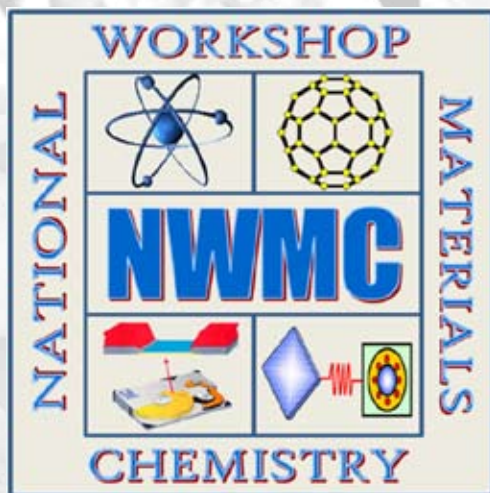


*Proceedings of*  
**DAE-BRNS**  
**5<sup>th</sup> NATIONAL WORKSHOP**  
**ON MATERIALS CHEMISTRY**  
**(NANO & COMPOSITE MATERIALS)**  
**NWMC – 2019 (NCom-Mat)**



**November 8-9, 2019**

*Venue*

Manipal University Jaipur  
Jaipur-Ajmer Expressway  
Jaipur, Rajasthan 303007

*Organised by*

Society for Materials Chemistry (SMC)  
C/o Chemistry Division, BARC  
Mumbai - 400085

&

Department of Chemistry  
School of Basic Sciences  
Manipal University Jaipur  
Rajasthan 303007



**NWMC - 2019**





**Proceedings of DAE-BRNS  
5<sup>th</sup> National Workshop on  
Materials Chemistry (Nano & Composite Materials)**

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Web site: [www.smcindia.org](http://www.smcindia.org)

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Manipal University Jaipur, Rajasthan 303007

November, 2019

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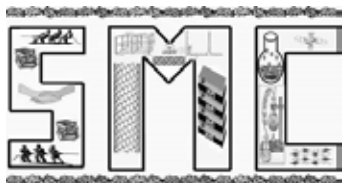
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## SOCIETY FOR MATERIALS CHEMISTRY (SMC)

Society Reg. No. – Maharashtra State, Mumbai, 1229, 2008 GBBSD

Public Trust Reg. No. F-38063, Mumbai Dt. 29-8-2009

Office Address:

C/o Chemistry Division

Bhabha Atomic Research Centre, Mumbai-400 085, India



### *Message*

I am happy to note that Department of Chemistry, School of Basic Sciences, Manipal University Jaipur, in association with Society for Materials Chemistry (SMC) is organizing the 5<sup>th</sup> DAE-BRNS National Workshop on Materials Chemistry focused on Nano & Composite Materials (NCom-Mat) during 8-9 November, 2019. This is for the first time that the NWMC is being organized away from the SMC Headquarters in Mumbai.

Nano and composite materials have taken a central stage in advancement of materials science in recent times with an emphasis to design and synthesis of new materials with unique properties which can be exploited for various applications. The spectrum of nano and composite materials is very wide covering diverse areas in energy, environment and health. In particular, interest in new catalytic systems for industrially and environmentally important reactions, materials for energy and health care which may range from sensors to drug delivery, is growing rapidly.

The Society for Materials Chemistry (SMC) is making an impressive progress since its inception in 2007 with Chemistry Division, BARC, Mumbai as its Headquarters. The Society is a registered public trust with more than 1200 life members. SMC has been promoting education, advancements and applications in materials chemistry through various platforms like biennial symposia-‘Interdisciplinary Symposium on Materials Chemistry’ (ISMC) and national Workshops (NWMC) as well as thematic symposia. SMC publishes ‘SMC Bulletin’ both thematic and contemporary topics in materials chemistry on regular basis and also arranges series of lectures by eminent scientists.

I take this opportunity to express my sincere gratitude to all the members of the Society for their support and cooperation in the growth of SMC. It will not be out of place to acknowledge the painstaking efforts and enthusiasm of the organizers of 5<sup>th</sup> NWMC. I am confident that the deliberations in NWMC – 2019 (NCom-Mat) will educate students and young researchers.

I extend my best wishes to the success of the 5<sup>th</sup> NWMC.

V.K. Jain  
President, SMC





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Government of India  
Bhabha Atomic Research Centre  
**Chemistry Group**

**Dr. Sudhir Kapoor**

Outstanding Scientist, DAE &  
Associate Director (D),  
Chemistry Group,  
B.A.R.C.

Ref: CG/NWMC-2019/

October 18, 2019



I am delighted to know that 5th DAE-BRNS National Workshop on Materials Chemistry (NWMC-2019: NCom-Mat), focused on Nano and Composite Materials is going to be held during at Manipal University, Jaipur during 8-9 November, 2019, which is jointly organised by Society for Materials Chemistry (SMC), C/o Chemistry Division, BARC and Manipal University Jaipur.

Conventionally material's chemistry plays an important role for betterment of human life. The never-ending quest of human beings to search still better materials has led to the evolution of nano-chemistry, which is the prime-theme of this workshop. Nano and composite materials covers a wide range of materials in the Nano domain with potential application in key technological areas. I am informed that more than hundred young researchers from different parts of country will be attending the workshop, where different aspects of the subject will be covered by experts. I sincerely hope that the young minds will be enriched from the deliberations during the workshop.

I extend my best wishes to the workshop in achieving its objectives.

*Sudhir Kapoor*

(Dr. Sudhir Kapoor)  
Associate Director (D), Chemistry Group



**Dr. A. K. Tyagi**  
(FRSC, FNASc, FASc)  
Head, Chemistry Division  
Bhabha Atomic Research Centre  
Mumbai-400 085

Email: aktyagi@barc.gov.in  
Phone: 022-2559 5330



## MESSAGE

I am delighted to know that DAE-BRNS 5<sup>th</sup> National Workshop on Materials Chemistry, (NWMC-2019) is being organised at Manipal University Jaipur, by School of Basic Sciences, and Society for Materials Chemistry during November 08- 09, 2019.

It is now widely appreciated that various properties of the materials can be augmented by downsizing the particle size to nano-regime. Various properties of nanomaterials such as mechanical strength, electrical resistivity and optical absorption, just to name a few, are significantly different from that of the same material at the bulk-scale. Over the last few decades, scientists have been able to capitalise this aspect to develop smart materials having myriad applications in various fields such energy, medical and healthcare, electronics, catalysis, drug delivery etc. A typical example is flexible, bendable, foldable, rollable, and stretchable electronics which had been made possible only due to carbon nanostructures such as carbon nanotubes, graphenes etc. Another vital approach that has been adopted for tailoring of material properties involves compositing two or more materials having desired properties to obtain materials that have synergistic or antagonistic amalgamation of characteristics of its constituents as well as new properties originating from the behaviour of interface of the components.

There is no denying the fact that the next big technology is nanotechnology and I am really glad to know that a workshop on such an important theme is being organised for the benefit of young researchers and faculty members.

I heartily compliment the organisers for arranging the workshop on such a contemporary theme and I wish it a grand success.

Dated: 17-10-2019

  
(A. K. Tyagi)







**MANIPAL UNIVERSITY  
JAIPUR**

Prof K. Ramnarayan, *MBBS, MD(Pathology), PG Dip. Higher Education*  
*Chairperson*



## Chairperson's Message

With great pleasure I welcome you to **DAE-BRNS 5<sup>th</sup> National Workshop on Materials Chemistry (NWMC-2019) (NCom-Mat)** on **November 8<sup>th</sup> and 9<sup>th</sup>, 2019** at Manipal University Jaipur, jointly organized by Society for Materials Chemistry (SMC), Chemistry Division, Bhabha Atomic Research Centre (BARC) Mumbai and Department of Chemistry, School of Basic Sciences, Manipal University Jaipur.

NWMC-2019 is uniquely positioned to share experiences, talks, basic and applied aspects of material science and technology through the two-day technical sessions. Let this workshop would provide a robust platform for the academia, R&D and industry from across the country with the aim to assist industries to develop technologies that are reliable, safe and efficient and conserve resources and the environment for a better future.

The workshop of this stature has an important intangible outcome to be achieved and that is to foster future collaborations nationally and internationally. I do hope NWMC-2019 provides delegates and the supporting organizations rewarding experiences, both at technical and personal level with enhanced new friendships, apart from the value addition in competence and networking for carrying out one's responsibilities much more effectively. I hope the delegates will have a comfortable stay and they will enjoy the traditional Rajasthani hospitality.

