant caters to the drinking water requirements of 4 villages of the district. These efforts are a part of the Jal Jeevan Mission of Government of India to provide safe drinking water to households.

Arsenic Immobilization in Water

A 1000 LPH capacity community-scale arsenic removal plant with water ATM facility is operational at Ichhapur-I Village Panchayat, Dist. North 24 Parganas, West Bengal based on BARC know-how, which forms a part of DAE's Vision-6 project on “Deployment of Water Purification Technologies in Rural India”. The arsenic concentration was reduced from 400 ppb in feed water to less than 10 ppb in product. In this context, to assess any arsenic release from the arsenic bearing sludge into the environment, leaching of arsenic from field-sludge was studied and it was ascertained that leaching of arsenic is less than 2 ppb. Subsequently, arsenic bearing sludge was immobilized in both cement and concrete matrix and their compressive strength and leaching behaviour were analysed. The arsenic concentration in leachant was found to be less than 5 ppb, which is 1000 times less than prescribed TCLP limit (1 ppm).

Visual Detection of Arsenic in Groundwater

A simple visual colorimetric method based on arsenomolybdic acid-crystal violet ion-associate pair formation was developed for the detection of arsenic at about 10, 25 and 50 ug/L levels in

groundwater. The pair exhibits arsenic concentration dependent colouration. The reliability of the method is up to 90%. The high sensitivity is achieved by the preconcentration of arsenic on covellite (CuS). The use of benign and easily available chemicals, absence of any hazardous by-product, undiminished applicability in sunlight and rapidity are some of the major advantages of the method.

Granular Biofilter for Treating Waste Water in Rural Areas

A lab-scale granular biofilter was evaluated for biological wastewater treatment. The biofilter was operated in continuous mode for treating simulated wastewater. Stable and simultaneous chemical oxygen demand (COD), nitrogen and phosphorus was achieved during long-term operation.

Rapid Biocomposting

A technology for "Rapid biocomposting" was developed and transferred to 33 agencies in India.



Compact helical shaped waste converter, Shesha, for biocomposting of waste

Six products are already being marketed through online shopping portals. This has been an important contribution of BARC towards Swachh



Sludge hygienization facility set-up by BARC in Ahmedabad

Bharat Abhiyan. To manage biodegradable waste generated in smaller housing societies and restaurants, a novel, compact helical shaped waste converter (Shesha) has been developed and transferred to different companies.

Hygienization of Liquid Sewage Sludge

In SHRI facility, Vadodara a total of 181 batches of 7 m³ of liquid sludge was irradiated. The average solid percentage was ~7.5% giving yield of ~142.5 ton of irradiated sludge on dry weight basis.

Identification of Origin and Evolution of Groundwater Resources

An integrated isotope-geochemical investigation in the multi-aquifer system along the coastal tract of the West Bengal has been carried out to understand the evolution of ground water in relation to recharge, salinity sources, mixing behavior and residence time of the deep groundwater. The stable isotopic ($\delta^{18}\text{O}$, $\delta^2\text{H}$) analysis shows that the deep groundwater samples (>400 ft) fall along the Global Meteoric Water Line (GMWL), which indicates their meteoric origin. The tight clustering of the deep groundwater samples

Water-The Elixir of Life

- ✧ Kalpakkam-based Nuclear Desalination Demonstration Plant, equipped with MSF (multistage flash) and SWRO units, produced 145204 m³ of water from seawater source
- ✧ A Hybrid granular sequencing batch reactor for sewage treatment
- ✧ Ozonation-based process for treatment of oil contaminated saline waste water
- ✧ 100 L bench-scale ozonation reactor for dye degradation
- ✧ Radiation Grafting technique for treating water discharged from industrial dye units

along the GMWL indicates precipitation as the single source of recharge and negligible evaporation during their recharge. The deep groundwater samples (>400 ft) show enriched isotopic signature compared to the shallow groundwater (20 to 120 ft) samples implying the paleo-recharge of deep groundwater under dry conditions compared to the present day precipitation. The deep ground waters do not show any ingress of seawater till date. C-14 age dating of the water samples from South 24 Pargana district show two sets of paleo-recharge during ~ 37000 and ~21500 years BP. Deep groundwater from the East Midnapur district is also found to be old but is comparatively younger (5200 to 7700 years BP) compared to deep groundwater of South 24 Parganas district in West Bengal.

Agriculture and Food Technologies

Crops

Radiation induced mutagenesis along with recombination breeding has been used to develop six new Trombay crop varieties, which have been approved and notified for cultivation by the Govt. of India. This includes mustard varieties, Trombay Akola Mustard 108-1 (TAM-108-1) for Maharashtra; Birsa Bhabha Mustard-1 (BBM-1) for Jharkhand; Trombay Him Palam Mustard-1 (THPM-1) for Himachal Pradesh; groundnut variety, Trombay Akola Groundnut-73 (TAG-73) for Maharashtra; rice varieties Trombay Chhattisgarh Sonagathi Mutant (TCSM) and Trombay Chhattisgarh Vishnubhog Mutant (TCVM) for Chhattisgarh. Two new rice varieties Vikram TCR (VTCR) and CG Jawaphool Trombay (CGTJ) have been Gazette notified for commercial cultivation in Chhattisgarh. Towards dissemination of Trombay varieties, 303 quintals of groundnut varieties, 65 quintals of pulses and 80 quintals of rice varieties were produced and distributed to different seed producing agencies for popularization among farming communities of Gujarat, Karnataka, Maharashtra, Madhya Pradesh and West Bengal.

Biotechnological Approach for Crop Improvement in Ginger

In biotechnological approach for crop improvement, an efficient, rapid and reproducible micropropagation protocol for ginger has been developed. This protocol provides disease-free good quality planting material throughout the year. It can also be used in germplasm conservation of elite ginger varieties.

Crop Improvement in Banana

In banana, a novel tissue specific promoter was identified for stress tolerance. Promoter of *chalcone isomerase* gene (*MusaCHI-1*) of banana was functionally analyzed for its tissue specific, stress mediated and strong guard cell preferred activity.

Crop Improvement in Tobacco

Transgenic lines harboring $P_{MusaCHI-1}$ -*GUS* display prominent GUS staining in vascular region and guard cells of leaves which corroborates with array of *Dof1* binding cis-elements in $P_{MusaCHI-1}$ region. Studies done in BARC confirmed that exposure of salicylic acid strongly suppresses GUS expression from $P_{MusaCHI-1}$ in tobacco.

Large Scale Commercial Trial for Preservation of Onion and Potato through Gamma Irradiation

Long term potato storage is generally done at lower temperatures along with the application of chemical sprout inhibitors. A large scale commercial trial was undertaken wherein irradiated (gamma radiation dose: 73 Gy) potatoes (approx. 28 ton) were stored at relatively higher



Non-irradiated potatoes

Irradiated potatoes
(after 7 months of storage)

Low dose gamma irradiation of potatoes improves its shelf life

cold storage temperature without the application of chemical sprout inhibitors. Three different commercial cultivars of potato, namely 'Santana', 'Kufri Frysona' and 'HYSM' were included in this trial. Within 100 days of storage, complete sprouting was observed in non-irradiated potatoes whereas, no sprouting was noticed in irradiated samples. The irradiated samples were found to be in good condition till 7-8 months of storage. After 8 months of storage, these irradiated potato samples were further channelized to the processing industry for manufacturing new value-added products.

Onion undergoes extensive weight loss, microbial spoilage as well as sprouting during storage and these limitations affect the commercial storage of onions. A large scale commercial trial was undertaken with the prime objective of storing irradiated onions without applying chemical sprout inhibitors. Onion (approx. 15 tons) were irradiated [Dose (Dmin: 60 Gy)] and stored in a commercial cold-storage facility under specified conditions. As a result, onions remained fresh for 8 months without any sprouting.

Effectiveness of Irradiation Technology for Pest Disinfestation in Foodgrains and Lentils

As a superior alternative to fumigation, irradiation technology was utilized in the long-term preservation of foodgrains including wheat and different kinds of pulses. Even after 14 months of storage under ambient conditions, packaged and irradiated wheat was found to be free of pests even as it retained key quality attributes and grain integrity. In contrast, non-irradiated wheat grains completely spoiled due to extensive pest (*Sitophilus oryzae*) infestations. Besides, irradiated split chickpeas ('Chana dal') also remained pest-free even after 1 year of storage whereas the non-irradiated ones were completely spoiled within this time period.

Shelf-life Extension of Perishable Fruits

Plum (*Prunus domestica*) is an expensive fruit that

has a short shelf life. The potential positive role of in-house developed PVA-pectin film in extending the shelf-life of plum under storage in chilled conditions had been examined. It was found that the unpacked plum fruits were spoiled within 7 days whereas those packed in active films were in good condition even after 45 days of storage. Films developed with PVA, passion fruit peel and lemon peel pectin in the ratio of 2:1:1 with glycerol as the plasticizer exhibit excellent food packaging characteristics.

Furthermore, the functionality of PVA- pectin film in increasing the shelf life of strawberries was also ascertained. There was 39% weight loss in unpacked strawberry while in active packed samples, the weight loss was limited to just 20% after 15 days under cold storage. Similarly, reduction in hardness of unpacked strawberries was very significant during storage but very little change was observed in samples stored in pectin films. On the basis of the above indices, unpacked strawberry at chilled temperature had a shelf life of less than 7 days while those packed in active film were acceptable for up to 15 days.

Development and Commercial Deployment of Value Added Products from Perishable Fruits

Jamun fruits are highly perishable and seasonal in nature. A technology ('Delicious & Preservative free, Shelf Stable Natural Jamun Product') has been developed to derive a value-added and preservative free dietary fruit product involving radiation processing. The Jamun product developed through the BARC technology has been launched through a licensee of the technology at various online platforms.

Effectiveness of Radiation Processing in Ensuring Microbial Safety of Sweets and other Allied Products

The effectiveness of gamma radiation processing was demonstrated for Indian sweets provided by M/s Amul India. Gamma irradiation (3&5 kGy dose) ensured microbial safety in Amul Kesar Peda (MAP packed, without preservative) till 2 months,

Other Accomplishments

- ✧ Development of dosimeters for food irradiation facilities and up-gradation of the food package irradiator
- ✧ Preparation of Long lasting delicious Strawberry Candy Roll (SCR)
- ✧ Indigenous Deep Brain Stimulator (DBS) for treating brain neurological disorders

whereas the non-irradiated sweets were spoiled after 2 weeks. Gamma radiation (2 kGy) was found to be highly effective in eliminating 10^5 *Salmonella* Typhimurium cells /gm of beetle leaves without affecting its sensory attributes.

Kit for Detecting Melamine, a Milk Adulterant

The formulation of gold nanoparticle based colorimetric sensing kit was developed for the detection of milk adulterant, melamine in real milk samples. The prototype kit has been optimized for technology transfer. The sensor undergoes visual colour change in presence of the adulterant with detection limit of 500 ppb in milk-extract using ultrafiltration and 10-15 ppm in milk samples without any chemical pre-treatment.

Healthcare Technologies

Algorithm for Computation of 3D Dose Distribution for Bhabhatron

An algorithm to compute 3D dose distribution in inhomogeneous medium has been developed for the Bhabhatron-II teletherapy machine. It consists of a beam model of Bhabhatron-II and correction based algorithms for accounting the surface irregularities and patient-specific inhomogeneities. Functionality of the algorithm has been verified for various test cases and patient data. This algorithm would be a core component of the proposed Treatment Planning Software for Bhabhatron.

Development of Phantoms for Nuclear Medicine Imaging Applications

Nuclear Medicine (NM) imaging involves administration of trace amounts of

radiopharmaceuticals to study a wide range of physiological processes in the human body. NM imaging modalities are capable of providing extremely sensitive measures for a wide range of biologic processes. Recent introduction of fusion of diagnostic images from two complementary imaging modalities has revolutionized diagnostic imaging. A versatile total quality control phantom for the NM scanners has been designed and fabricated locally to evaluate various image quality parameters, including image uniformity, spatial resolution, low contrast resolution, pixel size, and slice width. The developed phantom consists of various inserts and sections to test almost all performance parameters of nuclear medicine imaging devices, including PET and SPECT.

Hydrogen Technologies

Compact Alkaline Water Electrolyser Plant for Producing Green Hydrogen

An additional gas purification unit (GPU) was integrated with the electrolyser plant for production of ultra high purity grade Hydrogen. Process intensification was carried out on De-oxo bed system for mitigation of impurity in the product stream and back pressure regulators have been installed for improving pressure equalizing of the gas streams. The technology was transferred to public sector oil marketing companies.

In addition to this, revamping activity of compact alkaline water electrolyser plant has been completed successfully. Cell module stacks have been connected to an electrolyser process skid, which has capacity for oxygen production up to 5000 NLPH, simultaneously with 10000 NLPH Hydrogen production. A new oxygen gas compressor capable of boosting pressure from 0.5

bar (g) to 150 bar (g) has been integrated with the revamped electrolyser plant to produce medical grade oxygen which would be bottled in cylinders for medical as well as industrial use within BARC.

De-oxo Catalyst for Hydrogen Purification Step of Alkaline Water Electrolyser

Supported noble metal catalysts for removal of oxygen impurity from hydrogen were developed



Alkaline Water Electrolysis Plant for production of Hydrogen and Oxygen

using different Pd/Pt compositions supported on γ -alumina. Selected catalysts were synthesized at larger scale (35g batch), characterized and evaluated. Trial runs with a selected Pd/ Al_2O_3 catalyst were conducted and the performance of the catalyst was found to be satisfactory.

Cu-Cl Thermochemical Cycle for Hydrogen Production

Work on development of a 4-step Cu-Cl thermochemical cycle for hydrogen production was continued. The feasibility of all four steps of the process - hydrolysis, thermolysis, electrolysis, and crystallization - was demonstrated at bench-

scale (3-10 NLPH of H_2). The membrane electrode assembly developed for electrolysis was found to perform satisfactorily for optimized process conditions.

Multi-tube Membrane Reactor

Tantalum alloy-based metal membrane has been fabricated using DC magnetron sputtering & tested for corrosion resistance in HI environment of IS thermochemical process. It has been found to be ~5 times more corrosion resistant than tantalum membranes. A multi-tube membrane reactor has been designed, fabricated & installed in metallic close loop IS thermochemical process for 150 LPH hydrogen production.

Materials for Thermochemical and Electrochemical Hydrogen Generation at Engineering Scale

Sulphuric acid decomposition over $\text{Fe}_{1.8}\text{Cr}_{0.2}\text{O}_3$ foam catalyst at 850°C was carried out at different acid flow rates. Based on these results, a smaller sized foam catalyst was selected for deployment in a metallic closed loop of I-S process for Hydrogen generation.

Electrocatalyst based Membrane Electrode Assembly

Pt-based electrocatalyst based-membrane electrode assembly (MEA) with an active area of $\sim 29 \text{ cm}^2$ was prepared for use in CuCl/HCl electrolyser at ChED. A current of $\sim 6 \text{ A}$ @ cell voltage of 1V could be achieved, which was comparable to that obtained with commercial MEA. The permeability of copper ions across the proton exchange membrane was also evaluated.

Membrane Diaphragm for Alkaline Water Electrolysis

Polysulfone-zirconia membrane diaphragm of 500 mm width was prepared using continuous diaphragm casting machine assembly for separator application (as a replacement of asbestos) in alkaline water electrolyzer. The samples are sent for testing and characterization.

Preparation of Electrocatalysts and their Alloys on Cu Foil Substrate

A series of electrocatalysts comprising metals (Ni, Co, Mo) and their alloys (Ni-P, Ni-Co, Ni-Mo, Co-Mo) were prepared on Cu foil substrate using direct electrodeposition method and evaluated for hydrogen evolution reaction under alkaline conditions. Among all, Ni-P alloys showed the highest electrocatalytic activity ($\sim 450 \text{ mA/cm}^2$ at -1.1V).

Molybdenum Carbide Dispersed on Carbon Electrocatalysts

Molybdenum carbide dispersed on carbon ($\text{Mo}_2\text{C/C}$) electrocatalysts with varying $\text{Mo}_2\text{C:C}$ ratio were synthesized and investigated for hydrogen evolution reaction under acidic conditions. The $\text{Mo}_2\text{C/C}$ (1:2) sample exhibited the best performance for HER.

Materials for Hydrogen Storage Applications

Ti_2CrV alloy samples were synthesized for deployment in the bench scale hydrogen storage device of integrated hydrogen production and storage test facility. Around 300 g of Ti_2CrV material has been prepared for storing 144 lit of hydrogen. The materials were prepared in 25 batches under argon atmosphere in Arc Melting setup. Homogeneity in phase and composition of these alloys has been confirmed by XRD and Energy Dispersive X-ray (EDS) analysis techniques.

Electro Catalytic Hydrogen Evolution of Ni modified Stainless Steel Mesh

Ni modified SS-304 electrodes for H_2 generation were developed by hydrothermal method to



Ti_2CrV alloy samples synthesized for deployment in prototype hydrogen storage device

simulate in situ redox conditions during corrosion studies. The electrochemical surface area estimated was in the range of 0.005 cm^2 . A significant reduction was seen in the over potential (280 mV at 10 mA/cm^2) as compared to other electrode materials. Further studies were planned to optimize the synthesis conditions for fine tuning the catalytic activity.

Specialized Technologies

Scanning Electron Microscope SEM-4

Integration of all sub-systems for SEM-4 has been completed. Vacuum testing of sub-systems was carried out satisfactorily to achieve vacuum of the order of 5×10^{-6} Torr. Testing of the electron gun was carried out successfully up to 25 kV. Mechanical alignment of SEM electron-optics was carried out using a laser beam. Images of standard calibration specimen have been obtained for magnifications up to 150,000 times, with imaging resolution of about 24 nm.

System for Separation of Non-condensable gas (Helium) from Hydrogen/Deuterium Loop

Experiments of electrochemical cell with 50% Hydrogen in Helium as feed gas were carried out at different operating temperatures and current densities, using Pt loaded MEAs as anode and cathode. Complete recovery of Helium from the feed gas mixture is observed at high current densities, which are consistent with theoretical predictions.

Metal Membrane for Separation of Hydrogen-Helium Mixture

Membrane permeator with alumina supported Pd-Ag (75-25 %) membrane (10 mm OD & 250 mm length) was developed and tested. The helium leak testing of the permeator was carried out. The leak rate of all the metallic and ceramic joints were found to be $\sim 10^{-6} \text{ mbar.lit/sec}$ and $\sim 10^{-4} \text{ mbar.lit/sec}$, respectively. The Permeator was tested in hydrogen and helium gas environment

individually. A hydrogen flow rate of ~1 ml/min was achieved at room temperature and no helium flow was detected.

Adsorption of Elemental and Ionic Mercury from Air and Liquid Effluent

Sorbent materials for mercury respirators cartridge viz., humic acid coated Fe₃O₄ nano-particles, calcium alginate biocomposite, bio-hybrid of silica and microbial cells were synthesized and tested for their suitability for the adsorption of elemental mercury from Hg-contaminated air. From the experimental study it was found that humic acid coated Fe₃O₄ nano-particles have an absorption capacity of mercury is 343.71 µg/g which is about two times that of activated charcoal particles.

Further experiments are being conducted with other materials for removal of metallic and ionic mercury from liquid effluent. For removal of soluble (zero-valent) and ionic mercury from liquid waste, a bio-hybrid material of nano-silica and *S. cerevisiae* cells was synthesized, characterized and its mercury adsorption capacity was found to be ~185.19 mg/g.

Development of Indicator Strips for UV based Detection of Hg Vapour in Air

For calorimetric detection of mercury, various materials were evaluated and a visible colour change was obtained in the presence of mercury vapour.

Compact Carbon-Sulfur Analyser

Testing and performance evaluation of a new compact Carbon-Sulfur Analyser (CSA) was carried out. In this connection, base line interference in SO₂ NDIR signal was observed during switching on and off operation of high frequency induction furnace for sample combustion. The source of this interference was traced using signal tracing and isolation of various stages and removed by incorporating additional RF filtration at IR amplifier during input stage. The in-house designed NDIR detectors for both CO₂ and SO₂ were assembled. Pneumatic control of induction furnace and pneumatic flow control of oxygen gas in Purge and Analyse mode was tested. Leak test of the overall system showed excellent results. After satisfactory performance with gaseous injection of known



Compact Carbon-Sulfur Analyser developed in BARC

concentration and volume of pure CO₂ and SO₂ gaseous samples, the system was tested with combustion of solid samples in an induction furnace. Optimization of detector performance for both CO₂ and SO₂ is being carried out.

Dissolved Oxygen Monitor

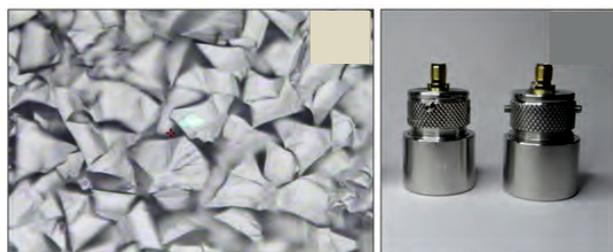
A dissolved oxygen (DO) monitor which has wide linear dynamic range of 1 ppb to 20 ppm was designed and developed based on the redox coupling of two metals with difference in their redox properties. The reduction current of oxygen is the measurable parameter for the determination of dissolved oxygen. The resolution of the system is 0.1 ppb at 2 ppm level.

Modelling of Plasma Incinerator

A lumped parameter-based code was formulated to obtain time-temperature profiles of plasma incinerator. The code was validated with the temperature-time profile data obtained in the actual run. The model can be extended to predict evolution of temperature with time during operation with coke and MSW beds.

Development of Large Area CVD Diamond Films for Optical and Nuclear Applications

Feasibility studies on CVD synthesis of large area diamond films for optical window applications were carried out. Using MPCVD system, a 2" diameter film was synthesized over Silicon substrate for 100 h in reducing environment. Mounting arrange was optimized to attain high substrate temperature (900 K). High quality polycrystalline diamond films (3 nos.) with thickness ranging from 15 m to 55 m were synthesized by plasma CVD route and processed.



Large area CVD diamond films developed in BARC for optical and nuclear applications

Two alpha detectors have been fabricated using CVD grown thick (55 m) as well as relatively thinner (28 m) diamond films.

Materials for Document Security Applications

Around 100g of up-conversion luminescent nanoparticles (taggants) have been prepared and delivered to SPMCIL, Dewas for extensive evaluation. The material has been tested with different types of inks used for currency/document printing. Based on the experiments carried out, concentration of the nanoparticles in inks has been optimised. Some of the issues such as interference of the nanoparticles with certain colours and bitterness of the ink etc, are addressed.

Development of Fluorophore Doped Plastic Scintillator Films

Plastic scintillators are widely used in radiation detection for nuclear applications. For in-house development of efficient plastic scintillators, polystyrene films were cast on a glass substrate from a styrene monomer with varying concentration of fluorophores PPO and POPOP. These films were also tested with suitable radiation sources. For a handheld beta detector, a film of 8 cm x 10 cm cast on plastic substrate was found to have an efficiency comparable to the imported scintillator.

Recycling Gold from Electronic Waste

With increasing utilization of gold in the electronics industry, accumulation of electronic wastes poses one of the biggest challenges to the environment. Therefore, recycling of the electronic waste for recovering gold has become vital. The Lennard-Jones potential based force Field for gold ion coupled with and FF in molecular dynamics simulation route was applied to study gold-water interaction and solvation structure.

Certified Reference Material of Dolomite and Bauxite

The first indigenous certified reference material (CRM) of dolomite (BARC B1101), was prepared

Niche Technologies

- ✧ Development of LLDPE/Flax fibre composite with reliable mechanical properties
- ✧ Synthesis, characterization and efficiency of nanoadsorbent for removal of Hg from liquid waste
- ✧ Crude Trichlorosilane Production Plant - for polycrystalline or solar-grade silicon used in the photovoltaic industry
- ✧ Revamping, commissioning, testing and performance analysis of TCS Distillation Plant
- ✧ Radiotracer investigation in a cross-flow reactor used for hydrotreating and hydrocracking in petroleum processing
- ✧ Demonstration of Combined Electrolysis and Catalytic Exchange process for Hydrogen isotope exchange reaction
- ✧ Development, characterization and performance evaluation Pt-PTFE catalyst for exchange reactions in spinning basket batch reactor



CRM of dolomite

jointly by BARC and AMDER. It is certified for Ca, Mg, Al, Fe, Ba and Sr and is traceable to international standards. The starting material is sourced from Tumallapalle area in Andhra Pradesh and is three times cheaper than the commercially available international standards.

Similarly, a certified reference material of bauxite (BARC B1201) has been prepared in collaboration

with public sector unit NALCO. The CRM is certified for nine property values that include Al, Si, Ti and Fe. The certification entailed an inter laboratory comparison exercise participated by 21 prominent analytical laboratories in the country and a comprehensive and rigorous statistical analysis. The material is traceable to international standards and will be released shortly.

Visual Detection Kit for Determination of Ethanol in Ethanol Blended Petrol

A simple colorimetric method for the on-site determination of ethanol in ethanol blended petrol has been developed. The method is based on phase separation and colour development and is applicable to petrol blended with up to 10% ethanol. The precision of the method is 12.5 % at 10% (v/v) ethanol blended petrol.

Robotic Welding System

The robotic welding system consists of two robotic arms equipped with a welding torch. In order to have access to the entire periphery of pipe geometry, a 90° welding torch was integrated with the robot for simulating the robot motion during root pass. Subsequently, a 90° welding electrode (with respect to torch housing) was installed, tested and integrated on robot and desired overlapping, while following circumferential path, was achieved. Tuning of control parameters for constant arc gap was also carried out.

Z-Theta System for Glove Box Applications

A Z-Theta system for transfer of radioactive powder inside the glove box has been developed in BARC. The system has two motions, namely vertical and horizontal sweep, and a payload capacity of 20 kg.

MRI/CT Scan Prototype for Experimentation using Neuro Surgical Suite

An MRI/CT scan phantom for validating neuro surgical suite has been designed and fabricated in BARC by using rapid prototyping method. The inner structure of the phantom was designed to accommodate reference markers for simulated entry and tumor points for the surgical biopsy needle.

Robotic Scrubber-dryer

A tele-operated robotic scrubber-dryer based cleaning machine suitable for wireless operation was developed in BARC.

Sensor-instrumented Miniaturized Robotic Gripper (SIMRoG)

A prototype instrumented miniature gripper and its control system have been fabricated and tested. The gripper comprises two miniature load cells, one flexi sensor, two strain gauges and one infrared sensor. The changes in sensor data can be viewed through graphs plotted by a Graphical User Interface.

Diode Mount Assembly for INDUS-2

Design and manufacture of Pin Diode Mount Assembly for INDUS-2 beamline of RRCAT was successfully completed.

Ultra High Vacuum (UHV) Chamber

A UHV Chamber was designed and manufactured in-house for the Photo-physics beamline. The chamber was qualified for Helium Leak Test with a leak rate in the order of 10^{-10} Pa*m³/s.

COVID-19 Technologies

Infrared Sensor based Instrument for Measuring Human Temperature

An infrared sensor based non contact human skin temperature measuring instrument



TaapDarshak

“TaapDarshak” has been developed in BARC. 38 units of the instrument have been given within and outside BARC for deployment as part of COVID-19 measures.

Development of CRISPR-based Diagnostics for Covid-19

Globally, healthcare took centre stage because of the sustained challenges posed by the Covid-19 pandemic to mankind and India is no exception to this. Committed efforts made by scientists of BARC have led to the successful development of a portable kit for accurately detecting Covid-19 infection in humans within 75 minutes. In this test,

viral RNA isolated from patient samples is converted into DNA. Two SARS-CoV-2 genes, N2 and E are specifically enriched in this step. These genes are detected with the help of CRISPR-Cas enzymes. Upon detection of the virus genes, a fluorescent signal is generated. A compact and portable instrument, BARC-CRISPR-Cube is developed to run this test and to visualize the positive signal. Salient features of the Covid-19 diagnostic kit are: The test is highly sensitive similar to RT-PCR; it is specific and avoids false positives; it does not require any high-end instrument like RT-PCR; the instrument is highly portable and can be operated with a battery and is suitable for use in remote areas.