My best wishes to all delegates, speakers, participants and organizers for the resounding success for this event.

**Dr K Ramnarayan**  
**Chairperson**  
**Manipal University Jaipur**







MANIPAL UNIVERSITY  
JAIPUR

Dr G K Prabhu, BE, MTech, PhD  
President



President's Message

I am glad to learn that the **DAE-BRNS 5<sup>th</sup> National Workshop on Materials Chemistry (NWMC-2019), (NCom-Mat)** is being organized at Manipal University Jaipur (MUJ) during November 08 - 09, 2019 by Society for Materials Chemistry (SMC), Bhabha Atomic Research Centre (BARC), Mumbai in association with Department of Chemistry, MUJ. It is my proud privilege to welcome the distinguished guests and delegates at Manipal University Jaipur – a premier academic institution of Northern Region.

The ever-increasing demand to conserve resources and environment and the need for developing sustainable materials to face increasingly demands remains not only a challenge for scientists but also engineers and policy makers. This workshop will foster an eco-system while deliberating the recent technologies and cutting-edge research to tackle the problems through a mutual partnership of academia and industry in order to overcome the impediments in translating basic science into technological reality.

The various thematic sessions will showcase important scientific advances and highlight impacts of new materials for development of sustainable technologies. I again welcome and invite all of you to attend the plenary talks and oral presentations to interact with the workshop participants during the sessions.

I would like to congratulate the Department of Chemistry for their initiative and hard work and wish the NWMC-2019 a grand success.

Dr. G.K. Prabhu  
President  
Manipal University Jaipur



# NWMC – 2019 (NCom-Mat)

## Chief Patron

Dr. K. Ramnarayan Chairperson MUJ

## Patron

Dr. G. K. Prabhu President MUJ

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Dr. V. K. Jain	Director CEBS, Mumbai
Dr. Sudhir Kapoor	AD Chemistry Group, BARC
Dr. K. I. Priyadarsini	CEBS, Mumbai
Dr. H. R. Kamath	Registrar MUJ
Dr. A. Mukhopadhyay	Dean FoS MUJ

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Convener	Dr. Sandeep Nigam, BARC, Mumbai
Co-convener	Dr. Rahul Shrivastava, MUJ
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Mr. Dalip S. Shekhawat	Dr. Prabhat Ranjan	Dr. Susruta Samanta
Dr. Debasis Behera	Dr. Pushpendra Kumar	

### Sub Committes - NWMC-2019

Sr. No.	Committee	Coordinators	Members
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2.	<b>Publicity Committee</b>	Dr. Nitu Bhatnagar	Dr. D. Behera Dr. M. Prabhu Dr. Santosh Patil Dr. Dalip Singh Shri K. Sandeep Rao
3.	<b>Registration Committee</b>	Dr. Naveen Kumar Dr. Susruta Samanta Dr. Deepak Tyagi	Dr. Abhijeet Singh Dr. Rajeev Mishra Dr. Rakesh Sharma Shri K. SandeepRao <b>Students:</b> Ms. Kruti K. Halankar Mr. Puruman Singh Rathore Ms. Jyoti Sharma Ms. Priyanka Pareek Ms. Khyati Malik Ms. Devanshi Ledwani
4.	<b>Accommodation</b>	Dr. Arunava Agarwala Dr. Susruto Samanta	Dr. Ajay Kumar Dr. Abhiroop Chowdhary Dr. K. C. Barick

			<b>Students:</b> Mr. Puruman Singh Rathore Mr. Abhishek Sharma Ms. Kanchan Mr. Tushar Mr. Bhanupratap Ms. Subhanushi Mr. Sandeep Rana
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6.	<b>Technical Committee</b>	Dr. Arunava Agarwala Dr. Susruto Samanta	Dr. Abhishek Sharma Dr. Mousumi Debnath Dr. Linesh Raja Dr. Garima Dr. Rashi Nathawat Dr. C. A. Amarnath <b>Students:</b> Ms. Kruti K. Halankar Ms. Mona Vajpayee Ms. Mumal Singh Ms. Shubhra Pareek Ms. Pranjal Mr. Divyansh Choudhary
7.	<b>Catering Committee</b>	Dr. Indeewar Dr. Pushpendra Dr. Michel Prabhu Inbaraj	Dr. Deepak Tyagi Shri K. Sandeep Rao <b>Students:</b> Mr. Neeraj Gaur Mr. Amit K. Sharma
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9.	<b>Printing</b>	Dr. Deepak Tyagi Dr. Adish Tyagi Dr. Rohit Jain	Dr. Sriparna Ray Dr. Ajay Saini <b>Students:</b> Mr. Puruman Singh Rathore Mr. Abhishek Sharma
10.	<b>Certificate</b>	Dr. K. C. Barick Dr. Sriparna Ray	Dr. C. A. Amarnath Dr. Adish Tyagi <b>Students:</b> Mr. Puruman Singh Rathore Mr. Tarun B. Kriplani Ms. Suman Yadav Mr. Ashish Sharma Ms. Shruti Sujit Ms. Hitlesh Ajmera
11.	<b>Cultural</b>	Dr. Babita Malik Shri Dheeraj Jain	Dr. Meenakshi Pilania Dr. Mousami Debnath <b>Students:</b> Ms. Kruti K. Halankar Mr. Manan Ms. Nandita Ms. Shivangi Tripathi
12.	<b>Photography and Media</b>	Dr. Deepak Tyagi Dr. Abhiroop Chowdhury	Dr. K. P. Mishra Dr. Rakesh Sharma Dr. Oinam Bedajit Meitei Dr. Dalip Singh Dr. Adish Tyagi <b>Students:</b> Aperture Club, MUJ

## प्रस्तावना

अनुरूप गुणों वाले पदार्थ के डिजाइन और विकास का हमारे रोजमर्रा के जीवन में अत्यधिक महत्व है और आधुनिक प्रौद्योगिकियों के लिए भी यह महत्वपूर्ण है। पदार्थ विकास के महत्व के संदर्भ में, पदार्थ रसायनिकी हेतु संस्था (पता: रसायनिकी प्रभाग, भाभा परमाणु-अनुसंधान केंद्र मुंबई), पदार्थ रसायनिकी पर द्विवार्षिक राष्ट्रीय कार्यशालाओं का आयोजन करती है जिसका उद्देश्य, पदार्थ विज्ञान के क्षेत्र को बढ़ावा देना और युवा शोधकर्ताओं को इस क्षेत्र की महत्वपूर्ण जानकारी उपलब्ध कराना होता है।

पदार्थ रसायनिकी पर 5वीं पऊवि बी आर एन एस राष्ट्रीय कार्यशाला, (एन डब्ल्यू एम सी-2019) का आयोजन विशेष रूप से नवोदित वैज्ञानिकों को नैनो और संमिश्रित पदार्थ का अवलोकन देने के उद्देश्य से किया गया है। कार्यशाला का मुख्य विषयनिष्ठ, नैनो और संमिश्रित पदार्थ के गुणों कार्यक्षमता, संश्लेषण, प्रसंस्करण, लक्षण वर्णन एवं ऊर्जा, स्वास्थ्य देखभाल, पानी व पर्यावरण के क्षेत्र में उनके अनुप्रयोगों के अध्ययन पर है। इस दो दिवसीय कार्यशाला में एक परिपूर्ण व्याख्यान और सात विविध सत्रों में तेरह आमंत्रित व्याख्यान शामिल होंगे। कार्यशाला में भारत के 50 से अधिक संस्थानों के लगभग 170 प्रतिभागी भाग ले रहे हैं, जोकि कार्यशाला के राष्ट्रीय स्वरूप को चरितार्थ करता है। हमें उम्मीद है कि इस कार्यशाला के विचार-विमर्श युवाओं के लिए लाभवान होंगे और उन्हें पदार्थ रसायनिकी विषय पर अपनी समझ का विस्तार करने का पर्याप्त अवसर देंगे।