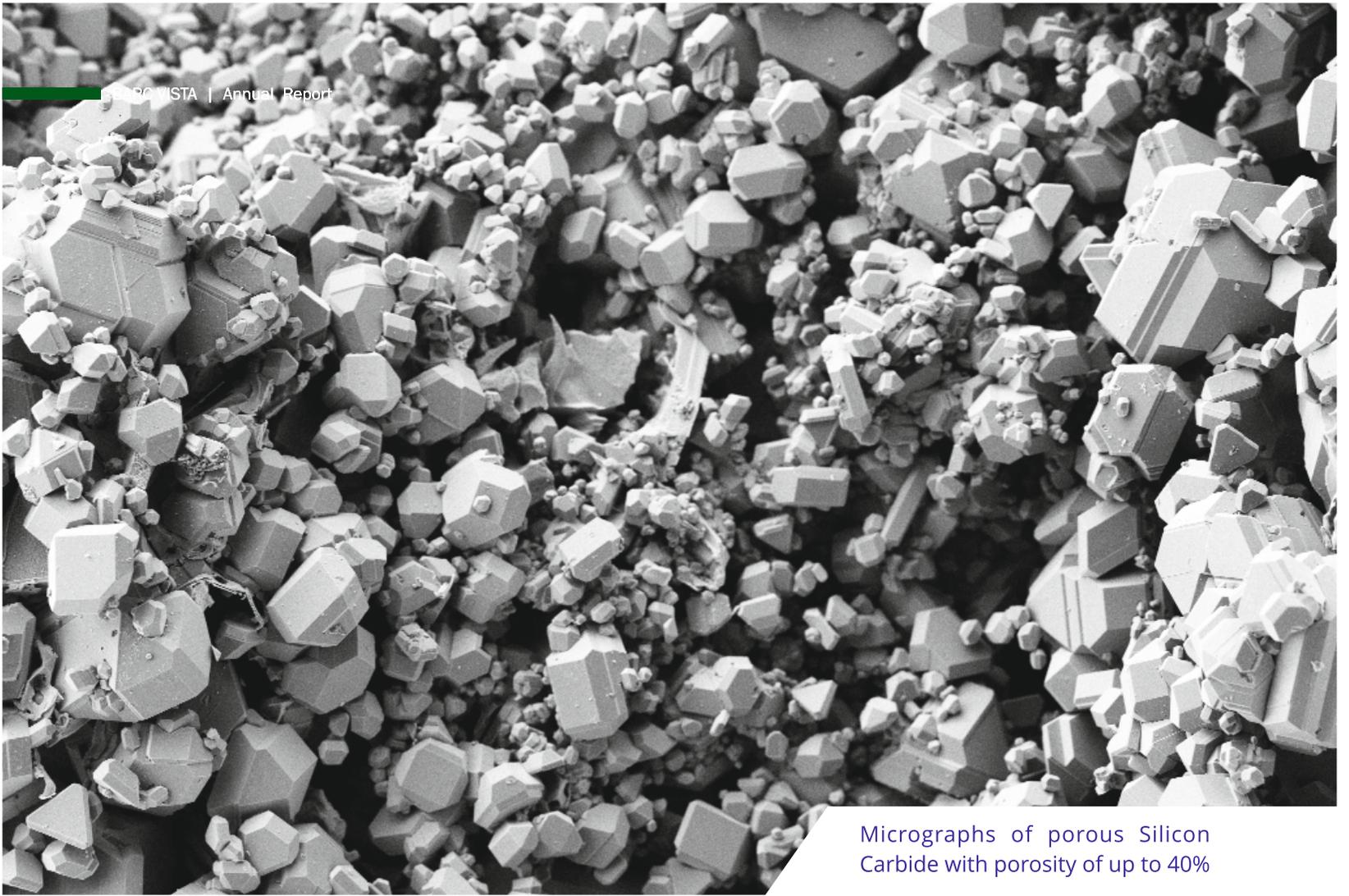


Kit for CRISPR-based detection of COVID-19



BASIC AND DIRECTED RESEARCH

BARC has highly competent workforce which is ingrained in pursuing specialized research in fundamental aspects of sciences to complement the inherently complex nuclear technologies. Over the years, research in basic sciences has expanded significantly from the traditional domains into new and emerging areas with a clear emphasis on ensuring directed outcomes that would contribute immensely towards improving the overall standard of living. In line with this philosophy, sustained efforts are underway in Physical Sciences, Chemistry, Biology, Water Resources Management, Radiotherapy and Radiopharmaceuticals, Mutation breeding for improved crop varieties, Food preservation approaches and Waste management to achieve the desired outcomes.



Micrographs of porous Silicon Carbide with porosity of up to 40%

Basic and Directed Research

Astrophysical Sciences

Monitoring of Gamma-ray Sources with the TACTIC Telescope

TACTIC (TeV Atmospheric Cherenkov Telescope with Imaging Camera) has been operational at Mount Abu, Rajasthan since 1997. During the observation spell 2020-21, the TACTIC telescope has been employed for observing the very high gamma-ray emission from sources within the Milky Way Galaxy and beyond. As the telescope is completing its successful operation of 25 years, activities related to the upgradation of its various subsystems have also been initiated. A prototype experiment has been set up to carry out the integrated testing of the data acquisition system of the TACTIC telescope with upgraded hardware components. The development of new software for the data archival is also completed. The preliminary requirements and preparation for onsite testing of Silicon-Photomultiplier based imaging camera are completed.

Phenomenological Studies in Astrophysics and Cosmology

A detailed phenomenological study has been performed on several galactic and extragalactic sources to understand the physical processes involved in the broadband emission from them. A methodology based on correlation between characteristics of the observed very high energy gamma-ray emission and redshift of the sources has been developed to estimate the distance of gamma-ray sources whose redshift cannot be measured through spectroscopic observations. An artificial intelligence based method has been proposed to predict the opacity of the Universe to very high energy gamma ray photon travelling over cosmological distances in the Universe. The cosmological evolution of the ultraviolet-optical-infrared background photons causing opacity to high energy photons has been studied using gamma-ray propagation effects up to redshift ~ 1 (Distance ~ 4.2 Gpc). The density of these low

energy background photons is an important cosmological quantity to estimate the total energy budget of the Universe. Evaluation of the cosmic ray neutron spectra has also been carried out at the Gulmarg observatory. It helps in the study of variations in the low energy neutron component in the atmosphere during the current solar cycle.

Synchrotron Beamline

Development and Utilization

BARC has been involved in the development of various kinds of beamlines based on synchrotron radiation sources (Indus-1 & Indus-2), at RRCAT for spectroscopic, x-ray imaging and structural studies of materials.

There are five beamlines on Indus-1 and seven beamlines on Indus-2 at RRCAT which have been developed and are being operated & maintained by BARC. These beamlines are being used by researchers from DAE, universities, national institutes including the entire gamut of IITs, CSIR laboratories and industry players. Two beam lines -undulator based Atomic Molecular and Optical Sciences (AMOS) beamline and bending Magnet-based Photo Emission Electron Microscopy (PEEM) beamline are under commissioning stage. AMOS beamline (6–800 eV) would be useful for photoionization, photodissociation and molecular dynamics in gas phase and soft x-ray EXAFS applications whereas PEEM beamline (100 to 8000 eV) will be useful for spectroscopic information at nm scale.

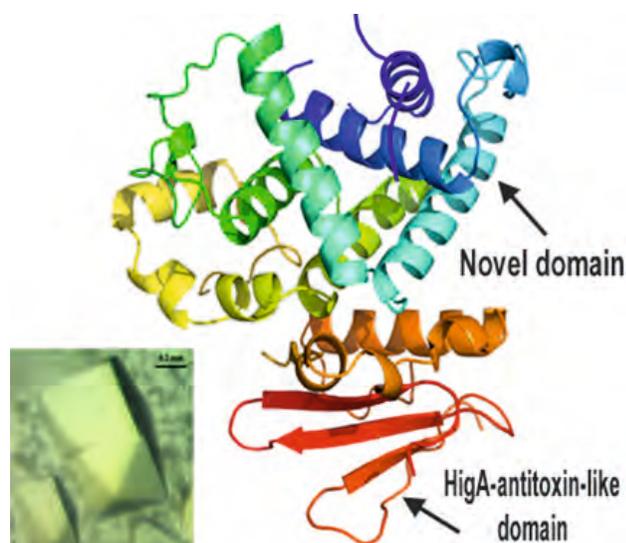
BARC has been carrying out R&D programs using these beamline facilities in the domain of atomic & molecular spectroscopy, multilayer science & technology, macromolecular crystallography, nanomaterials, functional materials etc. Some of the technologically important materials studied using these beamlines include potential materials for battery, catalytic materials, thin films for neutron mirror development and protein-inhibitor complexes.

High Pressure XAFS Results at Indus-2 Beamline

At the BL-9 (Indus-2) beamline, High Pressure XAFS (HPXAFS) data at BL-9 (Indus-2) was obtained from inside DAC for Nb_2O_5 . Results demonstrated systematic pressure-dependent Nb-O bond-length contraction with reasonably low uncertainties. This work warrants feasibility of HPXAFS experiments at BL-9.

Commissioning of Photo Absorption Spectroscopic Studies (PASS) Beamline at Indus-1

The PASS beamline is the 7th in the series of beamlines installed at the bending magnet port (BM03) of Indus-1 storage ring. Most of the beamline components are developed indigenously. The beamline is capable of performing photo absorption studies in the range of 55-840 eV (vacuum ultraviolet to soft X-ray) of materials, thin films and solid samples. This energy range covers the absorption spectra of low atomic number elements like C, N, O as well as L and M threshold of 3d elements, including Ti, V, S etc. The main components of the beamline consists of a plane grating monochromator (PGM) for selecting the desired X-ray energy, an ellipsoidal focussing mirror for focusing the monochromatic beam on to the exit slit and the experimental station. The plane mirror of the PGM accepts the incident beam with a



Crystal structure (2.3 Å) of a novel insecticidal protein-Txp40 from *Photorhabdus* bacteria solved by MAD method at BL21

horizontal and vertical acceptance angle of 3 mrad and 0.25 mrad, respectively and reflects the beam to the plane grating, which diffracts the monochromatic beam onto the focussing mirror. The plane mirror and grating gives a beam offset of 24.81 mm in vertical plane.

A facility has been successfully developed for *operando* X-ray Absorption Spectroscopy (XAS) measurements on electrode materials of Li-ion batteries using Indus-2 Synchrotron source. An electrochemical cell with kapton windows for transmission of X-rays as well as with sealing mechanism that ensures proper electrochemical performance of the battery has been developed in-house. The developments at the Energy Scanning EXAFS beamline (BL-09) at Indus-2 SRS are utilized for *operando* XAS measurements during the charging /discharging of the battery. The set up has been utilized for *in-situ* XAS measurements, on Li-ion batteries with LiMn_2O_4 as cathode material, *on* layer-structured lithium cobalt nickel manganese oxide ($\text{Li}[\text{Ni}_x\text{Co}_y\text{Mn}_z]\text{O}_2$) or LNMC electrode, which have lately emerged as one of the highly encouraging electrode materials. The measurements have been carried out simultaneously at Co, Ni and Mn edges and also on Fe_3O_4 nanoparticle based electrodes. This study is important for understanding the cyclic instability of the batteries during the charging/discharging processes and also to identify short-lived intermittent species.

VUV-IR Spectroscopy Studies using Photophysics Beamline Experimental Facilities

Photo-physics beamline at Indus-1 has been utilized for spectroscopic studies in the ultra violet (UV) and the vacuum ultra violet (VUV) regions. Few such molecules studied include 3-hexenol & 2-hexenal (biogenic and anthropogenic emissions by animals and plants into environment), ethyl-methyl carbonate (candidate solvent molecule in low temperature lithium batteries) and methacrolein (an important component of the atmospheric oxidation chemistry of biogenic

chemicals, which play a role in the formation of ozone). The UV-VUV absorption spectra required for understanding the photochemistry of these molecules and their potential applications are recorded using photophysics beamline. Detailed electronic and vibrational spectral analysis has been carried out on these molecules and interpretation of the spectral features is elucidated with the help of extensive DFT and TDDFT calculations. The analyzed UV-VUV absorption spectra of methacrolein recorded for the first time the potential energy curves required for understanding the nature of its excited states.

Crystal Structure of a Novel Insecticidal Protein using BL-21

The most commercially exploited bacterial insecticides which are considered to be toxic against mosquitoes and other insects are obtained from *Bacillus thuringiensis*, *Bacillus sphaericus* and *Clostridium bifermentans*. But over the years, the insect species have developed gradual resistance to the *B. thuringiensis* toxins. Hence there is an urgent need for the development of new biopesticides. In this regard, the novel Txp40 insect toxin proteins from *Xenorhabdus*/*Photorhabdus* bacteria have been cloned to understand their activity against a wide range of insect pests from lepidopteran (moths) and dipteran (mosquitos) species. Nonetheless, the precise mode of action of this toxin is not exactly known due to the fact that Txp40 proteins share no significant sequence match to proteins with known structures or functions, which clearly suggests that it is a novel toxin protein. Txp40 protein from *Xenorhabdus nematophila* was recombinantly purified and

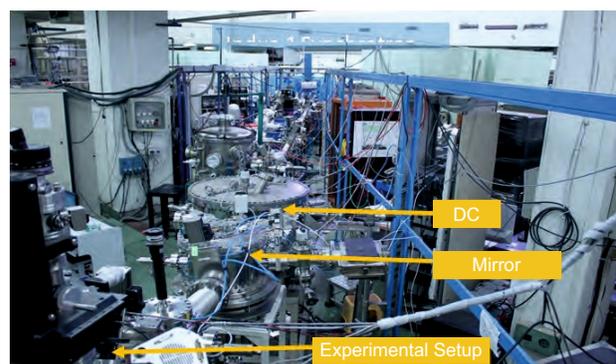
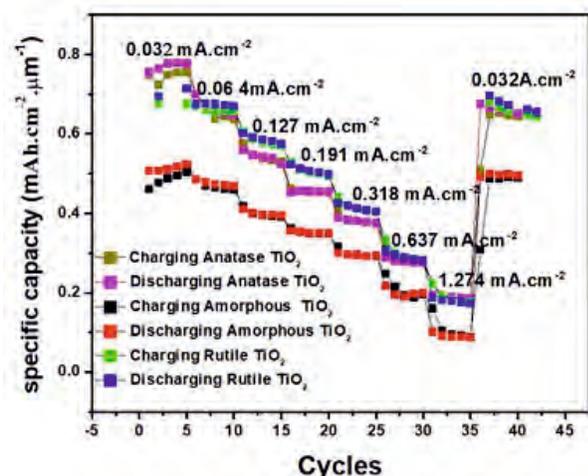


Photo Absorption Spectroscopic Studies (PASS) beamline

crystallized. To obtain phase solution selenomethionine (SeMet) was incorporated in the protein using recombinant technology so that its structure could be solved by multi-wavelength anomalous dispersion. The Txp40 is a monomeric protein and comprises two domains. Dali database search of all-alpha helical N-domain shows no significant structural homology to any of the structures in PDB suggesting a new protein fold. C-domain is an alpha-beta structure and shows significant homology to antitoxin HigA protein of *Proteas mirabilis* gut bacteria.

Development of Software for Analyzing Protein Sequence

The native folded state of protein is believed to be due to the amino acid sequence of the protein. Predicting the 3-D structure of the protein from its sequence is the famous "Protein Folding Problem". Other than the folding, various physico-chemical properties of proteins can be deduced by analyzing the sequence. Though a number of softwares are readily available in the market, they are either limited in calculating fewer properties or limited to only one sequence. However, PSA (Protein Sequence Analyzer) developed in BARC is capable of high-throughput analysis of considerable number of protein sequences and it provides a framework for statistical analysis of various properties of proteins. To make this, a new A cloud computing based web server has been developed in-house and was deployed in BARC so that the services of PSA could be exploited by the global



Cyclic performance of the coin cells at different current densities with TiO₂ electrodes under different phases

scientific community. The server has already started gaining global attention, which is evident from the fact that more than 800 jobs have already been processed. The high-throughput genomic sequences of the mutating SARS-CoV-2 virus have been made available through various world-wide consortia and GISAID efforts (<https://www.gisaid.org/>). Availability of such a huge and high-quality protein sequence data has made it possible to obtain the time evolution of various mutations. Millions of sequences deposited in GISAID from India and England have helped in obtaining the evolving nature of various mutations in SARS-CoV-2.

Lithium Batteries

Development of Li ion Batteries Assembled with TiO₂ Based Thin Film Electrodes

Li ion batteries have been developed with TiO₂ based thin film electrodes prepared using RF magnetron sputtering technique on polished SS substrates. Films with amorphous, anatase and rutile phases have been made in different coin cells. The cell containing rutile phase TiO₂ electrode showed the highest specific capacity of 1000 $\mu\text{Ahcm}^{-2}\mu\text{m}^{-1}$ after 700 cycles at a high rate of 100 μAcm^{-2} , which is the highest value reported so far. The studies on these cells showed that the batteries equipped with composite TiO₂/Fe₂O₃ anode have better structural stability of TiO₂ and better diffusion kinetics of Fe₂O₃.

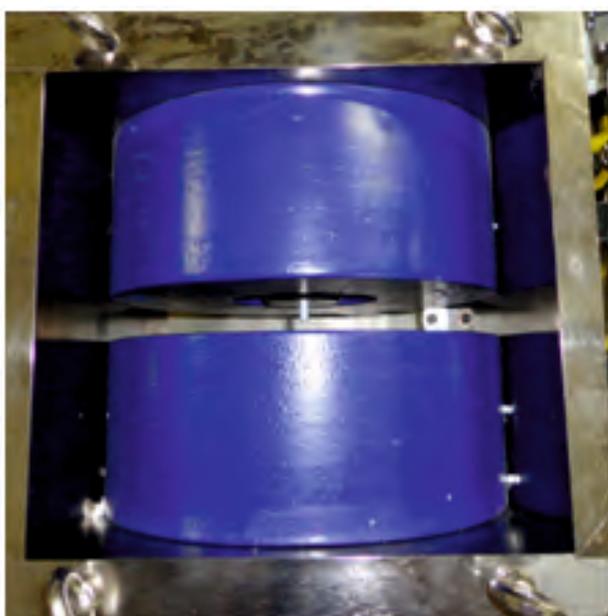
User-friendly GUI Software-PRISA- for Optical Analysis of Thin Films

A user-friendly software named "PRISA" has been developed for determining various properties such as refractive index, extinction coefficient, oscillator energy, dispersion energy, absorption co-efficient, band gap, and thickness of semiconductor and dielectric thin films deposited on transparent substrate only from their measured transmission spectrum. The thickness and optical constants of the films have been derived using Swanepoel's Envelope method. Both direct and indirect bandgap of the films are estimated from the

absorption co-efficient spectrum using Tauc plot. The software codes are written in Python and the GUI is programmed with tkinter package of Python. Finally, the developed PRISA was found to be much simpler and highly accurate as compared to the other freely available softwares.

2T Compact Electromagnet for Scanning EXAFS Indus-II Beamline for XMCD Experiments

X-ray magnetic circular dichorism (XMCD) uses differential absorption of polarised light (left and right circular oriented) in a magnetic field to examine structural properties of magnetic materials. Experiments have been carried out in this regard at the Scanning EXAFS Beamline (BL-09) of Indus-II synchrotron. A compact electromagnet generating 2T magnetic field in an air gap of 25mm with a footprint of 300mm x 300mm x 300mm is required to carry out XMCD measurements in BL-09 beam line of Indus-II. To achieve the requisite high magnetic field in compact dimensions high magnetic saturation material (FeCo alloys) was selected for magnetic poles and the pole edges have been optimized to achieve the required magnetic field and its uniformity with minimum Magnetomotive Force (MMF). Installation of the magnet with INDUS-II beam line is currently under progress.



2T compact electromagnet for Scanning EXAFS Indus-II beamline for X-ray magnetic circular dichorism experiments

Halbach based Permanent Magnet Dipole for Head Imaging

A portable 0.2 Tesla Halbach based permanent magnet dipole has been designed and developed for imaging of human body parts, mainly head, wrist and ankle as part of primary diagnosis. The magnet has a magnetic field uniformity over 2.5% in a spherical diameter of 200 mm. The uniqueness of this design is its in-built magnetic field gradient, which doesn't require separate gradient coils, associated power amplifiers and controls. Magnetic field gradient is required for spatial encoding of the images. By virtue of its high strength permanent magnets, the system is compact, lightweight, energy efficient and portable.

Mass Spectrometers and Spectroscopy

Thermal Ionization Mass Spectrometer (TIMS)

A compact Thermal Ionistion Mass Spectrometer has been commmisioned in BARC for the isotope ratio analysis of Lithium samples.



Halbach based permanent magnet dipole for imaging of specific body parts like head, wrist and ankle as part of primary diagnosis

Development of Process Gas Mass Spectrometers

Process Gas Mass-Spectrometer (PGMS) has been used for monitoring online isotopic ratio of Uranium isotopes in the enrichment plants. Two Process Gas Mass Spectrometers developed in-house were installed and commissioned at Rare Metals Project. The performance of the system was successfully evaluated with UF_6 standards prescribed for analyzing both enriched and depleted samples.

Utilization of in-house Metal Cluster Setup for Investigating Physics of Metallic Clusters

A new state-of-the-art Metal Cluster Setup laboratory was developed in-house for studying physics of bimetallic clusters consisting of few tens to hundreds of atoms, which are intermediate between molecules and bulk state of matter. It consists of an indigenously built laser ablation supersonic expansion-based setup for the generation of metal clusters and to carry out investigations by mass spectrometry and laser spectroscopy. The focus here has been to study these clusters as a function of their size and composition for understanding and developing the genesis and tunability of physical properties as matter is assembled from individual atoms towards functional nanomaterial and bulk systems.

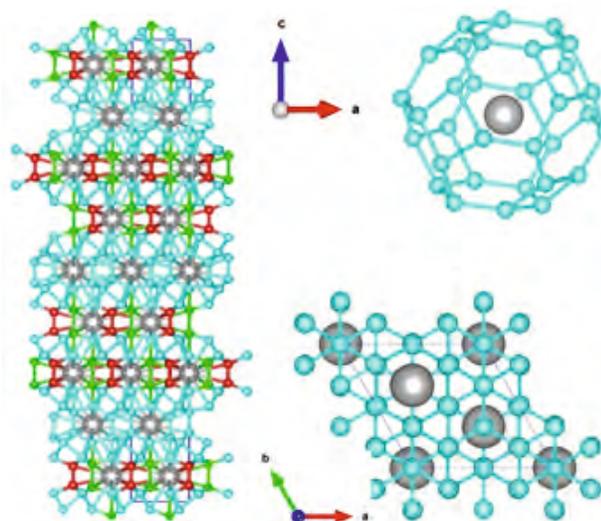


Process Gas Mass Spectrometer

The set up has been utilized to generate a range of metal and metal oxide clusters viz. LaO , Al , AlO , Co , $Co.NH_3$ in the size range of diatomic to 50-atom clusters. Mass spectrometric investigations proved that lanthanum clusters containing up to 50 atoms are stable. The geometric structures of 2 to 10 atom lanthanum clusters have been established through combined experimental and theoretical investigations.

Prediction of an Unusual Trigonal Phase of Superconducting LaH_{10} Stable at High Pressures

Evolutionary crystal structure searches in combination with ab-initio calculations, an unusual structural phase of superconducting LaH_{10} has been predicted in the pressure range of 250-425 GPa at 0 K. Inclusion of phonon zero-point and 300 K free-energy contributions shifts the transition pressures to higher values. The new phase contains three units of LaH_{10} in its primitive cell and is expected to become superconducting at a critical temperature of about 175 K.



The unusual structural phase of superconducting LaH_{10} predicted in the pressure interval of 250-425 GPa at 0 K.

Jet Cooled Laser-induced Fluorescence Spectroscopy of Tantalum Monocarbide: Observation of Ground State Vibrations and Low-energy States

Laser-induced excitation and dispersed fluorescence (DF) spectra of TaC molecule, produced in laser vaporization free-jet apparatus, was studied as part of investigations into its electronic structure. The DF spectra from the rovibronic bands yielded harmonic frequency of $769.1(1) \text{ cm}^{-1}$ for the ground electronic state. This value is distinctly different from the earlier reported value of 1064 cm^{-1} determined from the anion-photoelectron spectroscopy. Additionally, the reasonably intense dispersed fluorescence peaks between the displacement wavenumber 2400 to 5900 cm^{-1} are tentatively assigned to low-lying states predicted in the earlier *ab initio* studies.

Nuclear Physics

Reactor Antineutrino Studies

A large area plastic scintillator (PS) detector setup ISMRAN (Indian Scintillator Matrix for Reactor Anti-Neutrinos) has been fabricated and installed at Dhruva research reactor. Through measuring of antineutrinos, ISMRAN seeks to obtain answers to several outstanding problems which are of fundamental nature, including the existence of sterile neutrinos, reasons for excess antineutrino spectral yield and for monitoring reactor power in a non-intrusive way. Measurements have been carried out for the decay products of cosmic muons which are stopped inside the detector matrix, as well as cosmic muons passing through the full geometry. The measurements are expected to yield potential clues to several outstanding problems of fundamental importance, including the possible existence of sterile neutrinos, reactor antineutrino anomaly, explanation of peak in the positron spectra etc.

Utilization of Pelletron LINAC Facility

The Pelletron-Linac Facility consisting of an accelerator and a Linac has been kept operational round-the-clock with an aim to obtain various ion beams including, ^1H , $^6,7\text{Li}$, ^{12}C , ^{14}N , ^{18}O , ^{19}F , $^{28,30}\text{Si}$, ^{32}S ,

^{35}Cl . Proton irradiation of wheat and rice were performed under induced-mutation studies by employing the upgraded large area low flux Proton beam setup. This setup was also extensively utilized to carry out calibration studies of radiation-dosimeters to cater to specific requirements of the Indian Space Research Organisation. Experiments conducted on a trial mode with Americium-243 target have opened up fresh avenues in the pursuit of deploying a radioactive target at the accelerator facility.

Origin of Large Alpha Production in Nuclear Reaction with Weakly bound Nuclei

Investigations have been carried out in weakly bound nuclei to understand the role of projectile breakup to provide evidence of various clustering configurations of nucleons and to disentangle different reaction modes leading to breakup. A recent study using the BARC-TIFR Pelletron LINAC facility has resolved the origin of large alpha production in reactions involving weakly bound nuclei. To achieve an unambiguous experimental discrimination, a coincidence measurement between the outgoing alpha particles and gamma rays obtained from heavy residues has been performed for the weakly bound projectile ^7Li (alpha + triton cluster structure) on the ^{93}Nb target. For the first time the results provided direct experimental evidence on the dominant role of the direct cluster transfer of triton-from ^7Li to the target in large alpha production and not through a breakup process followed by fusion. Unraveling the reaction mechanisms with weakly bound nuclei is important not only from its fundamental aspect but is also a promising tool in other areas, including nuclear astrophysics and nuclear energy applications.