कार्यशाला की आयोजन समिति सभी आमंत्रित वक्ताओं के प्रति आभार व्यक्त करती है, जिन्होंने अपने व्यस्त समय के बावजूद, अपना बहुमूल्य समय और ज्ञान साझा करने के लिए सहमति व्यक्त की। बी आर एन एस द्वारा दी गयी वित्तीय सहायता के लिए हम उनके आभारी हैं। हम संरक्षक सदस्यों, सलाहकार समिति के सदस्यों एवं स्थानीय आयोजन समिति के सदस्यों द्वारा दिए गए बहुमूल्य सुझावों और उनके अथक प्रयासों के लिए आभारी हैं। हम इस कार्यक्रम के आयोजन के हेतु अपने समर्पित प्रयासों के लिए स्थानीय आयोजन समिति/ उप-समितियों के सभी सदस्यों एवं मनिपाल विश्वविद्यालय जयपुर, राजस्थान व रसायनिकी प्रभाग, भाभा परमाणु अनुसंधान केंद्र मुंबई के सभी कर्मचारियों के प्रति भी धन्यवाद अर्पित करते हैं।

हम सभी प्रतिभागियों के मनिपाल विश्वविद्यालय जयपुर में एक सुखद प्रवास और कार्यशाला के दौरान फलदायक विचार-विमर्श की कामना करते हैं।

(संदीप निगम)	(राहुल श्रीवास्तव)	(वी के जैन)	(ललिता लेडवानी)
संयोजक	सह-संयोजक	अध्यक्ष	सह-अध्यक्ष
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2019	2019	2019	2019





## PREFACE

Design and development of materials with tailored properties has utmost significance in our everyday life and are crucial to modern technologies. In view of the renowned interest in materials development, Society for Materials Chemistry (SMC) C/o, Chemistry Division BARC, organizes biennial National Workshops on Materials Chemistry to promote the field of material science to the young researchers and providing them key inputs required in the fields. The DAE-BRNS 5<sup>th</sup> National Workshop on Materials Chemistry, (NWMC-2019) is specifically aimed at giving an overview of Nano and Composite Materials to the budding scientists. The main focus is on physical basis of functionality, synthesis, processing, characterization, properties of Nano and Composite Materials and their applications in the field of energy, health care, water and environment. This two days workshop will consists of one plenary lecture and thirteen invited lectures encompassing seven diverse sessions. Around 170 participants from more than 50 institutes of India are participating in workshop, giving it a true national portrayal. We hope that the deliberations in this workshop will be an asset to the youngsters and give ample opportunity to expand their understanding of the subject.

The organising committee expresses its gratitude to the invited speakers who wholeheartedly agreed to share their valuable time and knowledge, in spite of their busy schedule. Financial support from BRNS is gratefully acknowledged. We are grateful to the patrons and members of the Advisory Committee and Local Organising Committee for their valuable suggestions and untiring efforts. We take this opportunity to thank all members of the Local Organising Committee/sub-committees and Manipal University Jaipur Staff and Chemistry Division staffs for their dedicated efforts towards organising this event.

We wish all the participants a pleasant stay at Manipal University Jaipur and fruitful interactions during the workshop

**(Sandeep Nigam)**  
Convener  
NWMC 2019

**(Rahul Shrivastava)**  
Co-Convener  
NWMC 2019

**(V. K. Jain)**  
Chairman  
NWMC-2019

**(Lalita Ledwani)**  
Co-Chairman  
NWMC-2019



**National Workshop**  
on  
**Material Chemistry (Nano & Composite Materials)**  
**NWMC (NCom-Mat) 2019**  
**November 8-9, 2019**

**SCIENTIFIC PROGRAMME**  
**Venue: Manipal University Jaipur**

<b>Day 1, November 8, 2019</b>	
<b>08:00 AM - 09:15 AM</b>	<b>Registration</b>
<b>09:30 AM - 10:15 AM</b>	<b>Inaugural Session</b> <b>Chief Guest: Prof. J. P. Mittal, DAE, Mumbai</b>
<b>10:15 AM - 11:10 AM</b>	<b>Plenary lecture by Prof. D. K. Aswal, CSIR-NPL, New Delhi</b>
<b>11:10 AM - 11:30 AM</b>	<b>Tea</b>
<b>11:30 AM - 01:00 PM</b>	<b>Invited talk-1: Dr. Sandip Dhara, IGCAR, Kalpakkam</b> <b>Invited talk-2: Dr. P. A. Hassan, BARC, Mumbai</b>
<b>01:00 PM - 02:00 PM</b>	<b>Lunch</b>
<b>02:00 PM - 03:30 PM</b>	<b>Invited talk-3: Dr. Y. K. Bhardwaj, BARC, MUMBAI</b> <b>Invited talk-4: Dr. A. K. Satpati, BARC, Mumbai</b>
<b>03:30 PM -03:45 PM</b>	<b>Tea</b>
<b>03:45 PM -05:15 PM</b>	<b>Invited talk-5: Dr. Rubel Chakravarty, BARC, Mumbai</b> <b>Invited talk-6: Dr. M.V. Shankar, Y. V. University, Kadapa</b>
<b>05:15 PM -05:45 PM</b>	<b>Quiz- for Research Scholar/PhD student</b>
<b>05:45 PM -06:00 PM</b>	<b>Tea</b>
<b>06:00 PM -07:00PM</b>	<i>Showcase of ChD activities by Shri Dheeraj Jain,</i> <i>Showcase of MUJ activities by Dr. Lalita Ledwani</i>

07:00 PM - 08:30 PM	Cultural Event
08:30 PM	Dinner
<b>Day 2, November 9, 2019</b>	
09:30 AM - 11:00 AM	Invited talk-7: Dr. Sayan Bhattacharya, IISER, Kolkata Invited talk-8: Dr. A. K. Chauhan, BARC, Mumbai
11:00 AM - 11:15 AM	Tea
11:15 AM - 12:45 PM	Invited talk-9: Dr. V. Sudarsan, BARC, Mumbai Invited talk-10: Dr. R. S. Dhaka, IIT Delhi, New Delhi
12:45 PM - 01:45 PM	Lunch
01:45 PM - 03:15 PM	Invited talk-11: Dr. Sameer Sapra, IIT Delhi, New Delhi Invited talk-12: Dr. Pushpal Ghosh, HS Gour Univ., SAGAR
03:15 PM - 03:30 PM	Tea
03:30 PM - 04:15 PM	Invited talk-13: Dr. Mahesh Kumar, IIT Jodhpur, Jodhpur
04:15 PM - 05:15 PM	Valedictory Session
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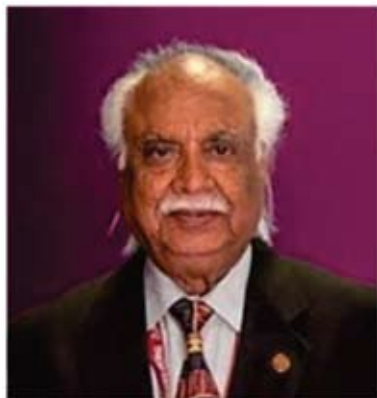
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## Chief Guest: Prof. Jai Pal Mittal



Jai Pal Mittal, after obtaining his MSc degree (1959) from the Agra University joined the Atomic Energy Research Centre's Training School and rose to be the Director, Chemistry and Isotope Group of Bhabha Atomic Research Centre (BARC), Mumbai. He obtained his PhD (1967) from the Radiation Laboratory, University of Notre Dame and later underwent post-doctoral training at the University of California, Los Angeles with WF Libby. Dr. Mittal was the DAE Raja Ramanna Fellow, BARC, Mumbai, Distinguished Professor, IIT, Bombay; and Honorary Distinguished Professor, University of

Pune, M.N. Saha Distinguished Professor (NASI), BARC.

Dr. Mittal initiated a school of modern Radiation Chemistry and Photochemistry research in India. He was responsible for setting up a nanosecond LINAC based pulse radiolysis system at BARC and setting up the nano, pico and femtosecond pump and probe techniques to study the chemical dynamics. His group initiated the infrared laser-induced Isotope Selective Photochemistry Research at BARC and succeeded in isotopic enrichment of the isotopes of hydrogen, carbon, uranium, etc. He has published about 300 research papers in peer-reviewed journals. Dr. Mittal has mentored a large number of student including 35 PhDs.

Dr. Mittal served on various research funding agencies of DAE, DST, UGC, etc. For years he guided the Basic Sciences Committees of Board of Research in Nuclear Sciences as its Chairman. After serving as the President of the Indian Society of Radiation & Photochem Sciences (1997-2001), he was elected as the President of the Asian Photochemistry Association (2003- 2008). He served the INSA Council as Member (1998-2000) and as Additional Member (2005-06).

Dr. Mittal is a recipient of Humboldt Research Award (2002), Senior JSPS Award, TR Seshadri 70th Birthday Commemoration Medal of INSA (1994), Golden Jubilee Commemoration Medal of INSA (2001), NR Dhar Memorial Medal of NASI, Goyal Gold Medal, Platinum Jubilee Award of ISCA. He was honoured by the Government of India in 2003 with Padma Shri, the fourth highest Indian civilian award. He was President of the Indian Chemical Society (1998-99), and National Academy of Sciences (India), Allahabad (2003-04). He is Fellow of the Indian Academy of Sciences, Bangalore and the Academy of Sciences for the Developing World, Trieste (2000).



*Plenary Lecture*





## Redefined SI units and their implications

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### Abstract

On May 20, 2019, the SI units of measurements were defined in terms of the fundamental constants. The SI units are the ultimate reference to any measurements and therefore, play a critical role in the national quality-infrastructure.

A quality-infrastructure of a Nation is comprised of internationally recognized metrology, standards and accreditation, which essentially is the basic enabling system of a nation for providing the conformity assessment (calibration and testing, certification and inspection). A robust quality infrastructure is built on a technical hierarchy and is essential for forming effective national policies and their implementation, to attract foreign investments, industrial development, international trading of products, food safety, environment and climate change, health, and efficient utilization of natural and human resources. As a result, a strong quality infrastructure contributes to the national economy and brings prosperity, health and well-being.



*Dr. Aswal joined BARC through the training school batch of the year 1986 (i.e. 30th batch) after completing M.Sc. in Physics (Gold medalist) from Garhwal University in 1985. He obtained Ph.D. in Physics from Mumbai University and subsequently carried out post-doctoral research work at Research Institute of Electronics, Hamamatsu, Japan. He is a condensed matter physicist of international repute and has made several outstanding contributions in the areas of molecular electronics, physics of organic films and their applications, thermoelectric power generators and gas sensors. He has edited three books, contributed 20 book chapters, published over 250 peer reviewed journal papers, filed three patents and secured the trademark of Bhartiya Nirdeshak Dravys (BND) – the Indian Certified Reference Materials.*

*Dr. D.K. Aswal has taken over the charge of Director, CSIR-National Physical Laboratory (CSIR-NPL), New Delhi with effect from 15th December 2015 maintaining lien with his position as “Outstanding Scientist” at Bhabha Atomic Research Centre (BARC), Department of Atomic Energy (DAE), Government of India, Mumbai. Dr. Aswal, during 2012-2015, has also served as Secretary, Atomic Energy Education Society (AEES), Mumbai, which is an autonomous institution under DAE.*

*His current focus is to enhance the Metrological capabilities of India at par with international standards for continuous improvement of the quality and safety of life in the country and making CSIR-NPL as a growth engine of the nation by supporting industries and strategic sectors through apex calibration facilities. As a member of “International Bureau of Weights and Measure (BIPM)”, France, “Asia Pacific Metrology Program, APMP”, and “International Union of Pure and Applied Physics, IUPAP”, he ensures that the country’s interests at international level are fulfilled.*



*Invited Lecture*



# Role of native defects for methane sensing in III-nitride nanostructures near room temperature

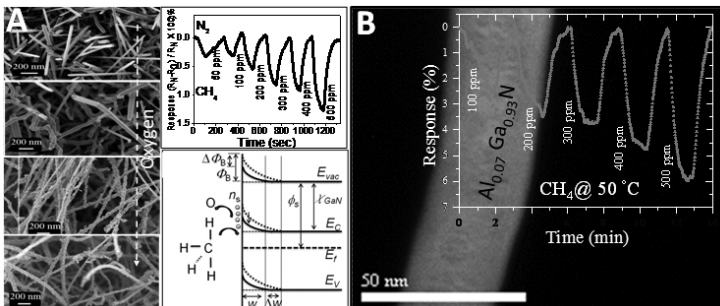
Sandip Dhara

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The underlying physicochemical processes involved in a chemical or gas sensor device operation are adsorption of chemical molecules, subsequent transfer and transport of charge on semiconductor surfaces. Owing to the high surface-to-volume ratio at the nanoscale, the semiconductor nanostructure surface usually shows complex behavior towards the above three fundamental processes, and hence alters the device performances unambiguously.<sup>1,2</sup>

We present a detailed study conducted on 1-D semiconductor nanostructures, in the context of understanding the above mentioned physicochemical processes which occurs during gas the sensing process. GaN and AlGa<sub>N</sub> nanowires (NW) with impurity (oxygen) induced surface defects are considered for this study.<sup>2,3</sup> The experiments and density functional theory (DFT) based simulations of electron energy loss spectroscopy (EELS)

studies are performed to understand the type of possible oxygen defects present in the impurity incorporated III-nitride NWs. The global resistive gas sensing measurements are performed on ensemble NW devices under methane gas. Charge transfer process in single GaN NW under methane exposure is studied by *in situ* scanning Kelvin probe microscopy. The global gas sensing behavior of ensemble NW is understood in terms of impurity induced



**Figure 1:**(A) Typical FESEM micrographs of GaN NWs grown under different concentrations of oxygen impurity; Gas sensing response and a schematic band diagram of GaN NW during the charge transfer process. (B) EELS imaging of typical Al doped GaN NW and inset shows Gas sensing response

defect complex ( $V_{Ga}-3O_N$ ) mediated localized charge transfer process in single NW (Fig. 1A). An enhanced sensing response is obtained in case of AlGa<sub>N</sub> as comparison to that of the pristine GaN NW (Fig. 1B) at near room temperature (50 °C) because of excess amount of carriers generated in the strong influence of native defects. Photoluminescence studies (not shown in figure) confirmed the presence of native defects in the AlGa<sub>N</sub> samples.<sup>4</sup>

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**Prof. Sandip Dhara** has completed his Masters in Physics from IIT, Kharagpur in the year 1989. He finished his Ph.D. from National Physical Laboratory, New Delhi in the year 1994 and joined IGCAR in the year 1996. He is a Fellow of Royal Society of Chemistry.

Presently he is the Head of Surface and Nanoscience Division, Indira Gandhi Centre for Atomic Research, Kalpakkam and Professor of Homi Bhabha National Institute. He was also visiting Professor in University of Valencia, Spain; Technical University of Chemnitz, Germany; and Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan. He was associate Professor in Electrical Engg. Dept, NCKU, Tainan, Taiwan during 2007-2008.

Dr. Dhara has published more than 300 research publications which include several review articles and two book chapters with several conference presentation. He has delivered more than 100 invited and plenary talks. He is the recipient of DAE-SRC outstanding researcher award for 2012. He is also in the editorial board of number of national and international scientific journals. Dr. Dhara is specialized in studies of light-matter interaction in the field of Near-field scanning optical microscopy (NSOM) and Tip enhance Raman spectroscopy (TERS). At present, he is involved in several national and international collaborative programs.

## Chemistry and applications of soft nanostructures

**P. A. Hassan**

*Chemistry Division, Bhabha Atomic Research Centre, Mumbai- 400 085.*

Self assembly of small molecules into complex hierarchical structures via non-covalent interactions offers an attractive route to develop size and shape selective nanostructures. The physical chemistry behind modulating the microstructure of self assembled materials by exploiting the intermolecular interaction will be discussed. Such nanostructures find potential applications in various industrial products or processes. One such example is the formation of viscoelastic fluids that exhibit both elastic and viscous response, analogous to entangled polymer solutions. This lecture will address the basic principles of creating viscoelastic fluids and gels using amphiphilic molecules and additives. The rheological behaviors of such fluids have been examined in the context of “living polymer” solutions and a systematic analysis of dynamic rheology will be presented. Another application of self assembly is to make surface functionalized nanostructures through non-covalent interactions for regulated delivery of drugs or proteins. Stimuli sensitive assemblies that can reversibly associate or dissociate in response to environmental changes have been fabricated, as a model system for self regulated drug delivery vehicle. Interfacial modification of magnetic nanoparticles via self assembly of amino acids and subsequent growth of peptide mimics leads to pH responsive drug delivery vehicle.