Observation of Rare Super Short Fission from Neutron rich ^{257}Md Nucleus at High Excitation Energy

Fission fragments from ^{257}Md nucleus populated by complete fusion of ^{19}F with ^{238}U have been measured in the range of excitation energies,

$E^* \approx 48$ MeV. The analysis of the mass and total kinetic-energy distributions infers on the presence of a rare fission mode called "supershort mode of fission", whose presence has been confirmed by measuring two additional reactions: $^{19}\text{F} + ^{232}\text{Th}$ and $^{18}\text{O} + ^{238}\text{U}$ first involving a different target and then a different projectile leading to compound nuclei ^{251}Es and ^{256}Fm , respectively, at similar excitation energies and comparing their mass & total-kinetic-energy correlation plots. The existence of considerable supershort mode of fission for the ^{257}Md nucleus up to high excitation energy ($E^* \approx 48$ MeV), observed for the first time, reveals that such rare fission modes for neutron-rich exotic nuclei are far off from the liquid drop model predictions even at high excitation energies.

Tunable Error-protected Qubit, Quantum Measurements, and Quantum Devices

An action principle formulation for the quantum Zeno effect (tunable $0-\pi$ qubit) has been formulated to show a possible practical error-correction method. The simulations of the cavity along with nonlinear elements like junction, have provided important design parameters for coplanar waveguides which are being fabricated at IIT Bombay Nanofabrication facility.

Resonance Dynamics in the Coherent η -Meson Production in the (p,p') Reaction on the Spin Isospin Saturated Nucleus

In the η meson production reaction, it was widely considered that the meson is produced due to the decay of $N^*(1535)$ resonance, i.e., $N^*(1535) N\eta$. This statement is shown true for the $N\eta$ invariant mass below 1.7 GeV. The resonance $N^*(1520)$ contributes dominantly to the η meson production reaction above the $N\eta$ invariant mass equal to 1.9 GeV.

Solid State Physics

Electron Doping of Geometrically Perfect Spin-1/2 Kagome Lattice by Graphene

A remarkable semiconducting behavior by innovative electron doping has been established in a structurally phase-pure barlowite (an electrical

insulator) system having geometrically perfect $S=1/2$ kagome (triangular arrangement of ions) planes by integrating with the reduced graphene oxide (rGO).

Study of Magnetic and Magnetotransport Properties of $\text{Bi}_{2-x}\text{Fe}_x\text{Se}_{3-x}\text{S}_x$ Topological Insulator

The observation of negative magnetoresistance (MR) in topological semimetals and topological insulators when a magnetic field is applied in parallel to an electric field (called longitudinal geometry), has recently attracted significant attention from the scientific community. The magnetic and magneto-transport properties of a family of topological insulators- $\text{Bi}_{2-x}\text{Fe}_x\text{Se}_{3-x}\text{S}_x$ - has recently been investigated where a change in the magnetoresistance (from positive to negative) has been observed with co-doping. The observed negative magnetoresistance behaviour has been attributed to the strong bulk ferromagnetic ordering.

Fine Tuning of Hydrogen Bond Strength in Crystals

Hydrogen bond interactions are one of the most enigmatic intermolecular interactions that play an important role in biomolecular processes, crystal growth and engineering, and soft condensed matter. They are considered as the 'master key interaction' of 'supramolecular chemistry' which goes beyond the molecules and offers an interface with biological and material science. Potassium dihydrogen phosphate crystals with small amount of ammonium ion substitution were grown and the variation of their hydrogen bonding propensities with temperature were investigated using spectroscopic as well as structural techniques. A small change in the crystal temperature as well as concentration of NH_4^+ ion are considered to affect hydrogen bond geometry which may result in a double well potential energy contour for these bonds. The dynamics of H atom was shown to be minutely dependent on the double well hydrogen bond potential which changes gradually with the decreasing temperature from predominantly inter

well dynamics to completely intra well dynamics within an intermediate precursor region where both inter well as well as intra well dynamics is important.

Multiple Kohn Anomalies in Alpha-Uranium

Using the state-of-the-art first-principles simulations of electron and lattice dynamical susceptibility and electron phonon interactions supported by inelastic neutron scattering experiments, it was conclusively shown that Uranium harbours multiple Kohn anomalies which meet the criteria set by Kohn, who, in 1959 had first proposed the strongest manifestation of the electron-phonon interactions.

Technical Physics Development of HPGe Detector

An HPGe detector was developed in-house from externally procured HPGe single crystal. The procured, high purity Ge crystal, was processed, initially, by cutting and polishing. Further, n-type and p-type contacts were fabricated on the crystals. The N-type contact of the detector was fabricated by Li diffusion and the p-type contact by Boron implantation. The fabricated diode crystal was chemically and physically passivated by chemical etching and deposition of amorphous

hydrogenated Ge film to decrease the surface leakage current. A leakage current of less than 1 nA at a reverse bias of 1 kV was achieved. The diode was then mounted on the cold finger of a liquid nitrogen cooled dipstick and tested for gamma radiation. The resolution of the acquired spectra is found to be 0.3% at 662 keV with line width of the ¹³⁷Cs peak around ~2 keV as compared to 1.5 keV with commercial detectors.

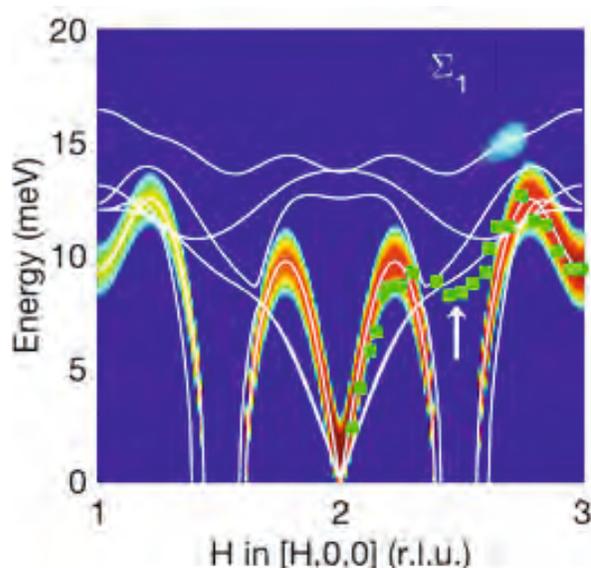
Development of Supercapacitors and Si Detectors

Supercapacitor devices store electrochemical energy where the energy is stored through adsorption of ions at the interface of active electrode materials and electrolytes. This process is known as electric double layer capacitance (EDLC). BARC is working on different materials like porous reduced graphene oxide, in combination with various redox electrolytes. Further, in collaboration with IIT, Guwahati, under a BRNS project, MXene hydrogel electrodes were developed for energy storage devices. The synthesis of these hydrogels at room temperature resulted in high performance supercapacitors, which offer gravimetric energy density of about 30 Wh/kg with gravimetric power density of about 1.1 kW/kg. The devices, however, did not show deterioration in performance even after 10,000 cycles of operation.

Work was initiated on developing supercapacitors using hybrid electrode materials which are composites of materials offering EDLC and pseudocapacitance. Nanocomposites of poly (3,4-ethylenedioxythiophene)-poly(styrene sulfonate) (PEDOT:PSS) and V₂O₅ were employed as electrode materials for fabricating coin cells of capacitance 1F that offer gravimetric energy density of 7 Wh/kg and gravimetric power density of 1kW/kg.

Development of “e-nose” to Discriminate H₂S and NO₂ Test Gases

A novel ZnO nanowires-based e-nose has been demonstrated successfully for its ability to discriminate H₂S and NO₂ test gases. Bar chart and principal component analysis (PCA) indicate the



Calculated phonon dispersion (solid lines) along with the measurements (square markers)

capability for producing qualitative as well as quantitative discrimination of two test gases. The e-nose system consists of three parts: multiple sensors (MS), data acquisition (DAQ) and pattern recognition algorithm (PRA). Multiple sensors were realized using ZnO nanowires (NW) grown using hydrothermal method. For this, the NW surface was modified by depositing a thin layer of Au, Cu, Ni and MgO (~10 nm) using physical vapor deposition methods. The addition of a thin layer of sensitizers on NW surface results in the formation of ZnO-CuO, ZnO-Au, ZnO-NiO and ZnO-MgO heterojunctions. A huge data repository was created in the process.

Titanium Hydride Targets for Portable Neutron Generator Applications

A process for fabrication of Titanium hydride (TiD_x & TiT_x) targets on Cu substrates for portable neutron generator applications has been validated. Titanium getter films of best quality having a thickness of ~3.5m possessing good adherence and having service temperature of ~500°C were deposited using thermal vapor deposition technique on a Cu substrate. For 3.5m thick and 12mm diameter Titanium film with active volume of $\sim 4 \times 10^{-4}$ cc, deposited on 16mm diameter Cu substrate, deuterium loading of 2.1 ($\pm 10\%$) standard cubic centimeters (scc) was achieved and this target gave a neutron yield of $\sim 10^6$ n/s in an indigenously developed portable neutron generator. Similarly, ~ 3 Ci ($\pm 10\%$) activity of tritium

was achieved for the same Ti thickness and it gave a neutron yield of $\sim 10^8$ n/s. Moreover, the thermal vapor deposition system was also suitably modified and optimized to achieve Titanium films up to 35 mm diameter (active layer). Efforts are already underway towards the development of Ti films for high yield ($\geq 10^{10}$ n/s) neutron generator applications.

On-line Coal Calorific Value Analysis

An on-line coal analyzer based on a pulse fast thermal neutron analysis method which uses both fast and thermal neutron activation for elemental analysis has been developed in BARC.

Polymer solar Modules and Pixelated Perovskite Solar Cells for Energy Harvesting

Si-based solar cells are extensively used in energy harvesting and have emerged as one of the most prominent green energy sources. However, owing to their expensive fabrication process, their use is constrained. Therefore, work on development of an efficient and economical solar cell technology solution was initiated in BARC. Large area polymer solar modules were fabricated with the device structure PET/HC-PEDOT: PSS/Active Layer/Al. The typical module has 27 devices (each device has ~ 0.1 cm² area) arranged in series on a single substrate (10 cm x 10 cm), which exhibited 15 V and 0.3 mA, under 1 sun illumination.

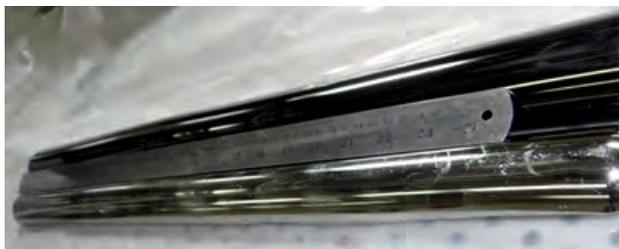
Other Accomplishments

- ✧ Operando structural studies on electrode materials of Li-ion batteries
- ✧ Development of Wire Beam Position Monitor for undulator-based Atomic Molecular & Optical Sciences (AMOS) Beamline, Indus-2 SRS
- ✧ Design and development of Band Pass filter for photoluminescence experiments on anti-counterfeiting experiments
- ✧ Understanding the molecular structure and intermolecular interactions of Curcumin during chemical complexation for potential biomedical applications
- ✧ Magnetic properties of $S=5/2$ anisotropic triangular chain compound $Bi_3FeMo_2O_{12}$ were investigated using neutron diffraction and neutron depolarization techniques at Dhruva reactor

Chemical Sciences

Ultra-purification of Materials

A new quartz assembly capable of refining 3 kg of sample at a time has been procured and assembled. Two zone refining experiments (TPMS-9 and TPMS-10) at slow scanning speed and under flowing hydrogen gas were carried out with 15 and 20 number of continuous passes. A new measurement system based on Hall Effect developed in-house in BARC was used to measure resistivity, Hall Coefficient, carrier charge concentration and the carrier mobility measurement of the latest zone refined germanium sample. A clear n to p transition, which is a signature feature of HPGe was observed around 200°C. At 80K, the average resistivity, Hall coefficient and carrier concentration of polycrystalline sample were found to be 80,000 ohm.cm, 8×10^7 cc/C and 3.5×10^{11} /cc, respectively. The purity of the sample was estimated from carrier charge concentrations.



Photograph of zone refined Ge rod

Recovery of Gallium from Bayer's Liquor

To improve the sorption capacity of resins towards Ga and V, sorption behaviour at different mass ratio of the resin beads to the volume of Bayer's liquor was studied. Further, 19L of functionalized resin beads were supplied to Heavy Water Board for undertaking a pre-pilot scale column operation. Resin samples from each batch were collected after completion of functionalization reactions. The FTIR study confirmed the successful incorporation of the required functional group, amidoxime, on the base polymer resin. The swelling characteristics of resins have been tested and found satisfactory. Thus, the resin supplied to HWB was found to be satisfactory in basic quality control experiments.

The concentration of NaOH in elute solution was optimized for better Ga recovery in electrolysis step. Dynamic light scattering (DLS) study was done with the Bayer's liquor (Spent liquor) provided by NALCO (a public sector undertaking of Govt. of India) to measure the suspended particle size distribution, which is important for pre-treatment process of Bayer's liquor. Reusability study at elevated temperature (55°C) with the developed resin was carried out up to 10 cycles. To regenerate the capacity, the used resin was treated with HCl and HNO₃ solutions, which led to a 3-fold increase in the sorption capacity. The used resin was also treated with NaOH solution to remove the adsorbed Vanadium, which might have been built up during sorption/elution cycles.

Thermal and Radiation Ageing Studies on Paint used in Nuclear Power Plant

Thermal stability of nuclear paint under inert (N₂) and oxidative atmospheres (air; air +5% steam) has been evaluated using thermogravimetric-mass spectrometry (TG-MS) technique. A method based on target factor analysis (TFA) has been developed for simultaneous determination of evolved organic components as well as to establish their concentration profiles over the applied temperature range. Paint pyrolysis under inert atmosphere is accompanied by continuous evolution of CO₂ up to 800°C. Different classes of organic molecules have been identified in the evolved gas. The major products that evolve in the major thermal degradation stage from 300-450°C include butanol, phenol and methyl isobutyl ketone. However, when paint is pyrolyzed under oxidative atmosphere it was observed that CO₂ is evolved in the major degradation step at 350-450°C. In this temperature range, gases such as butanol, phenol and methyl isobutyl ketone, isopropanol were also observed. The acceleration of the degradation process may be a fall out of the higher oxygen content in the atmosphere.

Gamma irradiation mediated ageing of nuclear paint was investigated by irradiating samples with 10-1000 kGy dose and analyzed by ATR-FTIR spectroscopy. At very low total dose (up to 10 kGy),

no significant change has been observed. In 20-60 kGy range, the chain-crosslinking phenomenon predominates, causing enhancement in amide (1650 cm^{-1}) signal intensity at the expense of carbonyl (1720 cm^{-1}) intensity. At higher doses of 80 and 100 kGy, the spectra becomes similar to that of the unirradiated one, which indicates that the chain crosslinking effect is being reversed by the opposing chain-scission reactions. At even higher dose, (of 200 kGy), the chain-scission becomes predominant which causes lowering of amide band as compared to the unirradiated paint. However, at 400-800 kGy the chain-crosslinking again seems to take pre-dominance over chain-scission which leads to an increase in amide band intensity even as it maintains the same carbonyl intensity. This might be due to oxidative conversion of CH_2 group directly attached to N-atom of amines into carbonyl moiety.

Reactor Water Chemistry

Studies Related to TAPS 1 and 2 Decontamination

A two-step process involving Nitric acid Permanganate (NP) and NTA-Ascorbic acid (NTA-AA) was suggested for TAPS-1&2 decontamination. Apart from the evaluation of the process under static conditions, it was also evaluated under flow conditions as per the directions of COSWAC. Chromium was found to dissolve mainly in the first step (oxidation by NP) while nickel and iron dissolved mainly in the second step (reduction and acid dissolution) by NTA-AA. Polished blank coupons of SS-316 and SS-304 were also exposed for the full duration of the experiment along with the tube specimen to obtain the corrosion rate, which was found to be 4×10^{-4} and 5×10^{-4} $\mu\text{m/h}$, respectively.

For optimization of the decontamination process, efficient dissolution kinetics of chromium containing transition metal oxides is essential. Hence, dissolution kinetics were probed with synthetic oxide (by sol-gel method) pellets $[\text{M}_x\text{Co}_{1-x}\text{CrFeO}_4]$ ($\text{M} = \text{Zn} \ \& \ \text{Ni}$) in oxidising and $(\text{CoCr}_x\text{Fe}_{2-x}\text{O}_4)$ ($0.0 < x < 1.0$) reducing formulation. In HMnO_4 medium Cr release was moderately linear

up to 2-3 h and later became saturated due to Cr depletion and *in situ* formed MnO_2 deposition on pellet surface. The Dissolution rate decreased upon Ni substitution whereas it increased with Zn substitution.

Chemical Cleaning of Structural Material Surfaces Coated with LiF-ThF_4

Decontamination of structural materials exposed to molten fluoride medium is an essential component of the Indian Molten Salt Reactor (IMSR) development program. It is required for the free release of the material as well as for evaluating the effect of exposure to the medium. A facility has been designed and developed to dip the structural material specimen in lithium fluoride and thorium fluoride eutectic mixture at a temperature of 650°C under an inert atmosphere of argon. The thorium fluoride coated Hastelloy-N and Inconel 690 specimens obtained from this facility were used in the subsequent dissolution studies. The efficacy of the chemical treatment was evaluated by alpha counting using a hand-held alpha detector and determining the aqueous thorium concentration by using Arsenazo III spectrophotometrically. A three-step formulation with first one of 2% CTAB, the second one of 5% KMnO_4 in 1.5 M H_2SO_4 followed by the third step of 5% EDTA, 5% ascorbic acid and 5% ammonium oxalate have been evaluated. A mixture of 0.1 M boric acid with 8 M nitric acid at 80°C has shown a rapid dissolution of the ThF_4 coating from the alloy surface. Thorium fluoride coating was completely eliminated through implementing two cycles of chemical treatment under the three step formulation.

Studies on Electro Catalytic Hydrogen Evolution of Nickel Modified Stainless Steel Mesh

Nickel modified SS-304 electrodes for H_2 generation were developed through hydrothermal method to simulate *in situ* redox conditions during corrosion studies. The electrochemical surface area of the electrodes was estimated was to be in the range of 0.005 cm^2 . A significant reduction in

the surface areas was seen in the over potential zone (280 mV at 10mA/cm²) as compared to other electrode materials. Thus, the catalytic activity towards HER was confirmed.

Healthcare Materials

Development of Nano-delivery Systems for Cancer Therapy and Bio-imaging

¹⁷⁷Lu-labeled NaGdF₄:Ho-Yb@m-SiO₂ upconversion nanophosphors (¹⁷⁷Lu-UCNPs) were developed for theranostic application. *In vitro* stability assessment showed that ¹⁷⁷Lu-UCNPs retain radiochemical integrity in saline and rat serum. From a whole-body SPECT/CT imaging (4 h after injection of ~ 18 MBq of ¹⁷⁷Lu-UCNPs in healthy Wistar rat), it is evident that they preferentially accumulated in the liver.

Glutamic acid-coated Fe₃O₄ magnetic nanoparticles (GAMNPs) were developed for combination chemotherapy using doxorubicin and methotrexate. The GMNPs show enhanced toxicity towards breast cancer (MCF-7) cells and exhibit good magnetic heating efficiency and transverse relaxivity indicating their potential capability in hyperthermia therapy and MRI tracking. Fe₃O₄@SiO₂ core-shell nanoparticles were explored for magnetic hyperthermia therapy in SWISS mice tumor model. Intratumoral injection of nanoparticles under the effect of AC magnetic field indicates a reduction in tumor size.

Nitroso-thiolated Fe₃O₄ nanoparticles were prepared for applications in chemotherapy. Nitric oxide (NO) release from developed nanocarriers (doxorubicin loaded nitroso-thiolated Fe₃O₄) in cancer cells were performed using Griess reagent at different pH levels.

The formulation showed higher toxicity towards cancer cells as compared to pure doxorubicin formulation. Up-and down-convertible LaF₃:Yb,Er nanocrystals with broad emission window from 350 nm to 2.8 μm were developed for bioimaging. The emission characteristics of Yb, Er codoped LaF₃ were compared with that of LaOF. The change in the emission behavior has been explained by calculated phonon spectrum, which indicates that

the highest phonon energy for LaF₃ is 438.88 cm⁻¹ while that of LaOF is 527.37 cm⁻¹.

Protein Conjugated Nanoparticles for Magnetic Hyperthermia Application

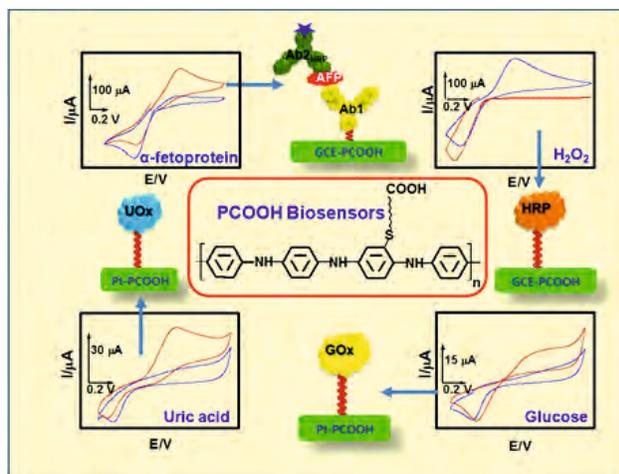
Hyperthermia using magnetic nanoparticles (MNPs) has been introduced clinically as an alternative approach for local treatment of tumors. The surface engineering of MNPs with bioactive molecules is extremely important for their design and subsequent application in hyperthermia. In this aspect, protein conjugated glutaric acid functionalized magnetic nanoparticles were developed for hyperthermia therapy. The prepared MNPs are biocompatible with normal cells and showed substantial cellular internalization in cancerous cells, suggesting their potential application in hyperthermia therapy.

Preparation of Super Bright Red Upconversion Nanoparticles for Bio-imaging Applications

Nanocrystalline materials emitting a single band red light under Near Infrared excitation have advantages in cellular imaging in biological windows, as agents for photodynamic and photothermal therapy. Highly monodispersed upconversion nanocrystals functionalized with folic acid for targeting tumor cells, were prepared and tested for cellular imaging under UV light and NIR excitation.

Development of Sensors for Healthcare Monitoring

A sandwich-shaped electrochemical biosensor was constructed using carboxylic acid functionalized polyaniline as antibody immobilization matrix. It was used for detection of liver cancer biomarker (α-fetoprotein (AFP)). The sensor displayed sensitivity of 15.24 μA (ng mL⁻¹)⁻¹ cm⁻², with good specificity, reproducibility (RSD 3.4%), wide linear range (0.25-40 ng mL⁻¹) and a low detection limit of 2 pg mL⁻¹. The sensor was validated by detecting AFP in human blood serum samples where the AFP



concentration obtained was found to be consistent with the values estimated using ELISA. Polyaniline was covalently modified by thiol-ene click chemistry to obtain carboxylic acid tethered polyaniline (PCOOH). Utilization of PCOOH for construction of enzymatic biosensor was demonstrated by covalent immobilization of glucose oxidase, uricase and horse radish peroxidase for the detection of the corresponding substrate glucose (G), uric acid (UA) and H_2O_2 , respectively. The biosensor displayed excellent sensitivity with a detection limit of 0.01, 0.001, 0.008 mM for G, UA and H_2O_2 , respectively.

Pharmacokinetics of Oral Formulation of 3'-3'-Diselenodipropionic Acid (DSePA)

The optimized clinical grade formulation containing DSePA, lactose monohydrate and magnesium stearate has been evaluated for stability under accelerated conditions (40°C, 75% RH) up to 1 month and long-term conditions (25°C, 60% RH) up to 3 months in sealed transparent glass vials. The assay confirmed >95% drug stability in the formulation.

Pharmacokinetics studies of the formulation containing DSePA, lactose monohydrate and magnesium stearate were undertaken in mice. The highest maximal concentration (C_{max}) of the DSePA formulation was observed in plasma (2.4±3.6 $\mu\text{g}/\text{ml}$) followed by lung (1.79 $\mu\text{g}/\text{g}$). The plasma elimination half-life of DSePA formulation was 14 h, which is about three times higher than that of plain DSePA. The synthesis of deuterated 3,3'-

diselenodipropionic acid (D-DSePA) was carried out and single crystals of D-DSePA were grown from methanol. The structure of D-DSePA shows highly disordered alkyl group. The deuterated DSePA exhibited better biocompatibility due to its slower metabolism (almost ~1.5 fold decrease in the rate of oxidation) as compared to normal DSePA.

Evaluation of ^{10}B containing Zinc Gallate based Nano-formulation against Tumor Induced in BALB/c Mice

The ^{10}B laden zinc gallate based nano-formulation was prepared and evaluated *in-vivo* against fibrosarcoma tumor induced in BALB/c mice and C57BL/6 mice. The mice were first treated with the formulation followed by irradiation of the tumor part with neutrons (20 minutes), an exercise which was repeated again. A 75% decrease in tumor size was observed within two weeks.

Exploring Organoselenium Compounds as Inhibitor of SARS-CoV2

Cellular thiols (GSH) are known to minimise organodiselenides, which may affect their antiviral activity during infections. In order to address this issue, inhibition of SARS-CoV-2 protein like M^{pro} by pyridine diselenide (Py_2Se_2) and diselenodipropionic acid (DSePA) was investigated in the presence of GSH. Results based on experiments done in BARC established that GSH does not alter the IC_{50} of Py_2Se_2 and DSePA for the inhibition of M^{pro} . Pyridine diselenide (Py_2Se_2) and nicotinamide diselenide (Nic_2Se_2) have been evaluated against human influenza A virus (WSN/A/33/H1N1 strain) infectivity using normal human lung cells. The results also indicated that Py_2Se_2 and Nic_2Se_2 treatment at 10 μM concentration inhibit viral infectivity by 60% and 80%, respectively. The mechanism of action of pyridine diselenide (Py_2Se_2) and diselenodipropionic acid (DSePA) as the potent inhibitors of SARS-CoV-2 was studied through circular dichroism (CD). The native viral protein exhibited 33.1% helix, 33% beta-sheets and 33% uncharacterized structure. Treatment with Py_2Se_2 and/or DSePA (0.15 nM to 5 μM) led to a decrease in

the helix content (by ~17%) with concomitant increase (by ~17%) in the beta sheet. This disruption in the structure was attributed to chemical modification of the cysteine residue present near the active site of the viral protein.

AIEgen-Protamine Assembly/Disassembly Based Fluorescence Turn-on Probe for Sensing Alkaline Phosphatase

A sensitive, fast, and simple AIE based fluorescence "Turn-on" sensor system has been developed to detect alkaline phosphatase (ALP), a crucial biomarker enzyme present in human blood. The sensing scheme is based on the fluorescence quenching of an AIEgen (BSPTPE)-Protamine (PrS) complex by an anionic quencher, hexametaphosphate (HMP), which also serves as a substrate for ALP. The method registers LOD of 15 $\mu\text{U/ml}$ of ALP in the linear concentration range of 0-40 mU/ml . The sensor exhibits remarkable specificity for ALP. The potential application of the sensing probe in real samples is demonstrated successfully in diluted human serum samples.

Treatment of Fibril-induced Neurodegenerative Disorders in A-mutant Drosophila Model using Ammonium Molybdate

Accumulation of Amyloid- (A) peptides in the brain plays a crucial role in the progression of Alzheimer's disease (AD). In this context, the ability of polyanionic molybdate as an additive to inhibit and degrade protein fibrils both *in vitro* (insulin protein) and *in vivo* (Drosophila fly model) has been validated. For *in vivo* condition, the inhibition and fibril degradation in Type II diabetes-induced fly and A 42-mutant of Drosophila by treating with ammonium molybdate has been established. The disappearance of fibrillar structures and recovery from neurodegenerative disorders in molybdate-treated Drosophila as compared to the untreated A 42-mutant fly, strongly corroborate the therapeutic ability of ammonium molybdate towards the treatment of Alzheimer's disease.

Development of Three-component Red-emissive Excited-state Intramolecular Proton Transfer (ESIPT) - Active Supramolecular Sensor for Biogenic Amines

Detailed time resolved emission spectroscopic studies were carried out for a three-component supramolecular sensor involving a water-soluble, ESIPT-active, red-emissive benzothiazole based probe (BTPICO), cucurbit[7]uril (CB[7]), and citrate-stabilized hydroxyapatite nanoparticles (Hap NPs) for its utility in the rapid and sensitive detection of spermine, spermidine and cadaverine in aqueous media.

Glycothiol functionalized Quartz Crystal Microbalance (QCM) for Lectin Recognition and Bacterial Detection

Indigenously synthesized glycothiol functionalized Quartz Crystal Microbalance (QCM) was used for selective capture of glucose binding lectin Concanavalin A in comparison to peanut Agglutinin (PNA) which is a galactose binding lectin. The functionalized QCM surface was found to be recyclable for over more than 4 cycles.

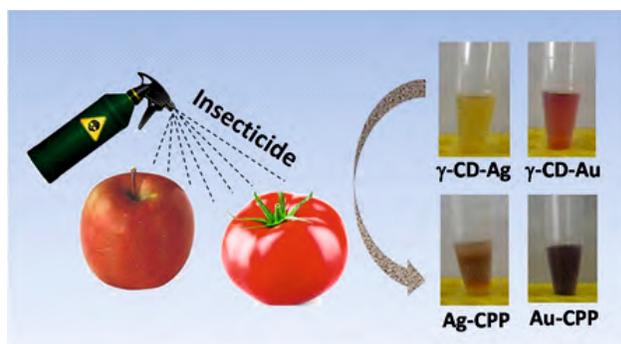
Development of Sensor for Heparin

An unsymmetrical cyanine-based probe molecule, TO-PRO-3, was used for the naked-eye detection of Heparin in aqueous and in complex human blood serum samples. The demonstration of naked eye Heparin sensing is based on a huge blue shift (~115 nm) observed in the absorption maximum, and marks one of the highest reported shift for any Heparin sensing system.

The shift in the absorption spectra has been attributed to the formation of H-aggregate of the dye molecules in the presence of Heparin. In addition, a tetracationic probe, tetrapyrrolium-tetraphenylethylene (TPy-TPE), was identified for sensing of Heparin by fluorescence method.

Silver and Gold Nanoprobes as Colorimetric and Raman Sensor for Detecting Traces of Pesticide "Chlorpyrifos" in Fruits and Vegetables

Studies have been carried out to demonstrate the applicability of silver and gold nanoprobes for the detection of pesticides. A facile one-step green synthetic approach, using γ -cyclodextrin (γ -CD), was employed to synthesize γ -CD-Ag and γ -CD-Au nanoprobes. The noble metal nanoprobes served as a platform for colorimetric and Raman sensing of chlorpyrifos (CPP). The colorimetric changes as well as enhancement in the Raman bands of CPP resulted due to the interaction of the metal particles primarily through the amine and phosphorothioate functional groups of CPP. The applicability of the nanoprobes was tested on apple and tomato. The methodology developed for pesticide detection is simple, fast, cost-effective and highly reproducible.



Colorimetric sensing of pesticide, chlorpyrifos (CPP) in fruits and vegetables

Materials

Document Security Applications

Around 100gm of up-conversion luminescent nanoparticles (taggants) have been prepared and delivered at SPMCIL, Dewas for extensive evaluation. The material has been tested with different types of inks used for currency/document

printing. Based on the experiments carried out, concentration of the nanoparticles in inks has been optimized. Some of the issues such as interference of the nanoparticles with certain colours and bitterness of the ink etc., are addressed. Documents incorporated with near infrared (NIR) based luminescent materials, printed at BNP, Dewas have been received and subjected to extensive characterization. Emission spectra recorded with NIR-PMT as the detector indicated the presence of nanoparticles in all the documents.

Relevant for Na and Li Ion Battery

Research efforts have been made to develop materials for high energy and power density, enhanced safety and low-cost lithium and sodium ion battery (LIB and SIB). Mo_2C nanoparticles dispersed over rGO electrode have been prepared and evaluated for use in SIB. The unique design of $\text{Mo}_2\text{C}/\text{C}/\text{rGO}$ nano sheets exhibits specific capacity of 498 mAh/g at 50 mA/g current density against sodium electrode. To develop stable carbon-based anode for Li-S battery, activated carbon materials derived from coconut shells were explored. The cyclic voltammograms for the samples showed an anodic peak at 2.5 V and cathodic peaks at 2.25 and 2V which were consistent with typical Li-S battery. The capacity after 100 cycles was 327 mAh/g and 522.3 mAh/g for the carbon samples heated at 400°C and 500°C, respectively, which corresponds to a capacity retention of 55% and 59%. The studies indicated that the sample obtained by heating at 500°C has superior as compared to the sample heated at 400°C, which was attributed to larger pore sizes in the former sample.

In order to circumvent the fading problem of $\text{LiNi}_{1-x-y}\text{Co}_x\text{Mn}_y\text{O}_2$ (Li-NCM111) cathode associated with dissolution of transition metal ions in electrolyte, surface coating of this cathode is attempted. A wet chemical method was used to

coat reduced graphene oxide (RGO) and Li_2MoO_4 on the cathodes and the electrochemical performance has been studied. Low electrode degradation (transition metal dissolution) and the fast diffusion of Li-ions/electrons (due to ionic and electronic conducting $\text{RGO@Li}_2\text{MoO}_4$ shell) have been observed.

Synthesis and Characterization of Ti-Codoped $\text{Y}_2\text{Ge}_2\text{O}_7$:Eu Phosphor

Ti-co-doped $\text{Y}_2\text{Ge}_2\text{O}_7$:Eu phosphor was prepared by solid state method using Y_2O_3 , GeO_2 , TiO_2 , Eu_2O_3 as reactants. XRD studies confirmed that Ti co-doped $\text{Y}_2\text{Ge}_2\text{O}_7$:Eu adopts tetragonal structure with space group P4_32_12 . The emission profile of Ti co-doped $\text{Y}_2\text{Ge}_2\text{O}_7$:Eu phosphor is similar to that of $\text{Y}_2\text{Ge}_2\text{O}_7$:Eu phosphor showing characteristic emission maximum at 614nm. The excitation spectra of the sample monitored for 614nm emission showed intense peaks in the soft UV region attributed to direct excitation of Eu^{3+} intra- $4f$ transition and a broad band around 260 nm owing to O-Eu charge transfer. The steady state luminescence results indicate that, Ti co-doping facilitates the direct excitation of Eu^{3+} in $\text{Y}_2\text{Ge}_2\text{O}_7$ by near UV LEDs.

Pd-dithiolate Complexes as Catalyst for Decarboxylative Sonogashira Reaction

The palladium dithiolate complexes $[\text{Pd}_2(\text{xantphos})_2(\text{SC}_{12}\text{H}_8\text{S})_2](\text{OTf})_4$ are used as catalysts for decarboxylative Sonogashira coupling reaction of phenylpropionic acid and 2-butyneic acid with various iodoarenes. Synthetic utility for the reported protocol is explored for the effect of various functional groups on the yield of corresponding heteroaryl alkynes. The current protocol showed excellent catalytic activity towards decarboxylative alkynylation reaction with high turn-over number (TON) up to 10^5 and turn-over frequency (TOF) up to 10^4 h^{-1} . The catalyst could be recycled up to six times without losing its catalytic activity. The *in-situ* generation of PdNPs was observed after the third recycle and the amount was significant after the sixth recycle, which was confirmed and characterized by PXRD, SEM, EDX and HR-TEM. The catalytic activity of the reaction is

attributed to the formation of palladium nanoparticles.

Synthesis of Nano-aggregates for their Application in Invisible Ink

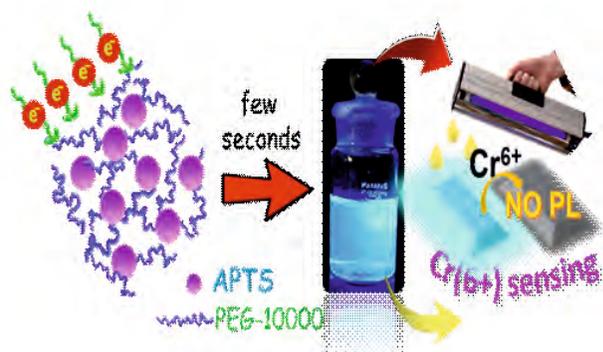
Tetracene and pentacene doped anthracene nanoaggregates are established as good invisible ink. Upon excitation with near UV light (350-390 nm) these nanoparticles provide green and pink emission which are demonstrated by making an ink and incorporation of the same in gel pens. Presence of DABCO molecule provides them better ambient stability from photo oxidation. Samples are observed to be stable for several months and observed to remain nearly unaffected by harsh acidic or basic condition. Synthesis of 10 gm of doped organic nanoaggregates for the application of highly fluorescent and stable invisible ink was completed.

Fluorophore Doped Plastic Scintillator Films

Plastic scintillators are widely used in radiation detection for nuclear applications. For the in-house development of efficient plastic scintillators, polystyrene films were cast on glass substrate from styrene monomer with varying concentration of fluorophores PPO and POPOP. These films were also tested with suitable radiation sources. For a handheld beta detector, a film of 8 cm x 10 cm cast on plastic substrate was found to have efficiency comparable to the imported scintillator.

Sensing of Chromium (VI) using Photoluminescent Polymer Functionalized Organosilicon Nanoparticles (PEG@OSiNPs)

Radiolytically synthesized PEG@OSiNPs shows emission yield of 35%, which quenches significantly in presence of dichromate ion only. Interference studies in the presence of various metal ions further demonstrated exclusive sensing of chromium (VI). Mechanistic investigations revealed the inner filter effect (IFE)-based quenching mechanism. The limit of detection (LOD) was

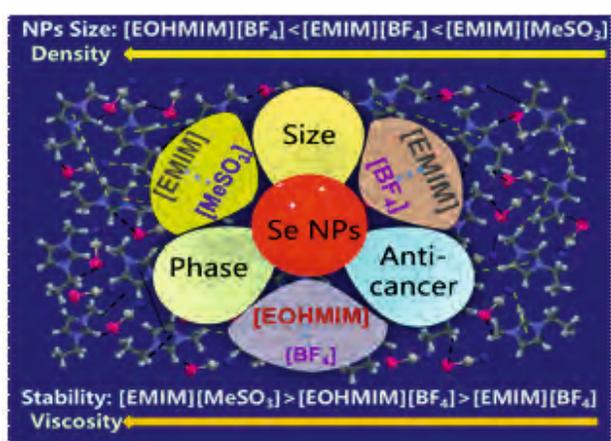


Electron beam induced synthesis of PEG coated silicon oxide nanocomposites for Cr (VI) ion sensing

determined to be $0.74 \mu\text{M}$. The present work using PEGylated silicon oxide nanocomposites for Cr (VI) ion sensing has various advantages such as facileness, low toxicity, bulk production, eco-friendly and time-efficient synthesis. To check the practical applicability of PEG@OSiNPs for Cr (VI) ion sensing in real-time scenarios, a paper kit has been developed. The visual detection limit for Cr (VI) ion using this paper kit was determined to be $\sim 55 \mu\text{M}$.

Electron-beam Assisted Synthesis of Amorphous-Se Nanoparticles in Room Temperature Ionic Liquids (RTILs) with Variable Ionic Moieties

The influence of the nature of cation-anion combination of RTIL on the phase and morphology of Se nanoparticles (NPs) prepared by electron beam irradiation was investigated. The size of Se NPs could be conveniently tuned by varying the cation-anion combination of the RTILs. It was observed that the density (or packing order) of RTILs plays an influential role in regulating the size



Radiolytic synthesis of amorphous Se nanoparticles in RTILs with different cation-anion combinations

of NPs, whereas their stability (against size variations) can be primarily associated with viscosity (of RTILs). In the meantime, with the introduction of -OH group in the cation, an overall improvement in the control over the size of the NPs, their polydispersity and the stabilisation efficiency of the RTIL was observed. The mechanistic studies based on pulse radiolysis revealed that the formation of NPs proceeds through the reaction of imidazolium cation-based transient species with SeO_2 .

Radiolytic Synthesis of Green Photoluminescent Cyclodextrin Passivated Tellurium Oxide Nanocomposites

In a first ever report, green photoluminescent Tellurium oxide nanocomposites (TeO NCs) have been prepared using electron beam irradiation route. The size as well as the photoluminescence properties of cyclodextrin (CD) functionalized TeO NCs could be tuned by varying the absorbed dose. The origin of the PL displayed by $\alpha\text{-CD@TeO}$ NCs has been attributed to the band gap radiative decay. Pulse radiolysis-based mechanistic investigations revealed the solvated electron-driven formation of Te NCs. Evidently, the role of $\alpha\text{-CD}$ is critical in directing the formation of TeO NCs, improving their colloidal stability, photoluminescence, and cellular uptake. The cytotoxicity studies showed a decrease in the proliferation of cells by $\alpha\text{-CD@TeO}$ NCs in both healthy and cancer cell lines, however, it was observed to be higher in the later one. More so, the observed aspect related to the selectively higher uptake of $\alpha\text{-CD@TeO}$ NCs in tumor cells can be utilized to achieve the differential toxicity in tumor versus normal cells.

Development of Sorbent Involving Simultaneous Grafting of Glycidyl Methacrylate on Polypropylene Non-woven Fabric

Glycidyl methacrylate (GMA) is an important intermediate in many chemical reactions to introduce new functional groups. GMA was grafted

on a poly-propylene (PP) non-woven fabric by using ⁶⁰Co gamma irradiation. The grafting yield was found to be ~120% in 1:1 acetone-water solvent system with 25 kGy of total dose having dose rate of 5.9 kGy/h.

discharge guidelines. So far 7 entrepreneurs have signed technology transfer agreements with BARC for building hgSBR based sewage treatment plants in the country. Patent application on “cultivating bio-beads from the microbes” was granted on 08 Nov 2021.

Environmental and Separation Science

Sewage Treatment, Full-scale Hybrid Granular Sequencing Batch Reactor Plant

A 0.15 MLD capacity hgSBR plant was operated without interruption in round-the-clock shift. The plant was fitted with hydro cyclone and disc filter to improve performance. Both the hydrocyclone and disc filters were working as desired and contributing to treatment performance. Various components and equipment of mechanical, electrical and instrumentation have been procured and erected for setting up 1.5 MLD hgSBR plant at Kalpakkam. Additionally, technical knowhow was provided to hgSBR technology licensees for setting up 0.6 and 0.5 MLD plants for BHEL, Trichy and Madurai Municipal Corporation, respectively.

The 0.15 MLD has been in operation for over a year at designed treatment capacity and meeting the

Sensors for Environmental Monitoring

A handheld H₂S sensor with an input voltage of 10V is developed for applications in oil and gas industry. For intrinsically safe operation of the hand held gas sensor electronics, input voltage needs to be brought down to 5 V. For such electronics, op-amps and microprocessor which work at 5 V supply are required. Op-amps for 5 V power supply is identified and the circuit is optimized. Analog circuit for current to voltage convertor of the sensor is also completed.

Nanostructured CeO₂ thin film was developed by Langmuir-Blodgett (LB) technique for highly sensitive and specific detection of NO₂ gas. These nanostructured CeO₂ thin film sensors showed sensitivity to NO₂ gas from 10 ppb to 12 ppm with fast response (2 mins) and recovery (40-50 mins). To get the specificity of the sensor for NO₂ gas,



Control panel & blower room



Control panels



Sewage before and after hgSBR



hgSBR tank



Sewage and treated water sumps, filtration system, drying bed

Parameter	Before	After
COD (mg/l)	450-600	<20
BOD (mg/l)	150-250	<10
TN (mg/l)	13-30	<5
TP (mg/l)	4-6	<2
TSS (mg/l)	150-200	<10
FC(/100ml)	10 ⁶	<200
pH	7-8.5	7-8.5

Quality of sewage before and after hgSBR

The components of 0.15 KLD hgSBR sewage treatment plant treating sewage from 320 houses at Kalpakkam, Tamilnadu and sewage treatment

several interfering gases were injected and it is observed that there is hardly any response with the same concentration of other gases suggesting a highly selective and sensitive NO₂ sensor.

Spray Coated NiO Nanoparticles for NO₂ Gas Sensing

In continuation to earlier work, thin films of Co doped (0, 2, 5, 10 and 20 at%) NiO nanoparticles were prepared by spray coating at room temperature on glass substrates using syringe pump. Deposition parameters were optimized to get uniform, homogeneous films. Gas sensors were fabricated by thermal evaporation of gold interdigitated electrodes. Spray coated films exhibited good reproducibility compared to drop-cast films. While all the sensors showed good sensitivity and high selectivity for NO₂ at 200°C, undoped NiO samples exhibited the highest sensitivity (six times conductance change for 10 ppm NO₂).

Synthesis of CuInSe₂ QDs using Diphenyl Phosphine with Application in Quantum dot Sensitised Solar Cell

CuInSe₂ affords extension of optical absorption towards NIR as compared to CdSe, thus leading to a better power conversion efficiency (PCE). CuInSe₂ quantum dots (QD) capped with diphenyl phosphine were prepared and they optimized the ligand exchange with MPA (mercaptopropionic acid) for sensitisation of mesoporous TiO₂ films. I-V measurements of copper indium selenide (CIS) solar cell module gave ~4% PCE.

Radiation Grafted Acrylic Acid on Polyurethane Foam for Toxic Metal Removal

Acrylic acid grafted polyurethane foam (PUF) was prepared by gamma irradiation and characterized by FTIR and TGA-DSC techniques. Grafted PUF showed sorption capacity of ~45 mg g⁻¹ and 200 mg g⁻¹ for Co and Pb respectively, which are significantly higher compared to the natural granular activated carbon (GAC).

Development of Thiol Functionalized Silica Microsphere Loaded Polymeric Hydrogel for Removal of Lead and Cadmium

The Current study presents a facile synthesis method for thiol functionalized silica microsphere loaded polymeric hydrogel. Silica microspheres were synthesised as core shell particles by sol-gel method followed by hydrolysis and condensation reaction to form the silica core. The silica was functionalised with thiol and the functionalized silica microsphere was subsequently impregnated into polymeric alginate matrix to form thiol functionalised silica microspheres loaded alginate hydrogel beads (SH-SiO₂MS-Ca-Alg). The developed components and final products were characterized by BET, FTIR, DLS and SEM-EDS. The developed SH-SiO₂MS-Ca-Alg hydrogel beads were used to remove lead and cadmium efficiently [72-97% for Pb; 60-85% for Cd at concentration range of 0.1-100 µg mL⁻¹ and optimum pH of 5-7] from aquatic medium. The sorption capacities evaluated for lead and cadmium from Langmuir isotherm were 127.99 and 70.68 mgg⁻¹ respectively. Uptake kinetics, isotherm, thermodynamics and intraparticle diffusion studies were carried out for both Pb (II) and Cd (II). Mechanism of Pb (II) and Cd (II) removal by SH-SiO₂MS-Ca-Alg hydrogel hybrid beads was proposed with the help of zeta potentials of SH-SiO₂MS at different pH along with fraction diagram of Pb and Cd.

Development of Covellite Based Arsenic Remediation Technology for Point of use Application and its Field Trials for Deployment

A covellite based adsorbent, christened 'Arsenil', was developed for the remediation of arsenic from contaminated groundwater. 25g arsenil remediates 25L water contaminated with 200 ppb arsenic in less than two hours, to WHO recommended level. In addition, the arsenil based arsenic remediation technology provides a complete and sustainable solution to waste (sludge) management wherein arsenic initially present in water is converted into a solid. It effectively eliminates any possibility of its re-entry

into water cycle and the treated arsenic powder is no longer an environmental hazard. The remediation technology is eminently suitable for household and point-of-use applications.

Visual Detection of Arsenic in Groundwater

A simple visual colorimetric method based on arsenomolybdic acid-crystal violet ion-associate pair formation was developed for the detection of arsenic at about 10, 25 and 50 ug/L levels in groundwater. The pair exhibits arsenic concentration dependent colouration. The reliability of the method is ~ 90%. The high sensitivity is achieved by the pre-concentration of arsenic on covellite (CuS). The use of benign and easily available chemicals, the absence of any hazardous by-product, undiminished applicability in sunlight and rapidity are the major advantages of the method. The method is potentially well-suited for the on-site testing of ground-water potability, under different regulations.

Development of Methods based on Single Molecule Spectroscopy for Actinide Biochemistry

In order to record single molecule dipole orientation and position imaging on cellular membrane, an objective type total internal reflection fluorescence microscopy for homogeneous sample excitation was developed. Fluorescence images were recorded with array detectors after necessary optical corrections for best possible resolution under diffraction limited condition. Attempts were made to image activated PE-labelled transferring receptors in lymphocytes with regular confocal fluorescence microscopy. After careful alignment and optimization of the setup, patterned images characteristic of the dipole orientation in the sample plane with respect to TIRF excitation under de-focused condition, were obtained. With focused imaging, a localization precision of 1.7 nm of individual bright spots was achieved through 2D Gaussian fit.

Atmospheric Degradation of Fluoroalkanes at Room Temperature: Reaction with OH Radical

Fluoroalkanes, an important class of VOCs, are released into the atmosphere due to their wide variety of uses. The rate coefficient for the reactions of fluoropentane and fluoroheptane with hydroxyl radical was determined at 298K using relative rate method. Pentane was used as reference molecule and the measured rate coefficients for fluoropentane and fluoroheptane were found to be as $(3.4 \pm 0.5) 10^{-12}$ and $(4.5 \pm 0.4) 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, respectively. The measurements suggest a long tropospheric lifetime of these VOCs, and hence their harmful effect on the environment.

Anomalous Hydration Dynamics in DMSO-Water Mixtures

Hydration dynamics of DMSO-water mixtures have been investigated at a number of intermediate compositions with varying mole fraction of DMSO (or D_2O) with 2DIR spectroscopy along with FTIR and time-resolved anisotropy measurements. While FTIR and anisotropy measurements show anomalous slow dynamics (spectral diffusion and reorientational relaxation) at DMSO mole fraction (X_D) of ~0.4, the spectral diffusion study, using 2DIR spectroscopy, revealed another anomalous region at $X_D \sim 0.2$, in addition to $X_D \sim 0.4$, which is responsible for the alteration of the activity of biomolecules in water-DMSO mixture. This slowdown of the water dynamics at such intermediate composition is attributed to the various DMSO-water structures formed via H-bonding which severely impedes the H-bond breaking and making pathways that exist for bulk water.

Kinetics of Reactions of 1,3-Dioxolane and Vinylchloroacetate with Cl Atom and O_3 : Relevance to Atmospheric Chemistry

1,3-dioxolane and vinylchloroacetate are volatile organic compounds, which escape into the atmosphere. To understand its degradation, its rate coefficient with the atmospheric oxidant Cl atoms was measured at 298 K and found to be

$(1.89 \pm 0.65) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The high value of the reaction rate coefficient implies that Cl atoms efficiently degrade 1,3-dioxolane. The rate constant for the reaction of Cl atoms with 1,3-dioxolane was determined at 298K using relative rate method, with cyclohexane as reference, and nitrogen as buffer gas. The value was found to be $(7.11 \pm 0.72) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. Similarly, the rate constant for the reaction of Cl atoms with vinylchloroacetate was determined at 298K to be $(3.2 \pm 0.4) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The rate coefficients for the reaction of VOC, vinyl chloroacetate, with an atmospheric oxidant O_3 were measured employing butene as a reference molecule. GC and GC-MS were used to measure the concentration of the VOC and identify the products. The tropospheric lifetime of the VOC was estimated. Results suggest this VOC is not very harmful to atmosphere.

Development of Multi Dimensional Spectroscopic Methodology: Investigation of Diffusion of Confined Water Molecules in Near Equilibrium Condition

The dynamics of confined water in a supramolecular host molecule, sulfobutylether-cyclodextrin (SBE-CD) has been investigated by ultrafast 2DIR spectroscopy, using 1-azido adamantane as the vibrational probe. The high affinity of the adamantane group for the cyclodextrin cavity places the probe into the cyclodextrin cavity which provides us an opportunity to probe the water molecules using the azido group present near the cyclodextrin cavity. The temporal dynamics of water molecules in the cyclodextrin nanocavity have been extracted using frequency-frequency correlation function from 2DIR measurements. Our results show a very slow dynamics of the water molecules around the azido adamantane probe in the probed time window, as compared to the bulk water.

Studies on Singlet Fission Process in Organic Nanoaggregates

Role of solvent temperature and polarity of

solubilizing organic solvents on controlling the size of nanoaggregates of singlet fission materials have been explored in detail. Nanoaggregate of 9,10-bis(phenylethynyl) anthracene (BPEA) prepared from DMSO yields small size distribution (average diameter: 100 -150 nm) while same prepared from THF solvents leads to larger sized particles (average diameter: 300-500 nm). Ultrafast transient absorption studies revealed that while both sized particles undergo ultrafast singlet fission to TT pair state in $\sim 1.5 - 2.0$ ps, the smaller particle leads to incomplete separation of the TT pair state to free triplet state. On the other hand, larger particles give free triplets with higher yield. Nanosecond flash photolysis experiments corroborate ultrafast dynamics showing size dependent yield of long lived free triplet state.

Vibrational Sum Frequency Generation (VSFG) Studies of Hydrophobic Molecules at Air-water Interface

The addition $(\text{UO}_2)(\text{NO}_3)_2$ to TBP solution does not change the VSFG spectra for the C-H vibrational modes of TBP suggesting that either the complexation of TBP with UO_2^{2+} ions does not alter the alkyl chains of the TBP molecule or that the complexation itself does not occur at the interface, but in the organic phase.

VSFG study shows that a centrosymmetric crown ether, di-benzo-18-crown ether, adopts a non centrosymmetric conformation on the air-water interface. Detailed analysis showed that there is an increase in the ordered alignment of water molecules by virtue of being stabilized in the ring cavity of the crown ether due to hydrogen-bonding interactions.

Bio-fouling Studies

Biological Waste-water Treatment

Bacterial strains capable of growing in the presence of toxic metalloids were isolated and identified and bacteria-laden granules were size-fractionated. Sulphidogenic activity of bacteria-laden granules was determined by incubating with sulphate in fed-

batch mode for 4 cycles under anaerobic conditions. After observing stable sulphidogenic activity, the experiment was continued under light condition for enrichment of green sulphur bacteria which is capable of sulphide oxidation. Experimental work was initiated on evaluating removal of toxic pollutants (Cr(VI) and antibiotics) by bacteria-laden granules. Lab-scale sequencing batch reactors were operated under different conditions for cultivating algal-bacterial granules for biological treatment of normal and saline wastewaters (without usage of seed sludge)..

Power Plant Biofouling and Microbial Biofilms Assessment and Control

Barnacles are the major macro-fouling organisms in the seawater cooling systems of nuclear power plants. For molecular understanding of biofilm formation potential, whole-genome sequencing data of *Amphibalanus reticulatus* was analyzed to identify functional genes responsible for fouling process. A total of 102 morphologically distinct bacterial strains were isolated from the coupons immersed in the seawater cooling system of MAPS and screened. Based on biofilm forming ability, 10 strains were short-listed for biofilm-barnacle larval interactions study. The antibiotic-susceptibility of biofilms for modulation of extracellular polymeric substances (EPS) content was determined in *Staphylococcus aureus* strains (V329, SA7, SA10, SA33 and M556) by growing biofilms at different glucose concentrations. Biofilms of V329 and SA7 strains had higher EPS production and exhibited higher tolerance to antibiotics (kanamycin, ampicillin and tetracycline).