*P. A. Hassan earned his M. Sc. Degree in Chemistry from Mahatma Gandhi University, Kottayam (1991 batch) securing first rank. In 1992, he joined Bhabha Atomic Research Centre (BARC) Training School. Currently, he is Head of Nanotherapeutics and Biosensors Section, Chemistry Division, BARC. He is an elected Fellow of the National Academy of Sciences, India (NASI). He was a visiting researcher at the Laboratory of Complex Fluids, University of Louis Pasteur, Strasbourg, France in 1995. He pursued his post-doctoral research on soft condensed matter at the Department of Chemical Engineering, University of Delaware, USA in 2000-2002. He has visited advanced neutron scattering facilities like National Centre for Neutron Research, NIST, Maryland, USA and Institute Lau Langevin, Grenoble, France. He has co-authored more than 140 research articles in peer reviewed journals. His current research interests include microstructure and dynamics of self assembly in supercooled solvents and development of nano drug delivery systems.*



# Radiation: An effective tool for polymer composite design and synthesis

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## Abstract

Polymers, ceramics and metals have considerably different properties; each offering a specific set of attributes. However, no single material or a class of material fulfills the diverse set of properties required for different applications. Therefore there has always been a need for development of novel combinatorial approaches wherein their functional advantages of the constituents are maximized and drawbacks are abridged. Composites comprise of two or more chemically distinct materials which when combined have properties better than individual materials. Radiation has proven to be an effective tool for synthesis and processing of polymer composites (PC) due to its inherent advantages. The ability of high energy radiation to crosslink polymer to form continuous polymer network has been exploited to crosslink the polymer component of PC which enhances the mechanical properties and structural integrity of PC. Radiation can also be used for surface modification of the filler component of PC. Surface modified fillers display better interaction with polymer and hence further enhancement of properties. Filler type and geometry, polymer type, interface in PC, and fabrication & processing protocol followed plays important role in determining final properties of polymer composites. At Radiation Technology Development Division (RTDD), BARC radiation processing of polymer composites has been explored extensively for wide range of applications viz. synthesis of flexible radiation attenuation PC, for synthesis of ESR dosimetry matrices, for absorbed dose indicators, as tensoresistors, as chemi-resistive sensors, and partially biodegradable composites. The talk will present an overview of different activities related to radiation processing of polymer composites presently being pursued in RTDD in close collaboration with industry and academia. The underlying principles and mechanisms of radiation-induced processing of composites and filler modification will be elaborated. Characterization of radiation processed polymeric composites and journey from lab to pilot scale of some products will be discussed.



**Dr. Y. K. Bhardwaj** joined Radiation Technology Development Section in 1989 after doing his M. Sc from University of Garhwal. He later did his Ph. D from the University of Mumbai. His research interest includes utilization of high-energy electron beam and gamma radiation for industrial applications. This includes development of radiation grafted polymer matrices, radiation processing of elastomer blends and composites and high-performance coatings. He has been actively involved in the studies on radiation polymerization/crosslinking of monomers/polymers, development of radiation processed hydrogels for healthcare and synthesis of fast stimuli-responsive hydrogels. He has to his credit more than 150 papers in peer-reviewed journals.



**Dr. K. A. Dubey** is working as a scientific officer in Radiation Technology Development Division, Bhabha Atomic Research Centre. He did his M.Sc. chemistry from Indian Institute of Technology, Roorkee, and Ph.D. from University of Mumbai. His research interest includes radiation processing of polymer blends, alloys and nanocomposites for advanced applications. Presently he is engaged in radiation processed biodegradable polymers, over current protection polymer-composite devices, polymeric strain sensors, toxic volatile sensors and high modulus nanocomposites.

# Investigation of Transfer and Transport Kinetics on the photoanode materials.

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## Abstract

Charge transfer and transport over the photo-anode materials is important in designing the efficient catalysts for generation of hydrogen and oxygen from water.  $\text{BiVO}_4$  is considered as promising photoanode material for solar water splitting [1]. Its performance is limited by slow water oxidation kinetics and poor charge separation [2]. To enhance water oxidation kinetics of  $\text{BiVO}_4$ , Oxygen evolution catalyst (OEC) has been incorporated on the surface of photoanode. Cobalt borate (Co-Bi) is known as an excellent catalyst for water oxidation [3, 4]. We have incorporated Co-Bi as OEC on the surface of  $\text{BiVO}_4$  to enhance charge transfer and transport efficiency and hence overall enhancement of water oxidation kinetics. Mo-doped  $\text{BiVO}_4$  was coated on FTO by spin coating technique using precursor solution followed by calcination. After formation of  $\text{BiVO}_4$ , Co-Bi has been incorporated on photoanode surface by photoelectrochemical deposition technique. Photoelectrochemical activity was performed by chopped light voltammetry, the increase in the photocurrent by 36% with the incorporation of Co-Bi indicated the suitable combination of OEC and  $\text{BiVO}_4$ . The onset potential was also found to shift cathodically on incorporation of the electro-catalyst. Charge transfer and transport efficiency were found to increase from 67% to 70% and 32% to 50% respectively upon incorporation of electro-catalyst. Results show that OEC facilitates separation of photogenerated charge and enhancement of interfacial charge transfer efficiency. Enhancement of Charge transport efficiency indicated that electro-catalyst works as hole collector and hence mobility of photogenerated hole increases many folds. Further interfacial charge transfer efficiency has been improved significantly with the associated improvements of relaxation frequency. The kinetics of charge transfer was measured from scanning electrochemical microscopy (SECM) technique. The probe was approached to substrate by probe approach technique (PAC) with different bias potential at the substrate and measure feedback current at the probe to study the hole transfer rate from substrate to the analyte. Along with the present materials some of the previous investigations on solar energy harvesting and storage will be discussed.

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**Dr. A. K. Satpati** is presently working as Scientific Office-F in Analytical Chemistry Division, Bhabha Atomic Research Centre, Mumbai. His research interest includes electrochemical investigation of thin films, biomolecules and interfaces. Fabrication of ultramicro electrodes for scanning electrochemical microscopy. He has been working on the development of composite materials and electrochemical investigations for efficient energy storage. He has investigated the Electrocatalytic and photo-electrocatalytic investigations of metal oxide composites for solar energy harvesting through splitting of water to hydrogen and oxygen. He has investigated electron

Transfer (ET) reactions in homogeneous and micro-heterogeneous media. Different series of coumarin and quinone dyes were used as the electron acceptors at their excited state and amines of different nature and structure as the donors, at their ground state. He has been working on development of analytical methods using voltammetry and developed many electro analytical methods and used them for the determination of metal ions at trace and ultra-trace levels. Development of modified electrode based on carbon paste and carbon nano-tube, thio-compound and DNA. Electrodeposition of thin metallic films. He is teaching electrochemistry and analytical chemistry in post graduate level since 2004. He is recipient of the following awards and recognition. "Young Scientist Award-2008" from Department of Atomic Energy, Government of India. Fulbright fellowship to carry out research work with Prof. Allen J. Bard in University of Texas Austin, USA during 2011 to 2012, Young associate of Maharashtra Academy of Sciences 2015 and member of National Academy of Sciences India (NASI) in 2018.

# Radiolabeled Inorganic Nanoplatfoms for Cancer Theranostics

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Over the last few years, a plethora of radiolabeled inorganic nanoparticles have been developed and evaluated for their potential use in cancer theranostics. Inorganic nanoparticles represent an emerging paradigm in cancer management, allowing the incorporation of various imaging modalities, targeting ligands, and therapeutic payloads into a single vector. A major challenge in this endeavor is to develop disease-specific nanoparticles with facile and robust radiolabeling strategies. Also, the radiolabeled nanoparticles should demonstrate adequate *in vitro* and *in vivo* stability, enhanced sensitivity for detection of disease at an early stage, optimized *in vivo* pharmacokinetics for reduced non-specific organ uptake, and improved targeting for achieving high efficacy. It is probably because of these challenges and other technological and regulatory issues, only a single radiolabeled nanoparticle formulation, namely 'C-dots' (Cornell dots), has found its way into clinical routine thus far. This talk will describe the available options for radiolabeling of nanoparticles and summarize the recent developments in cancer theranostics in preclinical and clinical settings using radiolabeled nanoparticles as probes. The key considerations toward clinical translation of these novel radiolabeled agents will be discussed, which will be beneficial for advancement of the field.



**Rubel Chakravarty** obtained his M.Sc. (Chemistry) degree from Banaras Hindu University, Varanasi in 2005 and joined BARC in 2006 after successful completion of 1-year orientation course (49<sup>th</sup> Batch, Chemistry) from BARC Training School. He obtained his Ph.D. degree in Chemistry from Homi Bhabha National Institute in 2011. He was a Fulbright Visiting Scholar at University of Wisconsin-Madison, United States during 2013-14. His research interests include radioisotope production, separation chemistry, nanotechnology and radiopharmaceutical chemistry. He is a recipient of several awards, including, the Young Scientist Awards from the

Department of Atomic Energy and Indian Science Congress Association. He has served as Principal Investigator and Co-investigator in several International Atomic Energy Agency (IAEA)-sponsored Coordinated Research Projects (CRPs). He has co-authored 1 book, 5 book chapters and 91 papers in peer-reviewed journals.

## Controlled synthesis of ultra-thin TiO<sub>2</sub> wrapped on CdSe core for stable and efficient hydrogen production under visible light irradiation

**Prof. M.V. Shankar, CChem, FRSC (London)**

*Professor & Chairman Board of Studies*

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Metal chalcogenide based semiconductor nanostructures are a promising candidate for photocatalytic or photoelectrocatalytic hydrogen generation. However, upon light absorption by metal chalcogenides generates photo-electrons and holes thus involved in red-ox reactions and any unutilized excitons destabilize the CdSe into ions that remain a grand challenge. My talk will elaborate the synthesis of one-dimensional capsule shaped CdSe nanostructure through surfactant mediated approach. In order to protect CdSe from photocorrosion, a layer of TiO<sub>2</sub> wrapped (shell) onto CdSe (core) nanocapsule via the post-synthesis process. The morphology studies confirm that a thin amorphous TiO<sub>2</sub> shell (3-8 nm) wrapped in all the three directions onto CdSe core and thickness of the shell can be controlled through modulating titania precursor concentration. The chemical environment of CdSe and TiO<sub>2</sub>@CdSe shell@core nanocapsule will be elaborated by using X-ray photoelectron spectroscopy, which ensures chemical bonding between TiO<sub>2</sub> and CdSe. The feasibility of pristine CdSe nanocapsules and TiO<sub>2</sub>@CdSe in transforming visible light to hydrogen fuel conversion was tested through photocatalysis reaction. The TiO<sub>2</sub>@CdSe nanocapsules generating a four-fold high rate of hydrogen gas (21 mmol.h<sup>-1</sup>.g<sup>-1</sup><sub>cat</sub>) compared to pristine CdSe (5 mmol.h<sup>-1</sup>.g<sup>-1</sup><sub>cat</sub>). This quantity is remarkably higher value compared to state-of-the-art CdSe nanostructured photocatalysis in associate with heterostructures, co-catalyst and passivation layers (ZnS, TiO<sub>2</sub>). Unexpectedly, the volume of H<sub>2</sub> gas generation (12 mmol.h<sup>-1</sup>.g<sup>-1</sup><sub>cat</sub>) is one-order reduced after filtering the UV light. In order to understand the role of shell@core, we have examined the photoelectrochemical and impedance analysis. The TiO<sub>2</sub>@CdSe nanocapsules showed high photoelectric current generation and less charge transfer resistance at electrode/electrolyte interfaces compared to visible light irradiation. These studies endorse that the chemically synthesized TiO<sub>2</sub> shell played a multifunctional role in (a) surface passivation from photocorrosion, (b) promoting photocharge carrier separation via tunneling process between CdSe and TiO<sub>2</sub> interface. As a result, at optimized experimental conditions TiO<sub>2</sub>@CdSe nanocapsules showed high conversion efficiency of 12.9% under visible light irradiation (328 mW.cm<sup>-2</sup>). My talk will facilitate the young scientists to design and develop highly efficient photocatalyst systems to realize the potential application for H<sub>2</sub> fuel production.

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**Dr. M. V. Shankar** is a professor of Materials Science and Nanotechnology at Yogi Vemana University, Kadapa, Andhra Pradesh, India. He is a Chartered Chemist and Fellow of Royal Society of Chemistry (FRSC), London. He has established Nanocatalysis and Solar Fuels Research Laboratory in YV University. The research group renowned for achievements in the area of photocatalysis and multi-functional application of nanomaterials, he has authored in refereed journals (72), patents (06), books (01) and book chapters (06) and conference papers with h-index of 28, average impact factor of 4.25 and 4300+ citations. He has chaired many national and international conferences, symposia, workshops and technical meetings. He has delivered several keynote and invited lectures. Prof. Shankar has very good R&D collaborators in the area of energy and environmental applications. He is an active member of various international organizing committees and serves as lead guest editor, guest editor, editorial board member and reviewer on various prestigious international journals. He has rich research experience in countries viz., France, Japan and Taiwan and recipient of several prizes, awards and fellowships.

## Zinc-air Battery by Perovskite Oxides

**Sayan Bhattacharyya**

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Rechargeable metal-air batteries have shown enormous potential for mobile applications due to their fascinating energy density as compared to metal-ion batteries, since oxygen is stored outside the battery until it is discharged. In Zn-air battery (ZAB), the reliable aqueous chemistry of Zn at all pH decreases the cost of device fabrication and operation as well as makes the device safer to handle. However their low power density is due to the sluggish  $O_2$  electrolysis through redox reactions in multi-electron pathways. To drive the oxygen evolution reaction (OER) during charging and oxygen reduction reaction (ORR) during discharge, the development of efficient and stable bifunctional electrocatalysts is necessary that can substitute the Pt/C-RuO<sub>2</sub> couple. Perovskite oxides of unit formula ABO<sub>3</sub> are potential low cost alternatives where B-site transition metal centers act as the active site and A-site influence the overall stability and tuning of electronic structure at the B-site. This lecture will address few persistent problems of perovskite oxides in order to articulate their bifunctional activity in rechargeable ZAB. Firstly, the loss of electrical conductivity at inter-grain boundaries is addressed by nanoparticle segregation. Secondly, local surface instability under sustained oxidative potential is resolved by coulombic interaction with a layered double hydroxide (LDH). Third, the problem of ending up with catalytically inactive bigger grains to obtain pure perovskite phases is deciphered by *in situ* ~10 nm crystalline particle growth on conducting substrates. Our air-electrode strategies enable low discharge-charge voltage gap, energy density of ZAB up to ~1000 mW.h.g<sub>Zn</sub><sup>-1</sup> with unaltered cyclic stability over 100h.





- *Sayan Bhattacharyya* obtained his Ph.D. with Prof. N. S. Gajbhiye at the Indian Institute of Technology, Kanpur, India in 2006.
- Postdoctoral research with Prof. (Emeritus) Aharon Gedanken at Bar-Ilan University, Israel (2006-2008)
- Postdoctoral research with Prof. Yury Gogotsi at Drexel University, USA (2008-2010)
- *Joined IISER Kolkata in April 2010 as Assistant Professor of the Department of Chemical Sciences, IISER Kolkata; Associate Professor (February 2015 to September 2019)*
- *Professor of the Department of Chemical Sciences, IISER Kolkata since September 2019*
- *He is the founder & chair of the Centre for Advanced Functional Materials at IISER Kolkata*
- *He is a Materials Chemist interested in photovoltaics, catalysis for energy, magnetism, and biological applications. A combination of wet-chemical synthesis and self-assembly of smart nanomaterials, structure-property correlation and device applications are used to attain these research goals*
- *In 2017, Dr. Bhattacharyya has been highlighted as one of the Emerging Investigators by the Journal of Materials Chemistry A, Royal Society of Chemistry.*
- *He has received several unsolicited media coverage on his scientific research work*
- *He is member of the American Chemical Society, American Nano Society, Chemical Research Society of India, Association for Iron & Steel Technology, and American Ceramic Society, USA*

# Graphene Composites of Conducting Polymers and their Application in Organic Solar Cells

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Conducting polymers (CP) have several advantages over conventional inorganic semiconductors however, these significantly lack in their charge carrier mobility values. Better charge mobility is very crucial for the development of flexible organic electronic devices and people are striving for it worldwide. Graphene, owing to its exceptional electrical and mechanical properties, is a promising material to be examined for its possible incorporation in CP matrix to achieve this objective. The graphene composites of the conducting polymers were prepared following an optimized procedure. The carrier mobility values were measured using electric field induced second harmonic generation (EFISHG) and field effect transistor (FET) transfer characteristics and found to increase significantly. These composites were used as an active layer in the fabrication of polymer solar cells and yielded about 20% higher efficiencies.