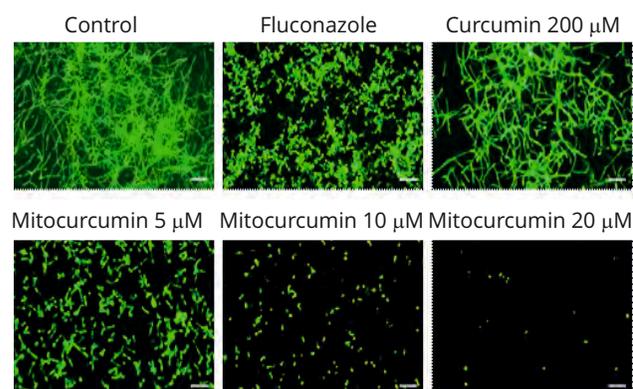
Imidazolium Ionic Liquids for Biofilm Control and Disinfection of Environmental Surfaces

Imidazolium ionic liquids were investigated for developing potential antimicrobial formulations for biofilm prevention. The imidazolium ionic liquids containing dodecyl to hexadecyl alkyl group on cation, effectively prevented biofilm formation in natural freshwater and seawater used in the tertiary cooling water system (CWS) of power

plants. Short term experiments (12 days) revealed that imidazolium ionic liquid with hexadecyl alkyl group can prevent biofilm formation in natural waters under re-circulating dynamic conditions. Apart from preventing biofilm formation in natural waters, the potent ionic liquid was evaluated for applications in disinfection of environmental surfaces. The chosen antimicrobial ionic liquid and its formulation prepared in ethanol were found to be suitable for disinfection of environmental surfaces such as wood, steel and glass. The effective killing and removal of bacteria from surfaces shows potential use in sanitizers. The results indicated that ionic liquids are promising for effective antimicrobial formulations.

Curcumin Compounds for Biofilm Control

The transition from yeast to hyphal growth is crucial in biofilm formation and virulence of *Candida albicans*. The activity of curcumin compounds on yeast to hyphal transition was studied at sub-MIC concentrations. In the presence of curcumin derivative, hyphal growth in *C. albicans* was strongly inhibited. Time-kill kinetics of *Candida albicans* cells by curcumin compounds was determined to establish the contact time required for complete killing. Cells were challenged with curcumin, curcumin derivative and fluconazole. Samples were drawn at regular time intervals and plated for viability assessment. Curcumin had not shown any killing activity. Fluconazole exhibited fungistatic effect but not killing. Curcumin derivative showed rapid killing activity on *C. albicans* cells. Complete killing was achieved by 9 and 6 h, respectively, with MIC and 5X MIC values.



Prevention of *Candida albicans* biofilms by curcumin compounds

Advanced Studies

Development of Theoretical Formalisms

Development and implementation of various important property modules for calculating some new properties of atomic and molecular systems more accurately has been undertaken in the DIRAC program package. The ground state molecular frame dipole moments of alkaline earth metal monofluorides and Group II-B-monohydrides have been computed using the Z-vector technique and the linear expectation value method within the four-component relativistic coupled cluster singles and doubles framework. In addition, by combining the Feshbach projection operator (FPO) formalism and the real-valued continuum remover potential, a novel technique is developed for computing the negative ion resonance energy and its decay width. Based on this method, a new molecular association mechanism has been predicted for unbounded systems at ambient light intensities.

Thermal Properties of UO_2 in U(V) State with Lanthanide Fission Products

Phonon spectrum is calculated for different Ln doped UO_2 lattice. Both harmonic and quasi-harmonic approximation is employed to calculate thermal expansion coefficients and specific heat capacity. The presence of Ln fission products introduces changes in phonon spectrum of pure UO_2 . Therefore, thermal expansion coefficients and specific heat capacity of Ln doped UO_2 show deviation from undoped UO_2 .

Mechanical Properties of U and U-Zr Alloy Fuel

Metallic fuels such as U-Zr alloy are considered for fast breeder reactors due to high thermal conductivity, low breeding time, and enhanced fissile atom density compared to ceramic fuels. However, the interaction of lanthanide fission products (FPs) with the fuel and cladding material is the main concern for fuel performance. This can cause degradation of mechanical properties

leading to cracks in the fuel rods. For the safe operation of nuclear reactors, the interaction of lanthanide fission products with cladding material should be restricted. For this purpose, first the α -uranium lattice is optimised and the mechanical properties were calculated. Then, U-Zr alloy structure is generated by substituting 10% of the uranium atoms in the lattice by zirconium atoms. This structure is optimized and mechanical properties like bulk modulus, Young's modulus and shear modulus are evaluated.

Computational High-throughput Screening of Metal Organic Framework (MOF) Materials for Xe/Kr Separation

Separation and storage of radioactive inert gases, Xe and Kr generated from the spent nuclear fuel reprocessing is one of the challenging issues. Metal organic framework (MOF) materials are shown to be promising candidates for gas separation and storage because of their tunable porosity and surface area. Computational high-throughput screening is carried out to identify the top performing MOFs for selective adsorption of Xe from Xe/Kr mixture. Adsorption of Xe/Kr gas mixture at 1 bar pressure and 298 K has been simulated using the grand canonical Monte Carlo (GCMC) simulations to check the Xe/Kr selectivity and loading capacity. Finally, 10 MOFs are found to have a Xe/Kr selectivity factor of greater than 50 and loading capacity of more than 2.0 mol/kg, which can be further considered for experimental validation.

Electronic Structure Investigation of TLD-100 ((Mg-Ti)-doped LiF)

Using Density Functional Theory, the defect structures of LiF in the presence of Mg and Ti has been investigated, which has been extensively studied by various experimental groups worldwide. The present study explored the crucial role of each dopant element, as well as lattice vacancy defects and successfully explained the origin of observed optical spectrum of Mg, Ti-doped LiF, which is commercially known as TLD-

100. This study paves the ways to design novel materials for radiation dosimetric applications.

Mo₂C as Electrode Material for Na-battery: A DFT Exploration

The potential of utilizing Mo₂C as anode material for Na rechargeable batteries was explored theoretically. It was concluded that the presence of sodium causes modification in the local geometrical environment of Mo₂C unit cell, especially at higher Na concentration (25%) i.e. significant volume expansion (~20%) takes place. The electronic properties of Mo₂C with and without the presence of sodium atom significantly differs indicating strong chemical interaction between them. Strong chemical interaction may lead to enhancement in stability thus aiding in storing more potential energy in the Mo₂C host, but at the same time may slow down the sodium movement

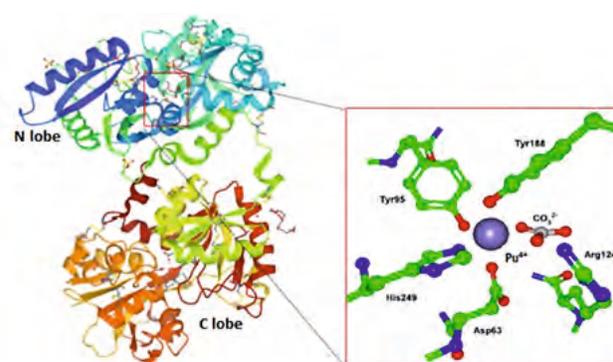
Electronic Relaxation of Photoexcited Open and Closed Shell Adsorbates on Semiconductors: Ag and Ag₂ on TiO₂

This work provides an insight into the dynamics and magnitude of relaxation rates for a surface with adsorbed open- and closed-shell Ag species, to determine whether the advantages in using them to enhance light absorbance remain valid in the presence of charge density relaxation. Different behavior can be expected depending on whether the adsorbate particles (Ag metal clusters in our present choice) have electronic open-shell or closed-shell structures. Calculated electron and hole lifetimes are given for pure TiO₂(110), Ag/TiO₂(110), and Ag₂/TiO₂(110). The present results, while limited to chosen structures and photon wavelengths, show that relaxation rates are noticeably different for electrons and holes, but comparable in magnitude for pure and adsorbate surfaces. Overall, the introduction of the adsorbates does not lead to rapid loss of charge carriers, while they show large increases in light absorption. This appears to be advantageous for applications to photocatalysis.

Proposing and Designing Suitable Synergistic Anion at the Binding Site of Serum Transferrin (sTf)

The binding of sTf with Fe and Pu is influenced by the presence of synergistic anion e.g. citrate anion. Till now, the force field parameters for citrate and non-standard residues of sTf are developed by employing electron polarizability. All Atom Molecular Dynamics (MD) simulations for all the two conformations i.e. Fe₂-sTf, and Pu₂-sTf with CO₃²⁻ as synergistic anion are carried out at pH 7.4. Equilibrium MD simulations were performed on each of these for 500ns. Average separation between two sub-domains of N and C lobes of the protein indicates that two lobes although structurally similar, behave differently with Pu(IV) at the binding site. Fe₂-sTf shows a closed conformation, whereas Pu₂-sTf exhibits a more open conformation.

Several extractants are known for the separation of minor actinides from lanthanides. Lanmodulins (LNs) are biomolecules that are known to be highly selective for lanthanide ions up to pico-molar concentrations. Multi-scale simulations were carried out to understand the binding and selective extraction of actinides through lanthanide binding tags (LBTs). Our calculations provide detailed insights such as solvation dynamics which can offer solutions and opportunities in bio-speciation of actinides.



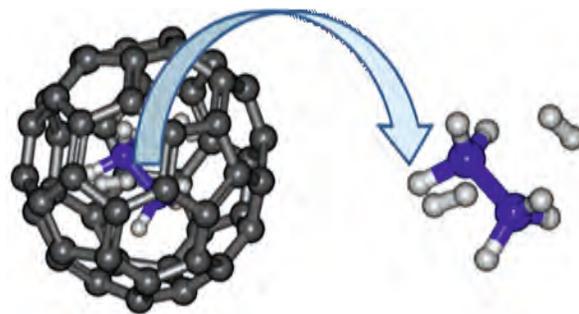
Plutonium binding site at serum transferrin

New Catalysts for CO₂ Reduction

Small molecule activation, in particular CO₂ reduction, is an important active research. Dioxygen binding to picket fence porphyrins (PFP) are considered as excellent bio-mimic to haemoglobin. PFP can be used to activate and reduce CO₂ through electronic structure calculations. The pendant amide arms of PFP anchor the CO₂ through hydrogen bonding. Decorating the Fe-catalyst with electron-withdrawing groups can shift the redox potential by more than 0.7V. This is unprecedented and is the most likely candidate for CO₂ activation. Calculations were also done to design a novel ligand for efficient CO₂ reduction. Studies on Ni-Cyclam ligands encapsulated in cucurbiturils indicate that redox active molecular orbitals are lowered, indicating the superior performance of the catalyst towards CO₂ reduction primarily due to favorable host-guest complexation.

Nanoconfinement as a Catalyst for the Formation of Ammonia and Nitrogen Hydrides

Nitrogen reduction is always a captivating topic among researchers due to its wide applications in the fertilizer industry and this process is, in general, achieved using the well-known Haber-Bosch method using iron as catalyst at 500°C temperature and 150–200 atmospheric pressure. Based on the density functional theory, a confined space in a nano-regime can stimulate the nitrogen reduction process leading to the formation of ammonia in the present of hydrogen without any catalysts. This unprecedented synthesis of ammonia or its intermediates in the absence of catalyst or energy-input in fullerenes is demonstrated for the first time to the best of our knowledge. The driving force for facilitating ammonia synthesis in fullerene-induced-confinement has been attributed to internal pressure effect. These results can have several implications in understanding various chemical processes in nanospace and it also strongly suggests that a suitable cavity size in the nano-regime is one of the essential parameters for such chemical reactions.



Formation of nitrogen hydrides under confinement in C60

Quantum Chemical Modeling of Unprecedented Photothermal Effects Observed in Water-filled Carbon Nanotubes

Carbon nanotubes can be ignited and reconstructed upon the exposure of the light from a normal camera photo-flash. During this experiment, the temperature of the system is estimated to be more than 1500°C which causes an unprecedented photothermal effect, leading to the generation of hydrogen molecules along with methane, CO₂, etc. In this work, an attempt was made to model this phenomenon using electronic structure theory based methods, by considering carbon nanocages and water molecules. These results reveal that confining few water molecules only leads to the hydrogen bonded water cluster inside the nanocage. Increasing the number of water molecules leads into opening of nanocage as well as destruction of carbon network structure. However, generation of hydrogen molecules is observed to be a rather difficult task which substantially relies on the concentration of water molecules present inside the nanocage.

Preparation of in-house Matrix Matched Hydrogen Reference Material

In order to prepare in-house matrix matched hydrogen reference material with hydrogen concentration of 100 ppm, inter laboratory exercises have been carried out using two different determination techniques. A Sample size of around eighty milligrams was cut from 9 different strips of Zircaloy – 2.5%Nb strips having uniform formation of zirconium hydride for estimation of hydrogen content. Analysis of more than 50 hydrogen

charged Zircaloy – 2.5%Nb samples were performed in five labs in BARC, using three different analytical techniques; IGF, DSC and HVEMS. Based on the measurements and statistical analysis, the hydrogen content was found to be 97 ppm ± 13ppm (1σ).

Isotopic Analysis of Lithium in Materials

A carbon beam induced gamma ray emission (CIGE) methodology beam was developed for the determination of the isotopic ratio of Li in materials. The method utilizes ${}^7\text{Li}({}^{12}\text{C},){}^{15}\text{N}$ (E = 5.25 MeV) and ${}^6\text{Li}({}^{12}\text{C},){}^{14}\text{N}$ (E = 2.33 MeV) reactions for the analysis. The method is unique and has been validated by analyzing lithium carbonate samples of several different Li isotopic composition. It provides measurements with about 10% uncertainty and has been employed for analyzing spodumene samples.

Analytical Services

High impact and specialized analytical services were rendered to DAE institutes and different research centres and industries across the country. Some important samples analysed include Ta, Co-W alloys, quartz powders, ferrocene, lead

lithium alloys, KKNPP Turbine oil, electrode materials, Al structural material, borated wood shielding, SS reactor material, carbon fibers, radiopharmaceuticals etc.

Determination of Carbon and Phosphorous in Material Surfaces with PIGE

An alpha particle induced-ray emission technique (AIGE) based on ${}^{12}\text{C}(\alpha,\gamma){}^{16}\text{O}$ nuclear reaction was developed to non-destructively determine carbon in steel. The method was validated by performing measurements on steel CRMs (e.g. steel 8J, 361 etc.). The method was applied for the analysis of a silicon-uranium alloy containing 800 ppm carbon.

Determination of Phosphorous and Lithium Isotopic Ratio in Materials by PIGE

The experiments aimed at developing a method for determining phosphorous using ${}^{31}\text{P}(p,p'\gamma){}^{31}\text{P}$ reaction with InP crystals serving as targets/standards were completed. Experiments have been initiated for the determination of the isotopic ratio of ${}^6\text{Li}$ and ${}^7\text{Li}$ in materials using proton and α -induced γ -ray emission spectroscopy.



Typical samples analyzed in BARC during 2021 (Hot spring gas, KKNPP Turbine oil, Electrode materials, Al structural material, Borated wood shielding, SS reactor material, Carbon fibers, Solution for radiopharmaceuticals)

${}^6\text{Li}(p,\gamma){}^7\text{Be}$, ${}^7\text{Li}(p,p\gamma){}^7\text{Li}$, ${}^6\text{Li}(\alpha,\gamma){}^{10}\text{B}$ and ${}^7\text{Li}(\alpha,\alpha\gamma){}^7\text{Li}$ are being utilized for this purpose while lithium carbonate powders containing natural and enriched (28 and 54%) ${}^6\text{Li}$ are used as reference targets.

Materials Science

Study of Structural and Energetic Properties of Actinides Doped BaZrO_3

The metallic wastes generated during nuclear reactor operation, including clads, wrappers, pressure tubes constitute high level nuclear wastes, which are immobilized by following a properly delineated process scheme. The alloy melting route using stainless steel (SS) and Zr alloys -- SS-15 wt% Zr, Zr-8 wt% SS and Zr-16 wt% SS was found to be a promising approach for immobilizing the metallic wastes.

Metallic wastes predominantly contain metallic fission products and oxide fission products. The oxide fission products present in the waste form a slag during the melting of the wastes by virtue of higher melting point than the metallic elements. Perovskite BaZrO_3 can be used as wasteform for this slag. Further, perovskite materials are also an important component of SYNROC material, which is a promising

alternative to glass for immobilization of high level nuclear wastes. The structural and energetic properties of BaZrO_3 in presence of actinides (Acs), including Th, Pa, U, Np, Pu and Am were studied by using the Density Functional Theory as implemented in the Vienna Ab-initio Simulation Package (VASP).

The solution energy of the actinides at Ba and Zr sites in BaZrO_3 phase were studied, which suggested that actinides, except Am, show preference to occupy the Zr site of the phase while Am prefers to occupy the Ba site. Further, the solution energies of the actinides at Ba and Zr sites in the BaZrO_3 phase suggest that their incorporation in BaZrO_3 is endothermic in nature. A very small change occurring in the structural properties on incorporation of actinides coupled with small positive solution energy suggest that the compound can be a promising waste material under the oxide fission products. Further, the study of elastic, defect and radiation properties of BaZrO_3 in presence of actinides is required to evaluate the performance of BaZrO_3 compound as a host material for oxide fission products.

Silicon Carbide Fibre through Processing of Polycarbosilane Polymer Precursor

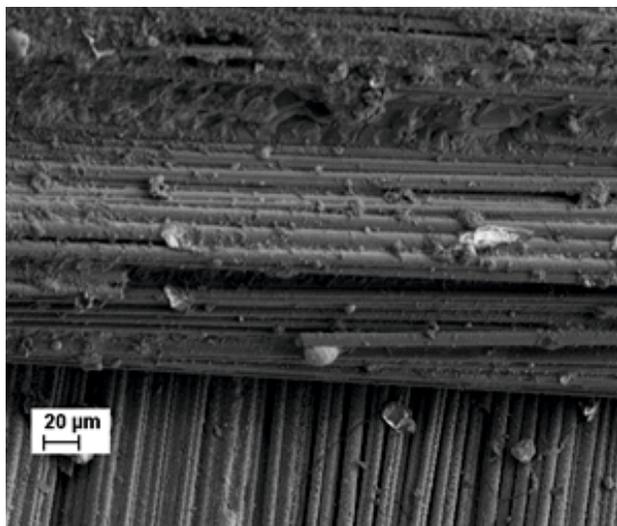
Solid Polycarbosilane (PCS) was extruded to fiber by spinning the molten PCS under nitrogen pressure through a single hole spinneret of melt spinning unit. A continuous fiber of about 5 m length was obtained without any surface defect. Fiber of different diametric configurations was produced by varying the diameter of the spinneret orifice, nitrogen pressure, winding speed and melt viscosity. It was subsequently cured by heating the fiber slowly in a flow of dry air in an oven at a temperature of 200°C . Heat treatment of cured fiber at 125°C for 30 minutes converted it into black lustrous SiC fiber.

Silicon Carbide Ceramics

Porous silicon carbide (SiC) can be used as hot gas or molten metal filter to assist the catalyst in



Melt-spun (green) fiber



Micrographs of reaction-bonded SiC fiber matrix composite

corrosive environment. In BARC, porous SiC was prepared by infiltrating molten silicon into carbon body, which was prepared by compacting the carbon soot. Depending on the initial compaction pressure, a sample was generated with varying amount of porosity (10-15%). The in situ reaction of Si with C was also exploited to generate porous SiC body with higher amount of porosity i.e. up to 40%. In-house made SiC fiber mat was successfully converted to SiC-SiC composite through Reaction Bonding technique.

Silicon carbide (SiC) based fibre matrix composites are among the proposed accident tolerant fuel tube candidate material in light water reactors post Fukushima scenario, owing to their high temperature strength, irradiation resistance, and reduced oxidation in comparison to Zircaloy. Incorporation of SiC fiber in the matrix helps to overcome low fracture toughness in SiC. Densification studies of SiC and SiC fiber reinforced composite has been carried out by Spark Plasma Sintering method.

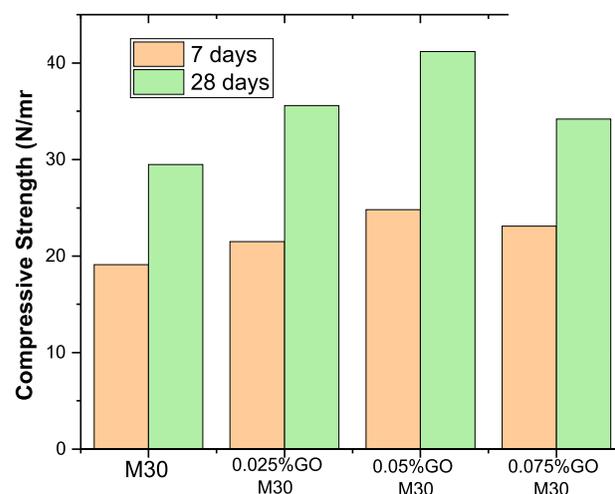
Transient liquid phase assisted densification of SiC particulate along with SiC fibre was carried out by using yttria, and alumina as a sintering aid by Spark Plasma Sintering technique at a temperature of 1900°C, 40 MPa pressure for a duration of 5 min. The in-house developed SiC fiber has fiber loading of 33% and the sintered sample had a density of ~2.88 (~90%).

Development of High Compressive Strength Graphene Oxide-concrete Composite

Cement composites (popularly known as concretes) are widely used in construction activities. Although several high-performance concrete materials are in vogue worldwide, their utility is constrained mainly due to their highly brittle nature. Calcium-silicate-hydrate (C-S-H) gels, the principal hydration products, are made up of nanocrystalline regions with the atomic structure resembling tobermorite and/or jennite.

Use of nanomaterials and nano-technology during the production of cements may lead to modification in structure of these materials at the nano-scale thereby improving their macro-properties.

Two mechanisms, namely seeding effects and filling effects have been summarized in the literature for enhancing the mechanical strength of cement composites by adding nano-materials to it. Firstly, the large specific surface area of the nano-materials can provide nucleation sites for hydration products. Secondly, the nano-materials can fill the pores within cement matrix to provide a compact microstructure.



Compressive strength of concrete without GO and GO-Concrete at 0.025, 0.050, 0.075 weight% GO, respectively.

From various nano-materials considered for this purpose, graphene oxide (GO) has shown tremendous potential as it can be produced in a cost effective manner and also the agglomeration (typical problem confronting the nano-materials) can be controlled by manipulating the functional groups attached to it.

GO was produced in-house by modified Hummers Method. The GO powder at different weight percentage (0.025, 0.050, 0.075) was mixed with concrete mixture (as per M30 composition) and standard blocks (150 x 150 x 150 mm) were cast. The compressive strength was checked after 7 days and 28 days of curing. Maximum improvement was seen with addition of 0.05 wt% GO resulting in a 40% increase in compressive strength over the normal M30 concrete. Fine cracks with few branches instead of a clean crack had been observed in the test samples of GO-concrete composites, implying that GO can delay the propagation of cracks by densifying the microstructure. Also the workability of the concrete, which was measured with the standard cone-slump test, improved with the addition of GO to it.

Development of Metallic W-coating for Tritium Permeation Barrier

Thick pore-free metallic tungsten coating is suitable for hydrogen and its isotopes as a permeation barrier in storage vessel as well as in first wall of fusion reactor applications. A suitable electrolyte comprising eutectic composition of tungsten trioxide and sodium tungstate was chosen to obtain metallic tungsten coating by molten salt electrolysis at 925°C. Electrolysis (Direct current as well as Pulse current) was carried out and the process parameters were established for depositing metallic bright, non-porous, adherent and uniform thickness coating on W in the current density range of 30 to 60 mA.cm⁻². The deposited W coating was characterized for its crystal structure, thickness uniformity, composition and top surface morphology. Further experiments are underway to investigate bond-strength, microstructural investigation and the capability to deposit thick W coating.

Fluorite - A Potential 'Accidental Dosimeter' Material

Natural CaF₂ is a potential thermo-luminescent material by virtue of its high ultraviolet transparency, linear response for a wide dose range and high luminescence sensitivity to gamma radiation. These inherent features make natural CaF₂ an attractive candidate for use in the accidental dosimetry. The effect of irradiation on the point defect formation and phase stability in CaF₂ is an important area of study.

A quantitative description of the cationic and anionic sub-lattice defects in natural fluorites in response to the long term self-irradiation and subsequent structural recovery as well as ex-situ electron irradiation was studied. For this purpose, naturally occurring fluorites having different colours (colourless, yellow, blue, purple, black and sea-green) were obtained from AmbaDongar in western part of India. Incidentally, the AmbaDongar Fluorite has been used earlier as an environmental dosimeter and hence it was selected for further studies for accidental dosimetric applications.

Detailed spectroscopic investigations done using X-ray photoelectron spectroscopy (XPS), Raman spectroscopy and Photoluminescence (PL) established that the yellow fluorites comprising the highest rare earth concentration have O₃ and O²⁻ vacancy type defect complexes contribute to its characteristic yellow colour. The green colour in sea green fluorite was attributed to presence of bivalent cationic dopants and F centres. These complementary techniques confirm the presence of metallic Ca colloids in blue, purple and black fluorites, which establish the fact that the fluorites had been subjected to radiation damage during the mineralization.

From XPS analyses of the metallic Ca content, it was concluded that the black and purple coloured CaF₂ were exposed to highest dose of self-irradiation from the associated pyrochlore whereas the yellow coloured CaF₂ to a minimum radiation. Even after

long term radiation exposure and elemental substitutions, the fluorite retained its crystal structure stability indicating its suitability in the aforementioned applications. Based on the observations, a suitable mechanism for defect production by radiation is proposed which suggests that the formation of metallic Ca colloids is due to knocking out of fluorine ions from their lattice sites. The confinement of the radiation damage only to the anionic sub-lattice was explained in terms of the higher displacement cross section for fluorine in comparison to Ca, and also requirement of lower energy to create fluorine displacements and vacancies.

Upon irradiation with 10 MeV electron beam under 5-10 MGy dose (carried out at EBC, Kharghar), natural and synthetic fluorites developed dark purple colour irrespective of their initial colour. Further investigations using spectroscopic techniques to map the dose-defect structure relationship are underway.

High Temperature Water Retention within Natural Serpentine

Serpentine rocks with different color indices were collected from different parts of India, including in Ukhrul and Kawatha areas of Manipur, Tummalapalle of Andhra Pradesh, Balasore in Orissa, Kudada in East Singhbhum, Tidding suture zone in Arunachal Pradesh, Rishabdev lineament of Rajasthan and Amgaongnessic complex of Maharashtra. It was noted that antigorite and lizardite are the dominant phases with some pyroxenes, olivines and iron oxides present within the rock. Representative samples were examined under optical microscopic, electron microscopic and spectroscopic techniques for identification of various serpentine phases such as lizardite, antigorite and chrysotile, and their mode of occurrences. Bulk compositional analyses were carried out using Energy and Wave-length Dispersive Spectrometers. Detailed mineral chemical analyses, including thermal analyses confirmed the presence of 10-15 wt% crystalline water in them.

Effect of Surface Burnishing on Mitigating Stress Corrosion Cracking of Machined Type 304L SS

Low plasticity burnishing is a surface modification technique which is used to mitigate stress corrosion cracking (SCC) by inducing surface compressive stresses. A controlled surface rolling (CSR) set up which works on this principle was designed and fabricated in-house and commissioned in BARC. The setup was used to study the effect of low plasticity burnishing in mitigating SCC of machined Type 304L SS by using ASTM G36 test (boiling MgCl₂ test). Machined Type 304L SS (150 x 150 x 5 mm) were subjected to surface burnishing (at 800 kg load, 10 mm/sec traverse speed and 20 passes) using the CSR setup, followed by ASTM G36 test for 24 h. The initiation of SCC cracks in machined region was clearly seen after the test while they were suppressed in machined region subjected to low plasticity burnishing. A reduction in the maximum height after CSR treatment is evident in the 3D optical profilometer image. A detailed parametric study and characterization of the surfaces after CSR treatment is under progress.