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# Glasses and Composites: Fundamentals and Applications

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## Abstract

Most commonly encountered classification of materials is based on their structure, namely the amorphous and crystalline phases. Both amorphous and crystalline materials (solids) can be either single phase or a combination of number of phases, the latter material is generally called as a composite material. There are many instances, wherein a synergistic mechanism operates and a composite material has many advantages over the corresponding single phase components. Composite materials find wide variety of applications and are commonly employed as catalysts, luminescent materials, glass ceramics, gas /hydrogen storage materials etc. In this lecture, composite materials such as glass ceramics, nanoparticles incorporated silica and multi component (phase) intermetallic alloys and their applications will be discussed.

Glass-ceramics consists of an amorphous phase embedded with single or multiple crystalline phases. They are produced as a result of controlled crystallization of glass with or without the addition of suitable additives (nucleating agents). Generally a glass ceramic consists of crystalline phases to the extent of 30-90% and the rest is glass. Glass ceramics can be prepared in such a way that the material possesses the advantages of both glass and ceramics. For example, glasses, in general, are brittle in nature and it is difficult to machine them. However, glass ceramics made with certain annealing conditions are machine-able. Typical example of a machine-able glass

ceramic is the one based on magnesium aluminosilicate (MAS) glass. By addition of suitable nucleating agents, crystallization of a phase called potassium fluorophlogopite can be achieved in the glass matrix. This phase is having tile like structure and is responsible for the machine-able property of the composite material. Presence of such phases can be identified and their relative concentration can be evaluated based on solid state nuclear magnetic resonance technique, using  $^{29}\text{Si}$  as the probe nuclei. Typical  $^{29}\text{Si}$  Magic Angle Spinning Nuclear Magnetic Resonance (MAS NMR) spectrum for MAS glass

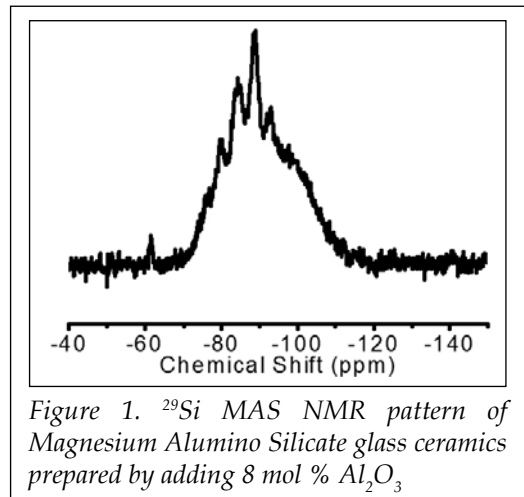


Figure 1.  $^{29}\text{Si}$  MAS NMR pattern of Magnesium Aluminosilicate glass ceramics prepared by adding 8 mol %  $\text{Al}_2\text{O}_3$

ceramic prepared with addition of 8 mol% of  $\text{Al}_2\text{O}_3$  is shown in Fig. 1. The sharp peaks in the NMR pattern are characteristic of Potassium fluorophlogopite phase. Depending up on concentration of this phase, machinability of the material is found to change. In addition to this optical and energy storage properties of representative composite materials will also be discussed in detail in the present lecture.



*Dr. V. Sudarsan* joined Chemistry Division of BARC in the year 1994 after graduating from the 37th batch of the training school. He received his Ph. D degree in Chemistry from Mumbai University in the year 2002 for his work on the structural aspects of inorganic glasses. Subsequently he worked for a period of two years at the University of Victoria, British Columbia, Canada in the area of structural aspects and luminescence of lanthanide ions doped in nanoparticles of inorganic hosts. Currently he is working on the optical properties of nanoparticles and glassy materials.

# Electrode materials in Na-ion batteries for energy storage applications

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In recent years, energy storage devices especially rechargeable batteries have become an integral part of portable electronic devices like mobiles, laptops as well being used at large scale in electrical vehicles (EV), hybrid electrical vehicles and power grids. Among various types of batteries, in the present scenario the only commercially established and feasible technology is based on Li-ion intercalation, mainly due to the advantage of high energy density, good rate kinetics and light weight. However, the major concern is due to the limited availability and uneven distribution of Li around the world, which evoke the urge among the researchers to look for other possibilities. Therefore, even after nearly three decades since first commercial battery was introduced, constant efforts are going on to search new electrode materials (negative as well as positive) for improving its electrochemistry. Among the alternative avenue, the Na-ion batteries are one of the potential candidates particularly for grid level storage due to its low cost and abundance on the globe, and therefore extensive research has been started in this field over past few years. In this direction, one of the major challenges is to find the suitable electrode materials and in particular a stable anode with high electrochemical performance

Transition metal oxides are widely studied as cathode as well as anode in Li/Na/K ion batteries. In this talk, I will discuss our recent results on the Na/Li-ion diffusion and electrochemical performance of NVO as anode material in Na/Li-ion batteries with the specific capacity of  $\sim 350 \text{ mAhg}^{-1}$  at the current density  $11 \text{ mA g}^{-1}$  after 300 cycles for Li-ion battery. Remarkably, the capacity retains  $\sim 200 \text{ mAhg}^{-1}$  even after 400 cycles at  $44 \text{ mA g}^{-1}$  with Coulombic efficiency  $>99\%$ . The deduced diffusion coefficient from galvanostatic intermittent titration technique (GITT), electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) measurements for NVO as anode in Li-ion battery is in the range of  $10^{-10}$ - $10^{-12} \text{ cm}^2\text{s}^{-1}$ . In case of Na-ion batteries, the NVO electrode exhibits initial capacity of  $385 \text{ mAhg}^{-1}$  at  $7 \text{ mA g}^{-1}$  current rate, but the capacity degradation is relatively faster in subsequent cycles. We find the diffusion coefficient of NVO-Na cells similar to that of NVO-Li. On the other hand, our charge discharge measurements suggest that the overall performance of NVO anode is better in Li-ion battery than Na-ion. Moreover, we use the density functional theory to simulate the energetics of Na vacancy formation in the bulk of the NVO structure, which is found to be  $0.88 \text{ eV}$  higher than that of the most stable (100) surface. Thus, the Na ion incorporation at the surface of the electrode is more facile compared to the bulk.

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*Dr. Rajendra S. Dhaka is an Assistant Professor of Physics at IIT Delhi. He is interested in the property evaluation of strongly correlated materials. He obtained his doctorate in physics from the Surface Physics Laboratory, RRCAT Indore, working with Prof. R. R. Burman on "Electron spectroscopic investigation of metallic systems". After completing his Ph. D. he did his post doctoral research with Prof. Dr. J. Kirschner/Dr. F. O. Schumann at Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle, GERMANY on "Electron Pair emission from Solid Surfaces/Double Photoemission" and subsequently a second post doctoral research with Advisor: Prof. Adam Kaminski at Iowa State University, USA on "Angle Resolved Photoemission Spectroscopy of high Tc Superconductors". After completing his post docs Dr. Dhaka moved back to India and joined the Indian Institute of Technology where he currently works on "Property Evaluation of Strongly Correlated Materials". Along with research he is actively involved in teaching. He has also visited several countries as guest scientist. As recognition to his research work, he has conferred with many prestigious awards (ECR) Award, INSA Medal for Young Scientists in Physics, DAE Young Scientist Research Award (YSRA), by Board of Research in Nuclear Sciences (BRNS), INDIA, Young Faculty Incentive Fellowship, by Indian Institute of Technology Delhi (IIT/D), DAE Young Achiever Award (YAA), by BRNS*

# Hybrid nanoheterostructures with transition Metal Dichalcogenide for optoelectronic applications

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## Abstract

Transition metal dichalcogenide (TMD) nanosheets with defect-rich and vertically aligned edges are highly advantageous for various catalytic applications. Synthesis of TMDs using the colloidal techniques opens various possibilities to tune the electronic and optical properties of these 2D materials. As an example, we choose MoSe<sub>2</sub> nanosheets that have plenty of defects. The defect sites are responsible for adsorption on the surface thereby yielding excellent electrocatalytic hydrogen evolution and other catalytic activities on the surface.