Computation and Modelling

3-D Modelling of AHWR

3D modeling of Advanced Heavy Water Reactor (AHWR) was done using CATIA PDPLM software. 3D models of both critical and auxiliary systems, including Venturi meter for GDWP recirculation and cooling system, Gate valves, Fast Active Valve for SDS#2, air handling units of Diesel Generator building ventilation system, equipment and piping layout of AHWR GDWP Recirculation and Cooling System (GDWPRCS), passive valve for PPIS, ECCS, LESS ACW tank and desiccant chambers of D2O vapour recovery system, layout for heavy water addition and transfer system and moderator purification system, moisture separation tank, poison tank of SDS2 reactivity worth augmentation system and expansion tank of chilled water system and PPIS were prepared. Besides these, modelling of Service Building (SB), Fuel bundle assembly, Top End Shield, Re-combiner Unit of AHWR Moderator

Cover Gas System, SDS Reactivity Augmentation System Gas Tank, 2D drawings of diesel storage tank, bottom end shield top tube sheet & bottom tube sheet chemical feed tank, bottom end shield annular plate, MHT storage tank, main air receiver & bulk air receiver of compressed air system were also prepared.

Void Reactivity Experiments with (Th-Pu) MOX Fuel Pins in AHWR-Critical Facility

Structural components and High Density Poly-Ethylene (HDPE) blocks simulating different reactor coolant void conditions were fabricated and used for carrying out the coolant void related experiments with seven AHWR type (Th-Pu)MOX fuel pin cluster. Measurement of coolant void worth was carried out in AHWR-CF. The experimental cluster was placed at E5 location in core and the Critical height was measured in 0%, 33%, 50%, 66% and 100% voiding cases. The measurements were found to be in very good agreement with the predicted values. In order to perform physics experiments in AHWR spectrum, a representative core has been designed with the initial core cluster consisting of 2.1% Pu in (Th,Pu)MOX. The central 9 reference natural uranium clusters has been replaced with (Th,Pu)MOX clusters. The Plutonium requirement has been worked out as 6.29 kg for an active length of 100 cm of AHWR fuel.

Fitness-for-service Assessment of Pressure Tubes of Indian PHWRs

The state-of-the-art assessment methodologies for planar/volumetric flaws, as per Canadian Standard N285.8-2015, are numerically implemented in a GUI based ZIPTAS code. The permissible level of flaw size for a given loading for the pressure tubes of 220 MWe and 540 MWe Indian PHWRs was evaluated by using ZIPTAS.

CFD Simulation of Rod Bundle for DNB of PWR Rod Bundles

Semi-mechanistic models based on force balance analysis were developed for arriving at bubble

departure diameter and departure frequency. The DNB was predicted in vertical tubes at PWR operating conditions with a mean error of 4.5% when compared with the experimental data. This approach was extended further to predict DNB of rod bundles with square and hexagonal lattices for PWRs. The predicted values came in at 19.6% at 13.8 MPa. DNB results of hexagonal sub-channel were compared with both Look-up table were within 13.9%. Thus, the developed CFD model proved capable of predicting DNB in complex geometries of rod bundles like PWR rod bundles with reasonable accuracy.

Simulation Based Studies on IPWR

The control rod for 900 MWe IPWR was re-evaluated with ARCH for all control banks and individual bank worth was also re-calculated as part of LORA studies. In order to perform coupled neutronic -Thermal Hydraulics (TH) simulations using ARCH-TH for LORA in 900 MWe IPWR equilibrium core, homogenized cross section data in two energy group were generated with burn up for several fuel and coolant temperatures. Eleven coolant temperatures were considered between the range 290°C to 340°C and 19 fuel temperatures were considered between the range of 300°C to 1200°C. These data sets will be used to get the reactivity feedback effect in transients.

As part of the safety studies on 900 MWe IPWR, reactivity initiated transient due to 10th bank CR rod movement has been simulated for equilibrium core at BOC and EOC in the presence as well as in the absence of fuel temperature feedback. The variation of power with dynamic reactivity change has been studied with ARCH-TH Code.

The power distribution in the 1st reload of 900 MW(e) IPWR has been estimated over the second cycle. The second transition core is obtained by replacing 57 out of 151 fuel assemblies and applying envisaged shuffling scheme. The cumulative and differential worth of the working control bank-10 has been estimated for the BOC (0 FPDs), MOC (205 FPDs) and the EOC (410 FPDs).

IMSR

The experimental IMSR core with 5 MWth power was analyzed with DRAGON + ARCH code system for LEU and U-233 based fuels. The radial as well as axial flux distribution in the core for two groups of neutron energy has been evaluated at full power condition.

The numerical investigation of unprotected loss of heat sink accident (ULOHSA) in IMSR has been carried out with point kinetics code PATH with TH module. The rise in temperature in fuel salt and graphite moderator of average powered channel were found to be well below the prescribed safe limits.

As part of design of experiments for validation of codes and data for IMSR, pre-experimental analysis prior to performing integral Fuel Salt experiments in AHWR-Critical Facility was taken up. The inventory of materials, including fuel salt has been worked out as part of the design for the experiment. The main requirement includes enrichment of lithium to an optimum level in order to achieve a workable salt. The salt composition used here is 74% LiF and 26% UF₄. Natural Uranium requirement is about 3.6 kg and the LiF was estimated to be 1.1kg with Li enriched to about 350 g. The moderator in the Critical Facility core was assumed to be filled up to 225cm.

Design of Graphite Fuel Salt Interaction Facility

The Instrumentation and control systems of the Graphite Fuel Salt Interaction Facility were worked out so that the temperature and pressure in the autoclave are always maintained at constant level. Further, the instrumentation was done to facilitate proper handling of fuel salt inside autoclave, insertion of salt smoothly, start-up, normal operation and for preventing anticipated transients, including N₂ gas impurity, overheating and high pressure. Fabrication of the autoclave for carrying out similar studies at Trombay using the coolant salt has also been completed.

Dissociation and Recombination Kinetics of Hydrogen Isotopic Molecules with Coverage on Fe (100) Surface by DFT Simulations

The rate constants for dissociation of H₂ molecule on Fe surface was calculated to be faster than D₂ and T₂ molecule for 0.5ML coverage. The rate constant for re-combination of H₂ was calculated to be much slower than the rate of dissociation of H₂ molecule for 0.5ML coverage. The re-combination rate of heavier T is slower than that of D and H. In the case of 2.0ML coverage the rate of recombination of H₂ and its isotopic molecules are faster than the rate of dissociation of H₂ and its isotopic molecules.

Dissociation and Re-association Kinetics of Hydrogen Isotopic Molecules on W (100) Surface by DFT Simulations

The activation barriers for dissociation and re-association of hydrogen isotopic molecules on W (100) surface were computed using combined DFT and NEB methods and the kinetics of H isotopes were studied by HTST. The predicted dissociation rate constants of H₂ molecule was seen to be faster than that of D₂ and T₂ molecule. Also, the calculated rate of dissociation of H₂ molecule was found to be slower than that of Fe(100) surface. Further, the computed rate constant for re-association of H₂ molecule was observed to be significantly slower than that of the rate of dissociation. Similar to Fe(100) surface, the re-association rate of heavier T is slower than that of D and H. The rate of re-association of H₂ molecule on W (100) surface was found to be slower than that of Fe (100) surface.

Diffusion and Permeation of Hydrogen Isotopes in Cr: First-principles DFT Simulations for IAEA

The behaviour of hydrogen isotopes in Cr was studied employing density functional theory. The lighter H atom was shown to have higher diffusion, permeability, solubility and rate constants than heavier D and T. The computed values of diffusion, permeability and solubility of H follow the experimental prediction.

Adsorption and Desorption Kinetics of H Isotopes in α -Ti

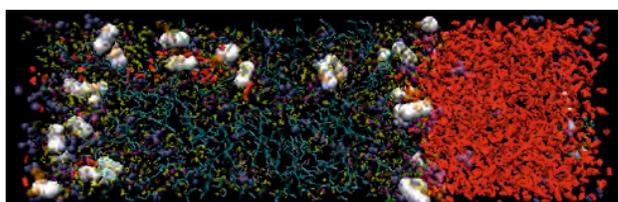
The adsorption and desorption kinetics of H isotopes on Ti (1000) surface were carried out by evaluating energy barriers using DFT followed by HTST. The rate constants for adsorption and desorption of hydrogen isotopic molecules were evaluated. The rate constant for desorption of H_2 from Ti surface is calculated to be much slower than the rate of adsorption of H_2 molecule. Further, the desorption rate of heavier T is slower than that of D and H.

Calculations of Distribution Constant (K_d) Profile of Uranyl ion by TBP

Extensive molecular dynamic simulations were conducted for aqueous (water + uranyl ion + nitrate ion + nitric acid) organic (tributyl phosphate (TBP) + dodecane) biphasic systems to gain molecular insights of PUREX process. An attempt was made to uncover the location of uranyl-TBP complexation by systematically studying the distribution of the complexes at the interface, mixed phase and the bulk phases. The experimentally observed bell shaped profile of distribution constant for uranyl extraction vs. acid concentration was captured for the first time by the MD simulations. The extraction of uranyl ions was predicted to be proportional to the interface thickness. The MD results show that the UO_2^{+2} -TBP complexation happens at the interface and not in the organic phase.

Multi-component Solvent Extraction (uranyl ion with 2-3 Competing Ions)

The MD simulations of TBP based UO_2 extraction was carried out. At the scaled temperature of 700K, results showed the extraction of UO_2 ions in the organic phase. Further, the equilibration run at STD

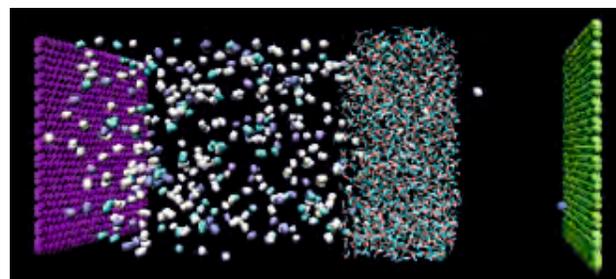


UO_2 (white) extraction in organic phase (blue) from aqueous phase (red)

(standard temperature and pressure, $T = 300K$, $P = 1atm$) are performed. In addition, the MD simulations of UO_2 extraction in presence of Zr ions, Fe ions and in the mixture of Zr and Fe are performed.

Direct Sequestering of Uranium using Maline Supramolecular Scaffold

MD and DFT simulations were performed to acquire diffusion, optimized structure, binding energy and molecular orbital diagram of U species in Maline to corroborate the experimental results and to shed light on the hydrogen bond network in Maline with aqueous dilution. Hydrogen bond analysis by MD simulation and luminescence studies (RCD/RC&IG) corroborates that as an aqueous chelator the diluted Maline behaves differently from its constituent malonic acid. The interaction of the UO_2^{2+} solution with Maline was observed to be endothermic and entropy-driven.



Snapshot representing H_2 (white), D_2 (ice blue) and T_2 (cyan) permeation through SiO_2 membrane

Permeation of Hydrogen Isotopes through Silica Glass Membrane

The silica membrane of density 2.0 g/cc (and thickness 30Å) was used to study the permeation of isotopes -hydrogen, deuterium and tritium. The permeability of isotopes was observed to be reduced in the order hydrogen > deuterium > tritium. Further, the MD simulations for permeation study of isotropic mixture of H-D, H-T and D-T are performed.

Anomalous Dynamics of Surface Water Surrounding Buckminster Fullerene

Molecular dynamics simulation has been carried out to elucidate energetic heterogeneity arising from well-defined surface structure of the

atomistic C60 which induces anomalous dynamics of the surrounding water. Using a model of water represented by a coarse-grained potential, which captures all anomalies of bulk water, the present study demonstrates that residence time and mobility of the salvation water follow a non-monotonic trend as a function of bulk density. The anomalous dynamics is shown to be a consequence of interplay between two opposing effects emanating from free volume and surface structure induced energetic heterogeneity. The present investigation, depicts the intricate reason behind anomalous dynamics of water molecules and demonstrates its correlation with energetic heterogeneity arising due to Van der Waals dispersion interaction between the non-homogeneously distributed carbon atoms of the Buckminster Fullerene and the water molecules around them.

Molecular Modelling of a Simple and Convenient Choline Oxidase Inhibition Based Colorimetric Biosensor for Detection of Organophosphorus Class of Pesticides

A simple and cost-effective biosensor design is highly desirable for the detection of organo phosphorus pesticides (OPs) due to their increasing environmental concerns. Mostly, OPs sensors rely on the inhibition of acetyl choline sterase activity and exhibit a narrow linear range of OPs detection. Thus, to find an alternative for acetyl choline sterase based expensive sensors with simple and improved platform, choline oxidase (ChO_x) inhibition based colorimetric sensor for OPs detection is designed. The current system records a LOD of 58l M with a linear range of 0–18 mM. Additionally, to find mechanistic insights, molecular docking and molecular dynamics simulations have been performed. The response has also been demonstrated in real water sample.

Modelling and Stress Analysis of Cryogenic Liquid Nitrogen Vessel

A 3-D model of the Activated Charcoal Beds and liquid nitrogen vessel with support is prepared for

analysis of coldbox system for purification of Helium gas stream. Symmetrical half model is considered to reduce computational time for finite element analysis. Structured mesh with minimum four elements across thickness is prepared. Different boundary conditions are applied over the model and finite element analysis is carried out as per ASME Sec VIII Div 2. The results ensure that all combinations of stresses across the stress linearization line are below the allowable limits, given by the code. It also identified the maximum stress locations and requirement of reinforcement. Overall, the vessel with given geometrical dimensions is qualified to be safe, as per the code.

2D CFD modelling and validation of electrochemical cell for Hydrogen-Helium separation using PEM membrane

A 2D CFD model involving coupling of multiple physics including charge, momentum, energy conservation and mass continuity equations has been developed for separation of Hydrogen from Hydrogen—Helium mixture in a PEM based electro-chemical reactor. Validation of the simulated results with in-house generated experimental data for hydrogen and helium separation has been carried out and found to be in well agreement.

Radiochemistry

Development of Porphyrin Compounds as Tumor Targeting Agents

Porphyrins are compounds well-known for their potential towards selective targeting of tumor lesions. To tune the characteristics and pharmacokinetics of porphyrins different derivatives were synthesized by introducing different functionalities. A water-soluble porphyrin bearing three carboxylic groups and one phenolic group at four meso positions was synthesized. The porphyrin compound was subsequently conjugated with a cell-penetrating peptide RKKRRQRRR (abbreviated as TAT) synthesized in-house using SPPS technique to enhance the cell

internalizing behavior of the porphyrin. Fluorescence and flow cytometry experiments demonstrated relatively higher cellular internalization of porphyrin-TAT conjugate in comparison to the porphyrin derivative. Cytotoxicity assay (MTT assay) revealed preferential light dependent toxicity for porphyrin derivative which was further enhanced upon peptide conjugation. Both porphyrin and porphyrin-TAT conjugate were observed to be capable of generating singlet oxygen, a highly reactive species required for photo-oxidation of toxic molecules and application in photodynamic therapy (PDT). Porphyrin and porphyrin-TAT were radiolabeled with ^{68}Ga (>95% radiochemical purity). ^{68}Ga -porphyrin-TAT conjugate demonstrated higher tumor uptake (6.32 ± 1.24 % IA/g) than ^{68}Ga -porphyrin (2.45 ± 0.88 % IA/g) during biodistribution studies in animal models (Swiss mice bearing fibrosarcoma tumors).

Synthesis and Development of Receptor-Specific Peptides

The peptide, DOTA-TATE binds to somatostatin receptors (SSTR) over-expressed in neuroendocrine tumors. ^{177}Lu -DOTA-TATE is a FDA (Food and Drug administration) approved and routinely used radiopharmaceutical for peptide receptor radionuclide therapy (PRRT) of SSTR-positive neuroendocrine tumors (NET). Experiments towards submission of proposal to DAE-RPC for manufacture and supply of 'DOTA-TATE kits, freeze-dried' (prepared using in-house synthesized DOTA-TATE peptide) for formulation of ^{177}Lu -DOTA-TATE were carried out. Six batches of kits were prepared and in-vitro cell binding assays in SSTR-2 expressing AR42J cells and in-vivo studies in nude mice bearing AR42J tumors were performed for all the six batches to establish the efficacy of the completely indigenously synthesized ^{177}Lu -DOTA-TATE radiopharmaceutical. Subsequent to completion of studies, the proposal was submitted to DAE-RPC seeking approval for the manufacture and supply of freeze-dried DATA-TATE kit for the treatment of cancer patients.

Development of Nitroimidazole-based Gold Nanoparticles as Tumor Hypoxia Targeting Agents

Tumor hypoxia is a situation where tumor cells are deprived of oxygen due to insufficient blood supply. Hypoxic tumors are associated with increased risk of metastasis and poor response to treatment. Nitroimidazoles (NIM) selectively accumulate in hypoxic cells through oxygen dependent process by undergoing a series of one-electron reductions mediated by nitroreductase enzymes. Gold nanoparticles accumulate passively in tumor cells by enhanced permeability and retention (EPR) effect. The prepared PEG2K coated gold nanoparticles were tagged with 2-nitroimidazole and DOTA and subsequently radiolabeled with ^{177}Lu . ^{177}Lu -DOTA-Au-PEG-2K-NIM displayed encouraging results in CHO cell lines with steady increase in hypoxia/normoxia ratio from 1.01 at 2 h post-incubation to 3.08 at 4 h post-incubation. In case of control, ^{177}Lu -DOTA-Au-PEG-2K, very low cellular uptake was observed both under hypoxic and normoxic conditions. Biodistribution studies in Swiss mice bearing fibrosarcoma tumor indicated fast clearance from blood and other organs at 3 h post-administration time point. Fast clearance of nanoparticles was observed from liver and kidneys.

Polymer Blends and Polymer Composites

Conducting ink synthesis was carried out by solution polymerization of aniline in presence of nanocarbon (CCB, CNT, and graphene) under standardized conditions. Various aniline and nanocarbon ratios were investigated to get high conductivity while maintaining optimal viscosity. The electrical conductivity of the conducting ink was ~ 1 k with lowest for CCB ink.

Polydimethylsiloxane (PDMS) and nanocarbon (CCB, CNT and graphene) based conducting nanocomposites based on) were prepared through compression moulding and crosslinked using gamma radiation. It was observed that the inclusion of nanofiller affects not only the mechanical and electrical properties of composites but also the thermal degradation temperature of nano-composites.

Nano-composites of SIS-5517, SBS 6414, SBS T-166 with NCB in the filler range 1-3% were prepared by optimizing various mixing parameters on Brabender Plasticorder at 150°C. The sheets of composites were also prepared by compression molding (Thickness 1-1.5 mm). It was found that the percolation threshold of NCB depends upon the styrene contents of elastomer. It was interesting to note that for elastomer with 40 wt% styrene percolation threshold was at 12.5 wt% while for 30 wt% styrene elastomer it was at 15 wt% of NCB.

Development of Piezo-Resistors

Free-volume affects elastic recovery of polymers. Different types of free volumes are possible in multiphase system; however, how radiation crosslinking and physical crosslinking caused by reinforcing fillers affects the free volume has been a topic of investigation. To investigate such effects, conducting polymer composites of Carbon nanotube (CNT) and poly (dimethyl siloxane) (PDMS) were prepared in different proportions and were crosslinked subsequently by gamma radiation. Piezoresistivity and tensoresistivity of composites were measured under compressive and tensile load. Free volume measurements were conducted on a series of composites. The findings revealed substantial reduction in the o-Ps intensity and a percolation dependent change in the lifetime of o-Ps.

Development of Shape Memory Polymer

Polycaprolactone (PCL) was blended with Ethyl Vinyl Acetate (EVA) in different proportion under molten condition (at 80°C) in Brabender Plasticorder. The blend of PCL: EVA (90:10 and 80:20) were further blended with a multifunctional acrylate trimethylol propane triacrylate (TMPTA) in different concentrations (2.5 and 5%). The sheets of 1.5 mm prepared in compression molding machine and irradiated in the dose range 10-100 kGy. The introduction of optimum proportion of TMPTA resulted in reduced crosslinking dose with a product of excellent strength and recovery. Modulus measurements were undertaken to

probe the mechanical integrity of the matrices. Dynamic mechanical analysis of these crosslinked PCL/EVA blends was carried out in temperature range 30-80°C. An increase of 3 times in storage modulus was observed when radiation dose increased from 10 to 40 kGy indicating that an absorbed dose can play a crucial role for designing PCL-EVA based robust matrices.

Thermal Studies for MSBR

The thermodynamic properties of $\text{NaCeF}_4(\text{s})$ have been studied which was identified as an interaction product of pseudo binary NaF-CeF_3 system for MSBR chemistry. CeF_3 is one of the burnable waste fluorides and Ce^{3+} is also the surrogate of Pu^{3+} . $C_p^\circ[\text{NaCeF}_4(\text{s})]$ has been measured experimentally with DSC and the Gibbs energy of formation, $\Delta_f G^\circ$ of $\text{NaCeF}_4(\text{s})$ has been determined using Solid Electrolyte Galvanic Cell (SEGC) with $\text{CaF}_2(\text{s})$ as solid electrolyte. The binary phase diagram of $\text{NaF}(\text{s})\text{-CeF}_3(\text{s})$ system has been calculated based on experimental thermodynamic data. To study the stability domain and coexisting phases of $\text{NaCeF}_4(\text{s})$, the chemical potential diagram of Na-Ce-F-O system and ternary phase diagram of Na-Ce-F₂ system has been calculated. In order to study the interactions between coolant salts and structural materials, thermodynamic properties of LiF-NiF_2 system has been carried out. The $\Delta_f G^\circ$ of $\text{Li}_2\text{NiF}_4(\text{s})$ has been measured with SEGC technique. The ternary phase diagram of Li-Ni-F₂ system and chemical potential diagram of Li-Ni-F-O system has been calculated in order to study stable coexisting phases of $\text{Li}_2\text{NiF}_4(\text{s})$ at the reactor operating temperature (600°C/873 K).

In order to study to understand the thermodynamic behaviour of fuel-coolant system, the pseudo binary phase diagram of NaF-UF_4 system was determined over full range of composition ($X_{\text{UF}_4} = 0$ to 1) by DTA measurements. C_v of Na_2UF_6 , $\text{Na}_7\text{U}_6\text{F}_{31}$ and NaU_2F_9 were measured. Thermodynamic (activity and activity coefficients) and kinetic (diffusion coefficients, activation energies etc.) parameters of UF_4 and ThF_4 in $\text{UF}_4\text{-ThF}_4\text{-FLiNaK}$ mixture were determined by various electrochemical techniques (CV, CP, and SWV in

temperature range 823 to 873 K for different compositions of UF_4 and ThF_4 . These kinetic parameters are important for efficient electrochemical pyro processing of MSBR spent fuel. A systematic investigation of thermal diffusivity (T_D) and thermal conductivity (T_C) of rare-earth fluorides is initiated to understand thermal behaviour of molten-salt-reactor fuels during burn-up. For the first time T_D of light rare-earth fluorides (LaF_3 to GdF_3) was determined, using laser-flash technique, in the temperature range, 300 –1100 K. Thermal conductivities of these compounds were determined by using the measured thermal diffusivity values, previously measured heat capacities and the sintered pellet densities. There was continuous decrease in the thermal diffusivities (as well as thermal conductivities) of these compounds with rise in temperature.

Depth Profiling Studies using Secondary Ion Mass Spectrometry (SIMS)

Quantitative depth profiling is an important part of material characterization. Two samples of pressure tubes from Madras Atomic Power Station were received for the depth profile analyses using SIMS. Depth profiling of various elements (Li, H, D, N, Cl, Ni, I, O, F, Cr, Mn, Fe, Cu, and Br) needed to be carried out in order to infer the cause of pit formation on the surface of the pressure tube. Depth profiles for most of the elements were analysed in MCS^+ -SIMS mode, so as to minimize the influence of matrix effects. A pristine Zr-2.5%Nb alloy was also analysed under similar conditions. By comparing the results in various samples, it was observed that the elements viz., Cl, F, Br, and Fe were present in higher concentration in the corroded pit sample compared to other samples.

Samples of 316LN stainless steel and modified 9-Cr 1-Mo steel exposed to sodium in BIM loop for 50,000 hours at IGCAR, Kalpakkam were analysed by SIMS for carbon depth profile. The SIMS profile obtained for sodium exposed 316LN steel shows a significant diffusion of carbon into the matrix up to a depth of nearly 45 μm in the specimen and the

surface concentration of carbon is estimated to be 0.9 wt%. 9Cr1Mo alloy sample showed the diffusion of carbon for a depth of about 30 μm and the corresponding surface concentration carbon was ~0.3 wt%.

Chemometrics and Artificial Neural Network Studies

Accurate determination of uranium content in the molten salt fuel mixture is a necessary step in its quality control. Though laser-induced breakdown spectroscopy (LIBS) provides direct elemental analysis of solid samples, the major limitations of this technique are the non-linear phenomena in LIBS signal due to matrix effect, self-absorption, etc. In order to overcome this limitation, a hybrid chemometrics model of the partial least squares-artificial neural network (PLS-ANN) was used to quantify the U in the salt-fuel mixture. Several parameters viz., spectra pre-treatment procedure, factor number of PLS for ANN input, number of hidden neurons and layers in ANN, activation function, and number of ANN iterations were optimized. The collective advantages of data dimension reduction from PLS and the nonlinear processing ability from ANN, improved the accuracy of LIBS quantitative analysis for U from $\approx 7\%$ to $\approx 4\%$ precision using this hybrid model.

Development of Analytical Methodology for Determination of Cadmium in Control Rod Material

The control rod material was dissolved using dilute HCl and a few drops of H_2O_2 . The solution was then diluted up to 100 mL and heated on a hot plate for some time to ensure complete removal of H_2O_2 . The mixture was then cooled and 3g of tartaric acid was added into it. The addition of tartaric acid makes the precipitation process selective for Cd (II) by generating more stable complexes with interfering elements viz., Al, Cr, Mn, Fe, Co, Ni and Sn. The pH of the solution was then adjusted between pH 7 and 8 by adding NaOH solution in the presence of a phenolphthalein indicator. Cd (II) was precipitated from the solution using 3% alcoholic

8-hydroxyquinoline solution. The crystalline precipitate of composition $\text{Cd}(\text{C}_9\text{H}_6\text{NO})_2 \cdot 2\text{H}_2\text{O}$ was filtered by using pre-weighed G3 glass filter crucible and washed with hot water and then with cold water. The solid mass was dried at 240-260 °C in the same G3 crucible. The cadmium content in the sample was calculated with stoichiometric factor: $\text{Cd}/\text{Cd}(\text{C}_9\text{H}_6\text{NO})_2 = 0.28052$.

Nuclear Chemistry

Studies on measurement of kinetic energy spectra and angular distribution of projectile like fragments in $^{19}\text{F}+^{89}\text{Y}$ reaction showed a dependence of the role of target structure in transfer reactions on the N/Z ratio of the projectile. An experiment was carried out at BARC-TIFR Pelletron-LINAC facility to investigate the role of single particle effects in fission product mass distribution in $^{35}\text{Cl}+^{165}\text{Ho}$ reaction. Studies on fission product mass distribution for the $^{28}\text{Si}+^{144}\text{Sm}$ reaction, calculated using the GEF code, were observed to be narrower compared to experimental mass distribution, indicating the role of fragment shell closure. Short-lived fission products were produced from $^{235}\text{U}(n, f)$ using pneumatic carrier facility at Dhruva reactor for detailed yield comparison from the GEF code to investigate the single particle effects, particularly of proton single particle effects. Measurement of angular distribution of projectile-like fragments in $^{19}\text{F}+^{89}\text{Y}$ reaction showed strong dependence of the angular distribution on the number nucleon transfer/pick-up. For stabilizing the polar orthorhombic (o) phase in observed ferroelectricity (FE) in thin films of HfO_2 , yttrium dopant has been used at three different atom% levels (3, 5 & 7) to look for extent of stabilization of o-phase in this oxide. All the monoclinic and o-phases present in the sample could be identified and relative population could also be determined by TDPAC spectroscopy.

PVC based Potentiometric Sensor for Eu(III) ion

The sensor for Eu(III) ion was prepared with diglycolamide-functionalized poly(propylene imine) diaminobutane first generation (G-I)

dendrimer as ionophore in presence of NPOE as plasticizer and NaTPB as ionic additive. The response of the sensor for Eu(III) was tested in the acetate buffer (pH 5.0), which showed a linear dynamic range with the slope of 7.1 ± 0.1 mV/decade. The response of the sensor was found to be fast (<10 s) and stable for 15 minutes. Another sensor involving of TPDGA showed preferential detection of Eu in presence of different cations and the interference can be tolerated up to 10 to 102 times of Eu(III) concentration in the solution depending on the cation where the order followed the trend: $\text{K}^+ < \text{Sr}^{2+} < \text{UO}_2^{2+} < \text{Al}^{3+}$. Polyether sulphone based scintillating polymer inclusion membranes (PES-SPIMs) with surface grafting of extractant (BMEP) were made for simultaneous pre-concentration and detection of Pu at low level.

Positron Annihilation Measurements (PALS) in Zeolitic Imidazolate Frameworks

The PALS spectra for both ZIF-67 and ZIF-8 were fitted with three ortho-positronium (o-Ps) lifetime components. The three components correspond to o-Ps annihilation in micropores, mesopores and inter-granular spaces. It was seen that with the increase in CO_2 pressure o-Ps lifetimes corresponding to all the three states decrease and saturate at a particular pressure for both ZIF-67 and ZIF-8 samples. The behaviour of corresponding intensities is however, distinct for ZIF-67 and ZIF-8. It is interesting to observe that even at the highest CO_2 pressure, the o-Ps lifetimes show finite values indicating that the whole pore volume is not utilized for CO_2 adsorption. The role of varying pore aperture and flexibility on CO_2 gas adsorption is studied by PALS measurements under varying CO_2 pressure. o-Ps lifetime is observed to decrease with the increase in CO_2 pressure due to filling of the pores. However, the decrease in o-Ps lifetime depends on the blm content in the frameworks indicating the role of pore aperture and flexibility on CO_2 adsorption.

ZIF membranes with mixed linker frameworks (ZIF- 7_x -8) show higher separation selectivity and low permeance of gases. Stiffened phase of ZIF- 7_x -8 ($x = 0, 20.6, 52.6, 79.4, 90.4, 97.2$ and 100%)

membranes have been deposited over Si substrate using a fast current driven synthesis method. In those with low blm content the synthesized frameworks was determined using ^1H NMR. The lattice structure and chemical bonding have been investigated using XRD and FTIR. The average pore size as well as relative porosity have been evaluated using PALS which confirms the fine tuning of pores in the frameworks as a result of ligands mixing. Crystalline structure and morphology have been characterized using XRD and FE-SEM. Changes in bonding pattern have been characterized using FTIR and Raman spectroscopy. Role of the pores interconnectivity and surface accessibility towards the permeance and selectivity of the gases, have been investigated by depth dependent Doppler broadening measurements.

Pulsed Positron Studies

Positron lifetime of Nitrile Butadiene rubber (NBR) and Polydimethylsiloxane (PDMS) were measured using the pulsed positron beamline. The resolution of the spectrometer was measured by recording the lifetime spectrum of a kapton foil. The choice of kapton was made because it has a standard lifetime of 380 ps. The resolution of the spectrometer was found to be described by a convolution of three gaussians- 0.535 ns (50%), 0.3925 ns(45%) and 3.6 ns (5%). Based on these measurements, the long lifetime of the NBR and PDMS were measured and compared to the corresponding bulk-PALS measurements.

External PIGE

In order to prepare in house reference materials (in kg scale) for isotopic composition of boron (IC, $^{10}\text{B}/^{11}\text{B}$ atom ratio) in B_4C samples, natural (19.8 at% of ^{10}B) and enriched (67 at% of ^{10}B) B_4C powder samples were mixed proportionately to get three different isotopic compositions (30, 40 and 50 ^{10}B at%). Using 3.5 MeV proton beam (in air) in external PIGE method for direct "as received" powder

samples wrapped in thin Mylar film, IC of boron was evaluated by measuring 429 and 718 keV of ^{10}B and 2125 keV of ^{11}B . The results are in good agreement with the calculated composition and the %RSD values from four replicates are in the range of 0.5-0.8% for enriched to natural B_4C samples. The external PIGE method is truly non-destructive as the samples are used for experiment as such and they can be returned after irradiation since no radioactivity is generated in the sample. Similarly the technique was used to determine low Z elements (Na, Mg, Al and Si- at minor and major levels) along with trace quantities of B and F in coal samples.

Gamma Ray Spectrometry

Analysis of complex Pu gamma-ray spectra having large spectral interferences from $^{235}\text{U}/^{241}\text{Am}$ under an Indo-US joint working group exercise was carried out using peak area analysis software PHAST, developed at BARC, to obtain the peak areas under the characteristic gamma-rays of various Pu, U isotopes along with ^{241}Am which were used to obtain isotopic fractions. For the determination of isotopic fractions, the code developed at BARC was employed, using ^{239}Pu (for samples with > 80% ^{239}Pu) and ^{241}Pu (for samples with < 80% ^{239}Pu) as reference. Results were comparable with those obtained using US based software FRAM and MGA.

Production cross sections of $^{66,67}\text{Ga}$, ^{65}Zn , ^{57}Co and ^{58}Co from their respective threshold to 50 MeV alpha energy were measured using natural copper targets and standard stacked foil irradiation method followed by high resolution gamma ray spectrometry.

$^{66,67}\text{Ga}$ nuclides are used for medical purposes, and the other produced radionuclides are considered as impurities and their production cross sections were measured accurately. The data was in good agreement with the literature, i.e. IAEA recommended data and TENDL-2019 database based on the TALYS-1.95 code.

Biology

Nuclear Medicines for Diagnosis and Therapy

PSMA-11, ligand for preparation of ^{68}Ga -PSMA-11, a Positron Emission Tomography (PET) based imaging agent used for diagnosis of prostate cancers was synthesized in-house as an import substitutes with a quality comparable to that of the commercial imported equivalent. The product has been validated, and is under process for Radiopharmaceutical Committee approval, and subsequent commercial production.

Up to 100 mg of PSMA-617, ligand for preparation of ^{177}Lu -PSMA-617, used for prostate cancer therapy, has been synthesized and supplied to BRIT for kit formation and supply to hospitals pan India.

Up to 1 g of Cu (MIBI)BF₄, used for preparation of $^{99m\text{Tc}}$ -sestamibi, used for myocardial perfusion imaging, has been synthesized and supplied to BRIT for kit formation and supply to hospitals pan India.

In a step towards 'Atma-Nirbhar Bharat', an indigenous, cost-effective technology for synthesis of o-tolylbenzotrile (OTBN), an advanced drug intermediate for anti-hypertensive-sartan drugs, has been developed. The technology is ready for transfer to industries.

Estimation of Alcohol Content in Alcoholic Products Through Easy Synthesis of BODIPY Dye

An easy and highly sensitive colorimetric technique was developed to measure ethanol/isopropanol in alcohol-water mixtures. A new dye has been synthesized indigenously. New synthetic methodology has been developed to tune its colour, fluorescence and solubility in different polar solvents. The dye is colourless and non-fluorescent in water, but after addition of ethanol/isopropanol, it develops cyan colour and becomes bright red fluorescent under UV irradiation which is easily and precisely detectable by spectrophotometric/ fluorimetric methods. Interestingly, the colour change is easily visible by

naked eyes. Importantly, the sensor is applicable for 0 to 100% (v/v) of ethanol/isopropanol in the mixtures with few seconds response time.

BODIPY Nanoparticle Based Near-infrared Fluorescent Sensor for Serum Albumin

Highly sensitive and selective near-infrared fluorescent bioprobes for serum albumin detection and quantification is in high demand due to the varied importance of serum albumins. Thus we have developed near-infrared emitting BODIPY dye as a turn-on emission sensor for serum albumin. Despite various outstanding photophysical properties of BODIPY dyes, their insolubility in water/biological media restricts their real applications, especially in biomedical fields. To overcome this issue, highly stable unadulterated BODIPY nanoparticles (BDP-NPs) were prepared in aqueous solution by self-assembly of the amphiphilic BODIPY dyes. The BDP-NPs were characterized by spectroscopic, NMR, DLS and TEM studies. The ability of the BDP-NPs for detection and quantification of the serum albumin was checked. It showed 150-fold fluorescence enhancement, high selectivity over other amino acids, porphyrin, proteins and various inorganic salts which remain as constituents in human serum. Finally, quantification of HSA in urine samples was done which showed that the bioprobe is applicable in clinically significant range with very low limit of detection (LOD) of HSA in urine. This clearly established the potential of BDP-NPs to quantify HSA levels in urine samples.

Synthesis of Dihydrobenzofuro [3,2-b] Chromenes as a Potential 3CLpro Inhibitors of SARS-CoV-2: A Molecular Docking and Dynamics Simulation Study

The recent emergence of the (COVID-19) pandemic caused by SARS-CoV-2 has raised significant global health concerns. More importantly, there are currently no specific therapeutics available to combat this deadly infection. The enzyme 3-chymotrypsin-like cysteine protease (3CLpro) is known to be essential for viral life cycle as it controls the coronavirus replication. 3CLpro could

be a potential drug target as established before in the case of severe acute respiratory syndrome coronavirus (SARS-CoV) and Middle East respiratory syndrome coronavirus (MERS-CoV). In the currently study, we wanted to explore the potential of fused flavonoids as anti-CLpro inhibitors. Fused flavonoids (5a,10a-dihydro-11H-benzofuro[3,2-b]chromene) are unexplored for their potential bioactivities due to their low natural occurrences.

Their synthetic congeners are also rare due to unavailability of general synthetic methodology. Here we designed a simple strategy to synthesize 5a,10a-dihydro-11H-benzofuro[3,2-b]chromene skeleton and its four novel derivatives. Our structural bioinformatics study clearly shows excellent potential of the synthesized compounds in comparison to the experimentally validated inhibitor N3. Moreover, in-silico ADMET study displays excellent drugability and extremely low level of toxicity of the synthesized molecules. In summary, we anticipate that the currently synthesized molecules could not only be a potential set of inhibitors against CLpro but that the insights acquired from the current study would be instrumental in further developing novel natural flavonoid based anti-COVID therapeutic spectrums.

A Novel Protocol for regioselective Crotylation

A novel protocol for the Bismuth metal mediated regioselective crotylation of aldehydes yielding α -homoallylic alcohols has been developed using [bmim][HSO₄] as a metal activator, as well as a mediator for regioconversion from the initially formed γ -regiomer. The present protocol minimizes the use of conventional solvents and proceeds with good yields and excellent regioselectivities.

Novel Pd-complexes based Catalyst in Suzuki Cross Coupling Reactions

Novel Pd-complexes derived from amido linked N-heterocyclic carbenes were synthesized, and used as a catalyst in Suzuki cross coupling

reactions. These catalysts performed reasonably well in case of an aryl bromide substrate with an electron donating group, which was otherwise not obtained with similar catalysts. The reaction mechanism was also deciphered.

Advanced Radiopharmaceuticals

RPC Development of Infection Imaging Agents

Studies were carried out to evaluate the potential of radiolabeled Ubiquitin (UBI) derived peptides as infection imaging agents and to elucidate the mechanism of interaction with bacterial membranes by ITC, DLS, QENS and competition assays. It was concluded by flow cytometry studies that UBI (1-59) kills *S. aureus* by causing membrane depolarization. UBI derived peptides restricted lateral movement of anionic phospholipids in bacterial membrane models. Detailed biological evaluation of ⁶⁸Ga-NODAGA-UBI derivatives in *S. aureus* and animal model bearing infection was carried out. Clinically relevant antibodies, trastuzumab and pertuzumab (targeting HER2 receptors on breast cancer cells) were identified and labeled with suitable radioisotopes with an aim to develop agents for radioimmunoscinigraphy (RIS) and radioimmunotherapy (RIT). During 2021, F(ab')₂-trastuzumab was prepared for formulation of ^{99m}Tc-HYNIC-F(ab')₂-trastuzumab as a SPECT imaging agent. Detailed studies were also carried out to develop ¹⁷⁷Lu-pertuzumab as a theranostic agent. In-vitro evaluation in cancer cell lines and in-vivo studies in animal model bearing HER2 positive tumors were done. Specific uptake of ¹⁷⁷Lu-pertuzumab in tumor was observed. Mechanistic studies to evaluate binding synergism of antibodies to HER2 receptors were performed and enhanced binding of ¹⁷⁷Lu-pertuzumab in presence of cold trastuzumab and co-localization of antibodies was observed.

Development of Drug Delivery Systems for Theranostic Applications

Liposomes serve as promising nano-cargos to deliver chemotherapeutic drugs and radionuclides

concurrently against cancer. Liposome conjugated with antibody trastuzumab (Lip-Ab) and liposomes (Lip) loaded with doxorubicin were prepared and radiolabeled with ^{99m}Tc . Protocol was optimized and SPECT imaging studies in animals bearing tumors were carried out to study the delivery of drug to the target. For combination radionuclide therapy, ^{177}Lu -labeled liposomes were loaded with drug doxorubicin were prepared and detailed evaluation in cancer cells and tumor bearing animal model were carried out.

In-vitro Evaluation of Bone Pain Palliating Radiopharmaceuticals

Several bone pain alleviating radiopharmaceuticals such as, $^{166}\text{Dy-NP}$, $^{177}\text{Lu-HA-NP}$ and $^{166}\text{Dy-DOTMP}$ were formulated as part of an ongoing program. Uptake of these formulations in mineralized bone and tumor cells were carried out. These radiopharmaceuticals showed >35% uptake in mineralized bone and insignificant uptake in tumor cells. These formulations also induced significant cell deaths as compared to the control cell populations.

Recovery of ^{90}Sr and Milking of ^{90}Y for Radiopharmaceutical Application

^{90}Sr is prominent fission product present in High Level Liquid Waste (HLLW). The Etrrium-90 (^{90}Y), daughter product of ^{90}Sr is β emitter with shorter half-life ($T_{1/2} = 64$ hrs) and have potential use for radio-therapeutic application. For the radio-therapeutic application, carrier free ^{90}Y should be extracted without contamination of other radionuclides. The process to recover pure ^{90}Sr (free from radio-chemical contaminants) from HLLW using multi step separation processes has been standardised. Bulk ^{90}Sr could be separated from HLLW along with actinides and lanthanides at the plant, using solvent extraction system at WIP, Trombay. Multi step separation processes are developed and demonstrated on a laboratory scale for obtaining purified form of ^{90}Sr . Around 2 Ci of ultra-pure ^{90}Sr solution has been recovered. The purified ^{90}Sr is followed by milking of carrier free radiopharmaceutical grade ^{90}Y from ^{90}Sr - ^{90}Y solution

using supported liquid membrane (SLM Generator) system. More than 30 batches of 150 mCi of ^{90}Y have been supplied to RMC for radiopharmaceutical applications. Till date, 10 patients are already administered with such recovered ^{90}Y solution at RMC.

Cancer studies

Investigating the Role of CHK1 Kinase in Regulating Topoisomerase 1 Dynamics

Topoisomerases, being essential enzymes involved in key cellular processes including replication and transcription, are attractive therapeutic targets in cancer therapy. It was shown that the CHK1i mediated TOP1 trapping on the genome is not inhibitor-specific by using inhibitors of other DNA damage repair pathway kinases ATM, ATR and DNA-PKcs. We have further demonstrated the physical interaction between CHK1 and TOP1 using co-immunoprecipitation and proximity ligation assay. Using in vitro plasmid relaxation assay involving nuclear extracts, we have also shown that total cellular TOP1 enzymatic activity is suppressed in the presence of CHK1i.

Synergistic Lethality in Breast Cancer Cells

Talazoparib (BMN673) is clinically approved for the treatment of BRCA-mutated cancers with homologous recombination deficiency based on the principle of synthetic lethality. PARPi treatment leads to replication associated DSB accumulation, that are repaired by HR which enhances chemoresistance. However, ~90% breast cancers are BRCA wildtype and hence are de novo resistant. RECQL5 physically interacts and disrupts RAD51 from pre-synaptic complex leading to impairment of HR. In the current investigation it was observed that the targeted inhibition of HR by stabilization of RAD51-RECQL5 complex by a pharmacological inhibitor of RECQL5 in the presence of talazoparib leads to abolition of functional HR with uncontrolled activation of NHEJ pathway proteins. Concomitant administration of BMN673 and 4a

leads to copious amounts of replication stress leading to prolonged G2/M arrest resulting in extensive DSBs leading to changes in nuclear morphology, chromosomal aberrations and ultimately to the demise of the cancer cells.

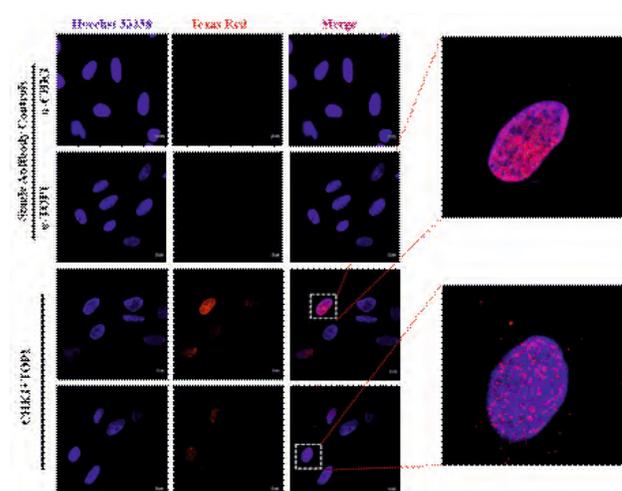
Synthesis of Peptide for Targeting and Diagnosis of Cancer

A 41-amino acid based pH-low insertion peptide was synthesized, purified, characterized, conjugated to zinc gallate (ZGO)-based persistent luminescence nanoparticles (NPs), and was used for specific delivery and precise detection of tumor *in-vivo* using a photon imager.

An efficient route of synthesis of *Alpinia Officinarum*-derived diarylheptanoids, an Anticancer Agent

An efficient synthesis of the *Alpinia officinarum*-derived diarylheptanoids was developed starting from commercially available eugenol. Among these, an α,β -unsaturated ketone showed a superior antiproliferative effect against human breast adenocarcinoma MCF-7 cells. Mechanistically, it acted as an intracellular pro-oxidant by generating copious amounts of reactive oxygen species. The impaired mitochondrial and lysosomal functions due to reactive oxygen species (ROS)-generation contributed to its apoptotic property.

A novel Fluorescent Probe for Selective



Detection of Fe⁺² in Cells

A BODIPY based novel fluorescent probe to selectively detect Fe⁺² in the live cells, based on a selective chemical reduction, has been developed, and has been validated *in-vitro*. The triplet, profluorescent nitroxide probe showed a turn-on sensing with a low limit of detection and high sensitivity.

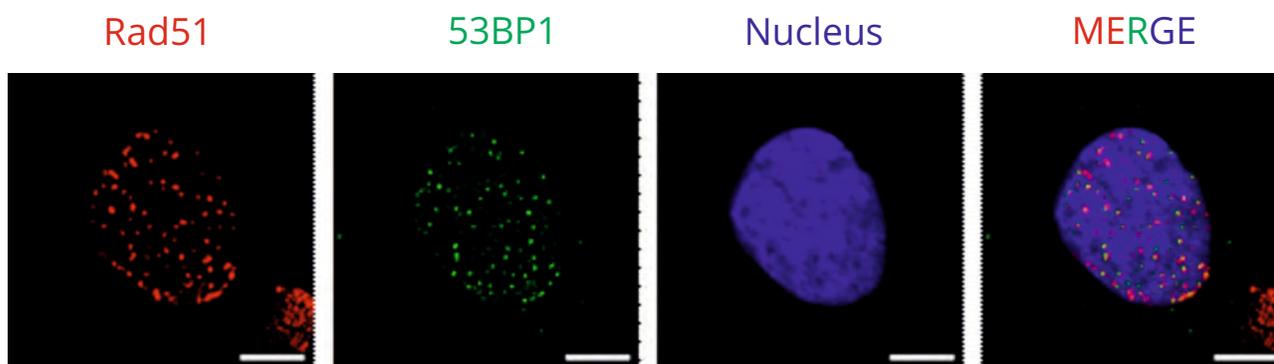
Development of DNA Aptamers for Targeting Cancers

Aptamers are single-stranded or double-stranded nucleic acids similar to antibodies for targeting important biomarkers over-expressed in cancers. They have gained relevance in recent decades due to ease of chemical synthesis, modification and manipulation. Additionally, the aptamer structure has high chemical stability, low molecular weight (10-14 kDa), and minimal immunogenicity. During 2021, selection of DNA aptamer against PD1 and HER2 receptor expressed on cancer cells was done by linking the respective proteins with protein-A-shepharose. Bound DNA sequences with Protein-A shepharose-PD1/HER2 were collected, purified and amplified in PCR to the extent they would be sufficient for a consecutive round of selection. Screened DNA aptamer against Pd1 and HER2 proteins have been sent for sequencing.

Biochemical Characterization of Human Translin

Translin is an evolutionarily conserved nucleic acid interacting protein. It binds to consensus sequences at chromosomal breakpoint junctions and mutation hotspots. It plays an important role in activation of RNA-induced silencing complex (RISC) and degradation of pre-miRNA substrates to alter the RNA population. Translin is over-expressed in malignancies such as testes cancer. 10 variants (found in different cancers) of this protein have been studied for their biophysical and biochemical properties.

These mutations span the protein length of the translin protein and fall in different regions of the



RAD51 and 53BP1 foci formation in SK-OV-3 cells in response to Talazoparib

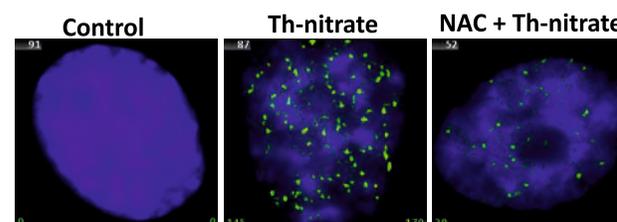
protein. These mutant proteins were generated through genetic engineering and checked the protein stability and DNA/RNA binding with all the selected 10 variants. All the proteins were expressed and found to be stable. Circular Dichroism analysis showed that the alpha helical component of the purified proteins was 86%, and the mutations did not alter the secondary structure of variant translin proteins. Dynamic Light Scattering (DLS) data also showed the protein preparation to be homogenous and the hydrodynamic ratio of the all the variant proteins was ~12.0 nm. Further, DNA binding analysis was performed by EMSA and the mutations did not alter the DNA binding ability of Translin.

Radioresistance of Cancer Cells

NGS analysis carried out in radio-resistant human lung cancer (A549) cells showed 545 differentially expressed genes. Gene enrichment analysis showed highest upregulation of cell-cell adhesion processes in radio-resistant cells. Interestingly, stem cell genes like PLIN2 and ALDH1A3 genes were also highly up-regulated in radio-resistant cells suggesting involvement of cancer stem cell features in the mechanism of radio-resistance. Radiosensitivity of cold atmospheric plasma was evaluated in different cancer cell lines, which showed human lung adenocarcinoma A549 cells as the most radiosensitive. Transcript profiling showed significant up-regulation of DNA repair genes ATM and BRAC1, both in directly CAP-irradiated as well as bystander A549 cells. CpG oligonucleotides in combination of radiation showed growth inhibition in non-targeted mouse fibrosarcoma.

Toxicity and Mechanism of Magnetic Nanoparticles for Improvement of Cancer Radiotherapy

Insignificant cardio-toxicity of liposomal targeted magnetic nano-formulation (cRGD-LMD) encapsulated with doxorubicin (DOX) was observed in terms of level of anti-oxidant enzymes (superoxide dismutase, catalase and glutathione-S-transferase) in heart tissues compared to animals administered with free DOX. Further toxicity studies showed maximum tolerated dose of cRGD-LMD as 15 mg/Kg for cRGD-LMD in mice. Acute dose toxicity of cRGD-LMD after intra-venous injection in rats showed insignificant change in gross physiological/pathological parameters. The median lethal dose (LD50) was found to be 22.8 mg/Kg body weight. These results suggest that cRGD-LMD was well tolerated in mice/rats. The mechanism of tumor growth inhibition by cRGD-LMD in combination with radiation and/or magnetic hyperthermia was found to involve increased expression of pro-apoptotic (viz., PARP, cleaved Caspase-3 and BAD) and decrease in pro-survival (viz., Survivin, P-AKT and AKT) proteins studied by Western blotting analysis.



Representative immunofluorescence images of untreated Control, Th-nitrate (10 g/ml for 24h) or NAC+Th-nitrate treated lung cells. Blue (DAPI) indicated nucleus and green indicated foci of gamma-H2AX, a marker of DNA-double strand breaks in nucleus. NAC treatment decreased number of gamma-H2AX foci.

Mechanism(s) of Th-232 toxicity in Human Cells

It is relevant to understand the mechanism of biological effect of Thorium in human cells, which would lead to the development of rational and efficient strategies for mitigation of its toxicity and enhanced detoxification/ decorporation. In this direction, mechanism of toxicity studies showed that Th-nitrate and Th-dioxide elevates intracellular level of ROS, which was inhibited by inhibitor of plasma membrane associated NADPH oxidase as source of ROS. Heat shock proteins (HSPs) are known to play a key role in cellular response against a variety of stresses including ionizing radiation and heavy metals. Differential effect of Th was observed on protein levels of HSP70 and HSP90 studied in human normal lung epithelial cells. A significant increase in gamma-H2Ax foci was found after treatment with Th-nitrate or Th-dioxide, which was found to be decreased by pretreatment with thiol antioxidant, N-acetyl cysteine (NAC).

Immune Stimulation by chlorophyllin

Chlorophyllin was found to improve the innate immunity in terms of higher phagocytic efficiency of macrophage cell line as well as in mouse peritoneal exudate cells. Chlorophyllin increased the uptake of bacteria by macrophages and enhanced the efficiency of phagosome acidification.

Development of Immune Markers for Radiation Exposure

Concanavalin A induced IL-2 release from splenic lymphocytes was correlated to lethal (8.5 Gy) and sub-lethal (4 Gy) doses of IR. After sub-lethal (4Gy) irradiation, IL-2 was suppressed at 4h time point but it recovered at 16h time point (green arrows). However, in response to lethal dose (8.5 Gy), suppression of IL-2 was seen at both 4h and 16h time points.

Epidemiological Studies for Assessing Risk of Low Dose and Low Dose Rate Radiation Exposure on Human Population

The human population residing along the monazite bearing Kerala coast are exposed to chronic low dose and low dose rate radiation due to Th232 deposits in its beach sand. The external gamma radiation level in this area varies from <1.0 to 45.0 mGy/year. The areas with a dose level of ≤ 1.50 mGy/year are considered normal level natural radiation areas (NLNRAs) and areas with >1.50 mGy/year, as high level natural radiation areas (HLNRAs). It provides ideal source for conducting large-scale epidemiological studies for assessing risk of low dose and low dose rate radiation exposure on human population.

Molecular and Cellular basis of Radioresistance in *Deinococcus Radiodurans*

Deinococcus radiodurans is known for extreme resistance to otherwise lethal doses of gamma radiation. Molecular basis of resistance to gamma radiation has been studied at various levels. The findings highlight (i) the existence of a new type of DNA damage response and cell cycle regulation that is similar to eukaryotic mechanisms and distinctly different from known mechanisms in other bacteria, and (ii) role of non-canonical secondary structure of DNA in radioresistance and regulation of gene expression in response to gamma radiation exposure.

Effect of Ser/Thr Phosphorylation on the Function of Cell Division Proteins

A Ser/Thr quinoprotein kinase (RqkA) characterized from *Deinococcus radiodurans* could phosphorylate its two cell division proteins FtsZ and DivIVA that play crucial roles in bacterial cell division. Phosphosites of these proteins were mapped mass spectrometrically and mutated with corresponding

phosphor-ablative and phosphor-mimetic residues. Transmission electron microscopy (TEM) of FtsZ mutants phosphor-ablative (ZAA) and phospho-mimetic (ZDD) suggested the negative effect of S/T phosphorylation on functional integrity of FtsZ. Real time dynamics of phosphomutants of FtsZ and DivIVA were monitored microscopically. Results supported in vitro results confirming the arrest of these proteins dynamics upon Ser/Thr phosphorylation by RqkA.

Bio-markers Identification in Neuroendocrine Tumors

Neuroendocrine tumors (NETs) are rare cancers that originate in specialized neuroendocrine cells present throughout the body. These tumors are often advance to metastatic stage at diagnosis which is based on serum chromogranine A levels and staining for proliferative marker Ki-67. The patients are treated either with radionuclide therapy, chemotherapy or both. Currently no biomarkers are available to predict which NET patients would benefit from the available treatment options. In a pilot study carried out in collaboration with Radiation Medicine Centre, whole blood transcriptome sequencing was carried out on 50 samples (12 Healthy, 38 NETs) to evaluate potential biomarkers. Among 4000 genes that were differentially expressed between the 2 sets (Healthy versus NETs), top 30 genes could segregate the samples correctly into healthy or NET groups.

Cellular and Molecular Understanding of the Microbial Responses Towards Uranium/Heavy Metal Toxicity

Under the context of cellular and molecular understanding of the microbial responses towards uranium/heavy metal toxicity, studies on bacterial motility and proteins important for maintenance of metal homeostasis such as PIB ATPase and metallothionein, were carried out.

Uranium tolerant soil bacterium *Chryseobacterium* sp. strain PMSZPI moved over solid agar surfaces by gliding motility thereby forming spreading colonies. PMSZPI genome harbored orthologs of all the *gld* and *spr* genes considered as core bacteroidetes gliding motility genes of which *gldK*, *gldL*, *gldM*, and *gldN* were found to be co-transcribed. The nutrient deficiency enhanced colony spreading whereas high agar concentrations and presence of motility inhibitor like 5-Hydroxyindole reduced the spreading. A detailed *in situ* structural analysis by bright field microscopy and scanning electron microscopy of spreading colonies revealed closely packed cells forming multiple layers at the center the of colony while the edges showed clusters of cells periodically arranged in hexagonal lattices interconnected with each other. PMSZPI colonies exhibited strong iridescence or structural coloration possibly as a result of periodicity within the cell population achieved through gliding motility. Presence of uranium reduced motility and iridescence and induced biofilm formation.



MEGA SCIENCE AND COLLABORATION

BARC is deeply engaged in high profile multi-lateral joint collaboration projects in the areas of high energy nuclear physics and technology involving the Large Hadron Collider at the CERN and Fermilab. Apart from its contribution to such high value and long gestation scientific ventures, BARC is committed to establishment of futuristic projects within the country, which include the setting up of a ground based Major Atmospheric Cherenkov Experiment telescope for exploring the gamma ray universe, and also a Neutrino Observatory (INO).



BARC supplied eight 7 kW, 325 MHz RF power amplifiers (RFPAs) in Fermilab, USA

Mega Science and Collaboration

MACE Telescope

The Major Atmospheric Cherenkov Experiment (MACE) Telescope set up by BARC in Hanle, Ladakh will aid the efforts for observing of a variety of Very High Energy gamma-ray sources, which can provide clues about the enigmatic jet formation process near black holes. MACE enables to explore astrophysical phenomena in the Universe that are not accessible to the terrestrial accelerators.

India based Neutrino Observatory

The India-based Neutrino Observatory (INO) project is aimed at studying the properties and interactions of neutrino in an underground laboratory in the south of India. The INO project would witness setting up of a flagship Iron Calorimeter (ICAL) detector and the Inter-Institutional Centre for High Energy Physics (IICHEP).

The copper coil for engineering module ICAL magnet of INO project for detection of high energy physics/cosmic particles working model has been completed. 76 pieces of conductors each in two sections (upper "C" section and lower "U" section) have been straightened and cut to size. The engineering prototype ICAL coming up at Madurai comprises 7 RPC detectors, integrated with gas set up and an energized magnet. The RPCs have started detecting cosmic muons. Their positions on "X" and "Y" coordinates are displayed on a screen at a capture frequency of 30 events per minute.



Oxygen free copper conductor spool for ICAL magnet of INO

CERN (European Council for Nuclear Research)

Indian partners from Department of Atomic Energy have been contributing significantly towards ALICE and CMS experiments at the CERN's Large Hadron Collider (LHC), including design and fabrication of several important detector components.

LHC - India

Indian scientists were involved in the design of several components for LHC manufactured through Indian industries. Some of the major Indian contributions to LHC are

- Superconducting corrector magnets
- Precision magnetic positioning system jacks
- Accelerator protection systems
- Quench detection electronics
- Vacuum system design for long beam transport lines and cryogenic systems.

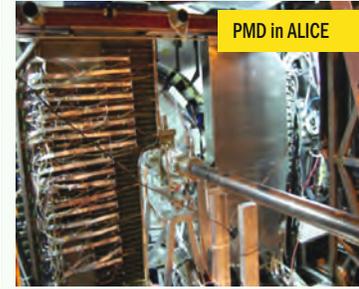
A Large Ion Collider Experiment (ALICE) - India

Protons and neutrons are made of quarks bound together by particles called gluons. LHC provides collisions between lead ions. Extremely high energy densities during the collision recreate conditions similar to those just after the Big Bang and the quarks are freed from the gluons, forming what is called the quark-gluon plasma (QGP). The collaboration has more than 1000 scientists from over 100 physics institutes in 30 countries. Indian scientists had a significant role in the ALICE Experiment leading to the discovery of QGP. Indian Hardware contributions to the ALICE Experiment are

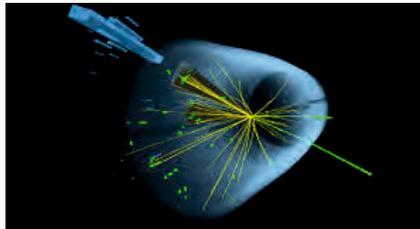
- Photon Multiplicity Detector (PMD)
- Muon Spectrometer
- MANAS chip
- Silicon pad detectors.



Alice Detector



Photon Multiplicity Detector based on proportional counter technology



Higgs Boson



CMS Experiment

CMS - India

The CMS (Compact Muon Solenoid) detector is built around a huge superconducting solenoid magnet generating a field of 4 Tesla, about 100,000 times the Earth's magnetic field. The CMS experiment is one of the largest international scientific collaborations in history, involving 182 institutes in 42 countries.

Indian scientists have played a major role in the CMS experiment, which is one of the two experiments that discovered the Higgs Boson.

They were responsible for Design and manufacture of Hadron Barrel Outer Calorimeter as well as on Silicon strip based pre-shower detector and RPC detectors.

Indian scientists have contributed to the physics analysis that led to the discovery of Higgs Boson and a detailed study of QGP.

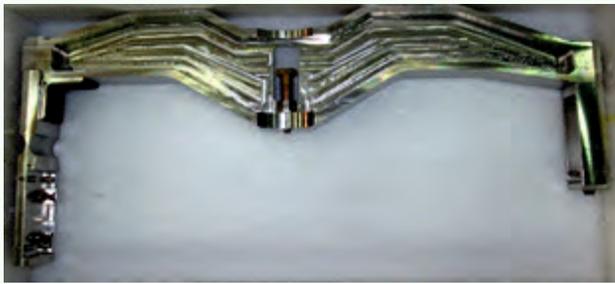
Experiments at CERN produce about 30 petabytes of data annually, shared by several institutions located around the world using Large Hadron Collider Grid (LCG).

Indian scientists contributed substantially to the building and operation of the LCG. India hosts two Tier 2 LCG centres at Variable Energy Cyclotron Centre (VECC) and Tata Institute of Fundamental Research (TIFR), in addition to several Tier 3 centers.

The two centres at VECC and TIFR process a large part of the LHC data.

The Indian Institutions And Fermilab Collaboration (IIFC)

Established in 2009 as part of an understanding between the Fermilab and the four Indian laboratories for collaborative R&D on superconducting radio frequency (SRF) technologies as applied to high-intensity proton linear accelerators. Advanced state of art solid state radio frequency (RF) power amplifiers, designed and developed by BARC are an integral part of Fermilab's beam facility in the US.



The SSR-1 Tuner made in BARC for superconducting RF cavities in SSR1 Cryo-module of FermiLab, USA.

Tuner for Single Spoke Resonator for superconducting RF cavities

Development of two units of SSR-1 Tuner was taken up in BARC under the IIFC. These tuners will be used to tune 325MHz SSR1 superconducting RF cavities in SSR1 Cryo-module for accelerating the H⁺ ion from 10.3 MeV to 35 MeV.

The tuner compensates for the uncertainties in the frequency shift of the cavity due to drastic cooling from 293K to 2K, and to minimize detuning caused by helium pressure fluctuations and micro-physics perturbations. Each Tuner consists of 32 manufactured items.

Trial assembly of the manufactured components has been dispatched to Fermilab, USA.



HUMAN RESOURCES, SCIENTIFIC INFORMATION RESOURCES AND TECHNOLOGY MANAGEMENT

BARC appoints scientific and technical manpower for its pan-India facilities through a carefully crafted testing process wherein selected candidates, mostly fresh graduate engineers, and masters from university systems are subjected to a rigorous program of training at its well-equipped Training School facility in Mumbai. BARC houses a large treasure of scientific literature which is stored in physical as well as in digital form to meet the requirements of the centre. Understanding the growing desire among users to increasingly access information virtually, it is continuously implementing new state-of-art technologies to ensure seamless access to first-hand high quality scientific data. To boost entrepreneurial zeal among the young generation, BARC has expanded its technology incubation infrastructure at its Mumbai campus and is also offering a wide gamut of technologies for mass production.



BARC Training School in Anushaktinagar, Mumbai

Human Resources, Scientific Information Resources and Technology Management

BARC Training School

Dr. Homi Jehangir Bhabha strongly professed that in order to achieve self reliance in nuclear energy sector, it is imperative to build a sustained pool of highly skilled human resources from the ranks of talented workforce which is readily available within the country. Keeping this in mind, he conceptualized the creation of specialized Training Schools in the Department of Atomic Energy (DAE) and the first BARC Training School was established in Trombay in 1957, as a centre for in-house training of professionals. Over the years, it has grown into an internationally acclaimed school of excellence with more than 9000 Scientists and Engineers graduating from it in flying colors.

BARC Training School runs two flagship programs - OCES (Orientation Course for Engineering graduates and Science Postgraduates) and DGFS

(DAE Graduate Fellowship Scheme) for which it picks young graduates from across the country through a carefully crafted selection process.

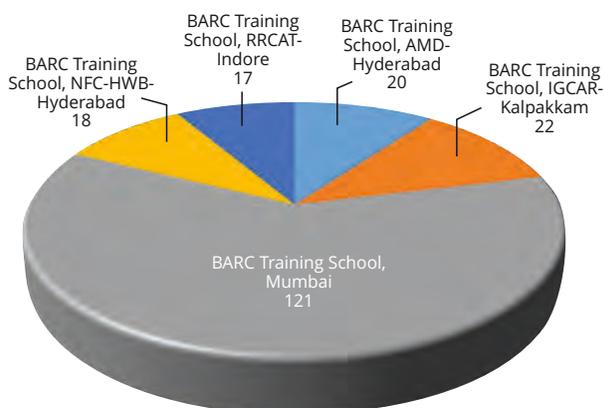
Recruitment

A total of 91 graduating TSOs of 64th batch of OCES/DGFS-2020 (57 engineering+ 14 physics + 7 chemistry + 7 biosciences + 6 RSES), after successful completion of training, were placed in various units of DAE. There were 8 Trainee Defence Officers, who passed out with this batch and were assigned to different Divisions/Units for undertaking project for MTech.

The linkage of BARC Training School programs with the Homi Bhabha National Institute (HBNI), a deemed-to-be-university of DAE, ensures

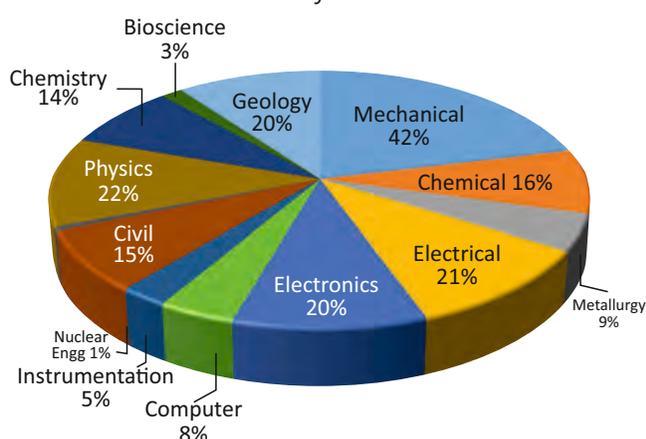
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OCES-2021 Total Numbers Selected for BARC Training School at different locations



Number of selected OCES/DGFS-2021 candidate for various BARC Training Schools.

OCES-2021 Total Number of Candidates Finally Selected



Discipline-wise total selection of candidates for OCES/DGFS 2021.

continuous availability of professionally qualified, well trained scientific and technical manpower for induction into various units of DAE.

Upskilling of Scientific and Technical Manpower

Under DAE's Continuing Education Programme (CEP) for upskilling of technical manpower working in the department, QUEST programme is conducted in BARC in which courses on varied themes, including on Process Modeling, Simulation and Optimization and Reliability Engineering have been offered during the year. Besides, it offers practical training and academic projects for students of BE/BTech/MTech/ME/MSc/MCA/JRF/SRF.

Collaboration with Educational Institutions

BARC offers collaborative Fellowship programs in Physical, Chemical and Life Sciences and several other domains under its tie-ups with Mumbai (CEBS) and Pune Universities and also with IITs and IISc.

Scientific Information Resources Publishing of Books

Publishing of scientific literature based on key R&D outcomes in BARC as well as in other constituent units of DAE on a regular basis is accorded top-most priority. During the year, HBNI has assisted BARC, IGCAR and AERB in their joint efforts to publish a 767-page comprehensive book titled "Physics of Nuclear Reactors" on topics related to reactor physics based on 60 years of experience of various experts and peers in DAE and it is intended for entry level scientists and engineers in nuclear energy arena. The book was edited by P. Mohanakrishnan, Om Pal Singh and K. Umasankari, and published by Elsevier/Academic Press.

In addition to this, BARC has published a book titled "Non Power Applications of Nuclear Technologies" in 2021. The book comprises 19 chapters, which highlight R&D activities in BARC in the development of nuclear technologies having widespread industrial applications. The 285-page book jointly edited by Dr. A.K. Mohanty, Director BARC and Dr. A.K. Tyagi, Chemistry Group Director, BARC, was granted ISBN recognition.

BARC Website

The official website of BARC has been equipped with the latest Content Management System based technology features which now make it highly mobile friendly. As a result of these measures, the website provides better navigation and rich experience for internet users, which is reflected in significant jump in number of visitors to the website. Over 51,000 users visit the website



Shri K.N. Vyas, Chairman AEC, Dr. A.K. Bharadwaj, Former Head AERB and Dr. A.K. Mohanty, Director BARC releasing the book Non-Power Applications of Nuclear Technologies on Founder's Day event in BARC Trombay.

consistently on a month-on-month basis with 95% of them accessing it through Android based devices.

Augmentation of Digital Resources

A fresh apex project - *Digital Resources for R&D Support* - was approved with an outlay of Rs 42.10 crore for implementation of advanced digital information resource platforms through acquisition of new servers and network devices in BARC. Access to knowledge resources of BARC Library digitally was made easy with the launch of upgraded version of Saraswati portal in November this year. BARC has employed Open Source Stack software based tools in overhauling the portal, which now hosts extensive archives of published scientific and technical literature.

Publications

R&D work carried out by the scientists and engineers of BARC is published regularly in its bi-monthly publication BARC Newsletter. During the

year, six issues of newsletter were published on various themes, including Nuclear Reactor Technology, Research in Physics, Atomistic Modelling and Simulations and Applications of Computational Fluid Dynamics in Chemical Engineering, Materials Science and Safety. These are available on the official website.



BARC Newsletter Issues published in 2021

Human Resources, Scientific Information Resources and Technology Management



BARC Central Library

Specific scientific works carried out in BARC are published in the form of reports regularly.

During the year, 31 Internal, 23 External and 05 Restricted reports were published. Three issues of in-house magazine - *Pulse* - of BARC Hospital were also released.

Nuclear News Web Digest is a latest initiative which has been introduced to keep BARC scientific community abreast of day-to-day happenings in nuclear energy arena. Articles published in various dailies are collated and featured in an easy-to-read format in the weekly Web Digest.

Management of Archives

Unique scientific reports, rare photographs, and published copies of conference proceedings and seminars are preserved and maintained properly through creating dedicated portals. Around 4300 reports which are considered quite unique have been archived so far in BARC.

International Nuclear Information Service

The International Nuclear Information Service (INIS) of IAEA in India has been augmented with journal articles, conferences and reports totalling more than 4000 in nuclear energy domain

published by multiple scientific agencies within the country during the year.

Foreign Language Translation and Interpretation

Translation of scientific documents from French, German and Russian into English as well as interpretation services are provided regularly to cater to the specific requirements of various groups of BARC and the constituent units of DAE.

Similarity Checking of Manuscripts

To ensure scholarly work of BARC scientists reflects originality, similarity checks are performed and reports were generated for 700 articles and 100 PhD theses during 2021.

Technology Management

BARC is actively involved in the deployment of technologies which possess non-power applications on a large scale, both industrial and societal.

The activities of BARC Centre for Incubation of Technology (BARCIT) have been reinvigorated through creation of state-of-art infrastructural facilities for carrying out technology incubation activities towards imparting entrepreneurial zeal among the young generation so that they increasingly transform their careers to become job-givers rather than being job-seekers. An MoU was inked for incubation of "Development of Carbon Nanotube-Boron Carbide (CNT-B4C) composite tiles by hot pressing and "Strong Motion Seismic Instrumentation system for Nuclear Power Plants" technologies. Further, it has advertised for potential partners in the incubation of "Handheld Gamma Spectrometer based on Cesium Iodide (CsI) Single Crystal" technology.

BARC has entered into several technology agreements with private parties in the areas of Nuclear Instrumentation; Industrial, Medical and

Environmental applications; and healthcare among others. As part of management of Intellectual Property Rights issues, a dedicated IPR cell has also been established.

Technology Transfer

About 210 different technologies of societal benefit across various fields of science and engineering are published by BARC for technology transfer and about 400 licensees are commercializing such technologies in urban and rural sectors of the country till date.

Under the 'Azadi Ka Amrit Mahotsav' drive, BARC is offering a one-time 75 per cent concession in license fee charged by it in return for transferring of technologies to interested parties, which is valid up to September 2022.

A total of 52 technologies were transferred by BARC to 78 parties pertaining to agriculture, radiation processing, medical, environment, engineering, chemical and water domains during 2021.

In addition to this, BARC released 31 new technologies into the public domain during the year.

Radiation technologies introduced by BARC into the public domain include 10 MeV Linac for Radiation Processing Applications; ANUSUCHAK, a dongle for detecting elevated levels of Gamma Radiation; Industrial Fluoroscope Technology; Radiation Monitoring Watch; Ultra Flexible Lead-Free X-Ray Shields and a Quick Scan Whole Body Monitor.

In the medical domain, the newly introduced technologies include HDR Brachytherapy System "Karknidon-I"; Taap Darshak- remote monitoring of human body temperature; Engineered Valveless Transparent Face Mask (EVTFM); A CRISPR-based integrated system for detection of Covid-19; ABS IMRT/VMAT Phantom - for pre-treatment dose verification in Intensity Modulated Radiation



Technology transfer of Engineered Valveless Transparent Face Mask (EVTFM).

Therapy (IMRT)/Volumetric Modulated Arc Therapy (VMAT). Engineering industry related technologies include Serial Coordinate Measuring Mechanism (SCMM); Process for production of copper selective polymeric resins; Production of high purity Copper Oxide nanoparticles from de-populated Printed Circuit Boards (e-waste) using novel Cu-selective ligand grafted polymeric resins & Synthesis of novel copper selective polymeric resins; Atmospheric Pressure Plasma Jet" technology; 100kW, 35kV Electron Beam Melting (EBM) Gun Column for Metallurgical Application; Liquid Nitrogen Based Transportable Refrigeration System for Vaccine - Sheetal Vahak Yantra (SHIVAY-V); Liquid Helium (LHe) Dewar; 10 kW, 15 kV Electron Beam Melting Machine and 2 kW Electron Beam Welding Machine. Environment related technologies are Dissolved Oxygen (DO) Monitor (Model-1); Upgraded NISARGRUNA - Biogas plant based on Biodegradable waste and Compact Helical Biodegradable Waste Converter - SHESHA. For chemical industry, BARC has made available Visual Detection Kit (VDK) for monitoring ethanol in petrol; Preparation of Pb-Li alloy by fused salt electrolysis; Accurate estimation of alcohol content in alcoholic products through easy Synthesis of BODIPY dye; Nano-Ni Coating on Difficult-to-Plate Upon Metals/Alloys.

Renewal of Technology Licences

The licenses granted to private parties for commercial scale implementation of the following technologies were renewed for additional 5 years. These include Inductively Coupled Plasma Mass Spectrometer (ICPMS), Fluoride Detection Kit for ground water (FDK) and Nitrogen oxides releasing wound dressing.

Advanced Knowledge & Rural Technology Implementation Program

57 licences were granted to various parties interested in 17 BARC technologies under Advanced Knowledge & Rural Technology Implementation (AKRUTI) program. The licensee partners are spread across Odisha, West Bengal, Bihar, Uttarakhand, Rajasthan, Tripura, Andhra Pradesh, Tamil Nadu, Uttar Pradesh and Maharashtra. A total of 12 AKRUTI Agreements were signed with various parties for deployment of BARC technologies in rural areas. Technologies that were of interest to them include delicious & preservative-free shelf stable natural jamun product; a post-harvest technology for the development of intermediate moisture shrimp; development of instant fish soup powder; Banana health drink and gluten free- multigrain pre-mix.

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OUTREACH

Being a highly reputed multi-disciplinary R&D centre for advancement of nuclear energy activities in the country, BARC is committed towards educating citizens on the positive benefits of nuclear energy in the long term. Students of all levels, Private persons, Defence staff, VIPs and members of the Press are provided multiple opportunities to visit BARC to gain first-hand knowledge on the day-to-day activities conducted in BARC.

Outreach

As part of the year-long Azadi Ka Amrit Mahotsav celebration in BARC to mark 75th year of Indian Independence during 2021-22, BARC has lined up several activities, including publishing of new scientific documents and books in bi-lingual form (Hindi and English), organise farmer-scientist interactions, conducting student seminars and lectures both online and offline, short films for popularizing atomic energy across wide strata of the society. Many of these activities have already been put into motion. Some of these are presented in a nutshell in this chapter.

Interactions between Farmers and Scientists

1. Workshop on fruit crops protection held at Krishi Vigyan Kendra (ICAR) situated at Kosbad Hill in Palghar, Maharashtra.
2. Workshop-cum-Distribution of seed kits to farmers for Popularization of Mutant Rice Varieties (Vikram TCR & CGJT) and field demonstration of these new rice varieties at Indira Gandhi Krishi Vishwavidyalay in Raipur, Chhattisgarh.
3. Workshop on Soil Health for Growers & Producers' Association held at the Department of Agriculture, Government of Uttar Pradesh in Varanasi.
4. Workshop on Peaceful Applications of Radiation Technology in Agriculture & Food Preservation & Demonstration of BARC Crop Protection Technologies was organized across various states of India, including at three locations in Rajasthan through Agricultural University of Rajasthan; at Palampur in Himachal Pradesh as well as in Odisha and Maharashtra.
5. Field demonstration on determining ammonia in aquaculture waters for the benefit of aquaculture farmers in Telangana and Andhra Pradesh by BARC scientists held under the auspices of NCCCM Hyderabad.



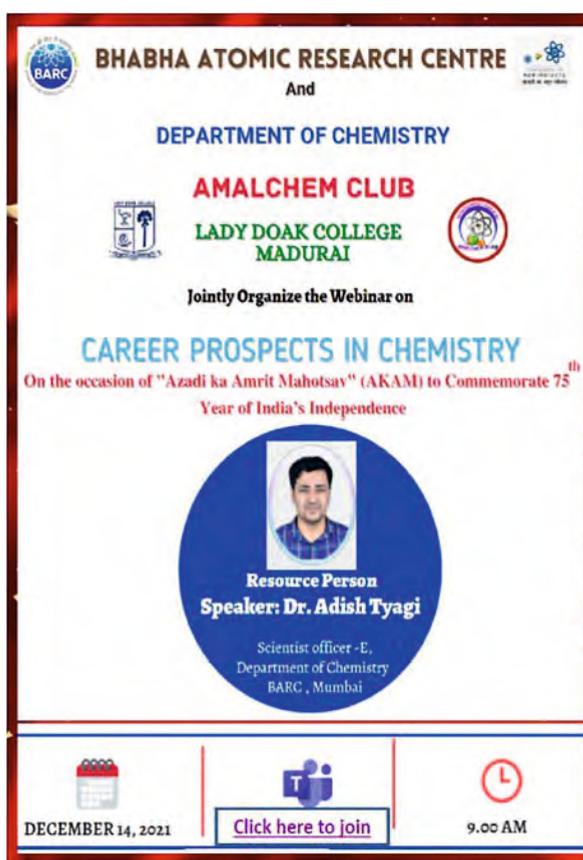
NCCCM Hyderabad organised workshop for the benefit of aquaculture farmers in Telangana and Andhra Pradesh

Student-Scientist Interactions

1. Lecture series on Career prospects in Chemistry by senior scientists of BARC Chemistry Group was held in online mode for the benefit of students of Department of Chemistry in Lady Doak College in Madurai.
2. Online lecture series on the topic - Chemistry for Societal Benefits - by scientists of BARC Chemistry Group.
3. Webinar on "BARC Technologies for solid waste management through biological route" for the students of SIES college of Arts, Science & Commerce College in Mumbai.
4. Seminar-cum-education program on Accelerators, Plasma and Pulse Power for students of colleges in the vicinity of BARC facilities in Mumbai and Visakhapatnam.

Public Awareness

BARC had chalked out a long drawn program for sensitizing people from all walks of life on the positive impact of nuclear energy. The Centre attracts wide range of audience from both India as well as abroad regularly, which includes scientists onboard joint collaborative projects inked under inter-governmental understanding and visits by VIPs. Besides this, BARC encourages students to visit its campuses, an initiative which aims to educate young minds on the positive impact of R&D activities in atomic energy. Highly experienced scientists and engineers interact and explain to students multi-disciplinary mode of research in BARC and their contribution to overall national development.



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Grain Irradiator facility

INFRASTRUCTURE DEVELOPMENT