Further, these defects can be employed as seeding points to grow other materials on them. Cu<sub>2</sub>S in these defect sites leads to a Type-II semiconductor heterojunction that allows for charge separation and therefore the MoSe<sub>2</sub>-Cu<sub>2</sub>S forms a superior material for generation of photocurrent.

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*Dr Sameer Sapra is interested in the development of materials for energy generation; photovoltaics and photocatalysis being the main forte. He obtained his doctorate in chemistry from the Indian Institute of Science, Bangalore working with Prof DD Sarma on the electronic and optical properties of semiconductor nanocrystals in 2004. After completing his PhD, he was awarded the Alexander von Humboldt fellowship to carry out research on the luminescence properties of quantum dots at the Ludwig Maximilian University at Munich. From there he moved to the group of Prof Dr Alexander Eychmueller in Dresden. After researching for three years on the luminescence properties, Sameer moved back to India and joined the Indian Institute of Technology where he currently works on the various aspects of nanomaterials - his interests ranging from basic size and shape dependent studies, synthesis of new materials such as those based on transition metal dichalcogenides, light emitting materials, photovoltaic devices and photocatalytic applications including hydrogen and oxygen evolution reactions. Along with doing research, he teaches various courses in Physical Chemistry and Materials Chemistry and mentors a number of postdoctoral fellows, PhD, master and bachelor students. He has over ninety publications in reputed international and national journals with an h-index of 34 and has authored four book chapters*



# Facile Synthesis of Energy Efficient Nanomaterials from Ionic Liquids

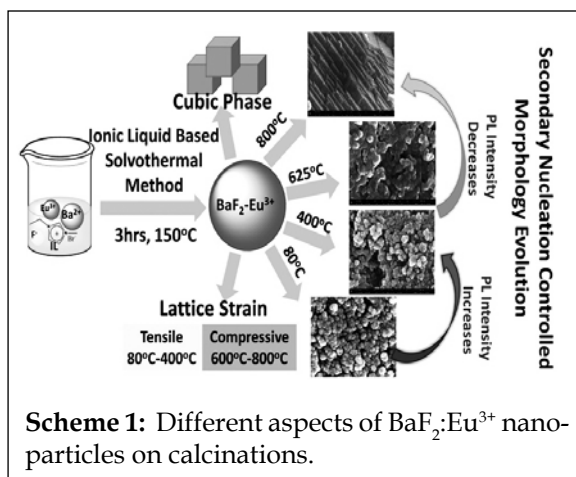
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Ionic liquids (ILs) which are normally described as “green” and “designer solvents” draw a tremendous attention in academia and industries. Normally ILs are composed of distinct cations and anions and they are a widely tunable class of compounds with interesting properties like negligible vapor pressure, wide liquidus range, good thermal stabilities, considerable electrical conductivities and wide electrochemical window. Though they are extensively used in organic catalysis, electrochemistry, f-element separation and many other applications, their use in inorganic materials synthesis has just started but holds great promises.

In my research group, we are developing IL based “green” synthesis to prepare next generation phosphor materials for energy efficient and environmentally benign lighting; rare-earth based optoelectronic materials with improved property or property combinations. We are also focusing on new generation semiconducting nanomaterials devoid of toxic metal ions and useful for catalytic/photocatalytic degradation of toxic dye molecules. In addition, we are also working on graphene based composite materials interfacing with rare-earth doped luminescent materials. In most of the research problems, ILs are not only used as solvent, templating agent but sometimes as a reaction partner also. For example,  $[C_4mim]BF_4$  IL can be used as a solvent, templating agent and source of fluoride ions to prepare rare-earth ion doped ternary and binary fluoride materials.

The range of materials are quantum cutting useful for energy efficient and environmentally benign lighting as well as upconverting useful for photonic and biophotonic applications. Keeping in mind about the fascinating applications of our “smart” materials, our endeavor is also to unravel the structure property relationship controlled by tuning ionic liquid properties. Two important topics which will be covered in my lecture are given below.



Herein, phase pure, template free rare-earth ( $RE^{3+}=Eu^{3+}, Ce^{3+}$ ) doped  $BaF_2$

nanoparticle are synthesized using ionic (IL) liquid assisted solvothermal method. Here IL is used not only as capping/templating agent but also sometime as a reaction partner. As-prepared cubic shaped  $\text{BaF}_2:\text{Eu}^{3+}$  nanoparticles are calcined at different temperatures such as 200°, 400° and 800°C. Interestingly, lattice strain, morphology and optical property are drastically changed at 800°C. Lattice strain is changed from tensile to compressive strain beyond 400°C calcinations temperature. At high temperature, cubic-shaped morphology is changed to step like structure due to secondary nucleation. Thereafter, photoluminescence excitation and emission intensities are completely vanished at 800°C. Thermally stimulated luminescence (TSL) and thermally stimulated exo-electron emission (TSEE) measurements are performed to understand the role of defects in luminescence quenching.

In another attempt, phase tuned quantum confined  $\text{In}_2\text{S}_3$  nanocrystals prepared solvothermally using task-specific ionic liquids (ILs) as structure directing agents are reported. Selective tuning of size, shape, morphology and, most importantly, crystal phase of  $\text{In}_2\text{S}_3$  is achieved by changing the alkyl side chain length, the H-bonding and aromatic  $\pi$ -stacking ability of the 1-alkyl-3-methylimidazolium bromide ILs,  $[\text{C}_n\text{mim}]\text{Br}$  ( $n=2,4,6,8$  and 10). In addition it is noticed that, source of sulphur precursor and their concentration plays a pivotal role to obtain the phase pure materials. It is observed that crystallite size is significantly less when ILs are used compared to the synthesis without ILs keeping the other reaction parameters same. At 150°C, when no IL is used, pure tetragonal form of  $\beta\text{-In}_2\text{S}_3$  appears however in presence of  $[\text{C}_n\text{mim}]\text{Br}$  [ $n=2,4$ ], at the same reaction condition, a pure cubic phase crystallizes. However in case of methylimidazolium bromides with longer pendant alkyl chains such as hexyl ( $\text{C}_6$ ), octyl ( $\text{C}_8$ ) or decyl ( $\text{C}_{10}$ ), nanoparticles of the tetragonal polymorph form. Likewise, judicious choice of reaction temperature and precursors has a profound effect to obtain phase pure and morphology controlled nanocrystals. Furthermore, the adsorption driven catalytic and photocatalytic activity of as-prepared nanosized indium sulphide is confirmed by studying the degradation of crystal violet (CV) dye in presence of dark and visible light. Maximum 94.8 % catalytic efficiency is obtained for the  $\text{In}_2\text{S}_3$  nanocrystals using tetramethylammonium bromide (TMAB) ionic liquid. Analysis reveals that along with electrostatic interaction, molecular structures of dye molecules have also significant impact on adsorption capacity which finally governs the catalytic (even in the dark) and photocatalytic efficiency of nanocrystals.

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# Real time detection of $\text{Hg}^{2+}$ ions using $\text{MoS}_2$ functionalized AlGaIn/GaN HEMT for water quality monitoring

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## Abstract

The Molybdenum disulfide ( $\text{MoS}_2$ ), a two-dimensional transition metal dichalcogenide (TMDC) material received considerable attention due to their semiconducting electronic properties and ultrahigh surface to volume ratio. Moreover, the detection of mercury ions in water can also be realized using the strong binding affinity of  $\text{MoS}_2$  towards  $\text{Hg}^{2+}$  ions. In this work, we report, the application of  $\text{MoS}_2$  as a functionalized material on the gate region of AlGaIn/GaN high electron mobility transistors (HEMT). The  $\text{MoS}_2$  was prepared by simple hydrothermal approach. The structural and morphological analysis was carried using scanning electron microscopy, X-ray diffraction, and Raman characterization. The AlGaIn/GaN HEMT are normally on device due to availability of two-dimensional electron gas (2DEG) at the heterointerface AlGaIn/GaN. This 2DEG can be modulated by change in electronic properties of  $\text{MoS}_2$  during exposure of  $\text{Hg}^{2+}$  ions. By exposing  $\text{MoS}_2$  functionalized AlGaIn/GaN HEMT in  $\text{Hg}^{2+}$  ion solution, the gate potential varied due to formation of Hg-S complex and electrostatic interaction which in turn change the drain to source current ( $I_{\text{DS}}$ ). Here the concentration of  $\text{Hg}^{2+}$  ions was varied from 1 ppt to 10 ppm and corresponding change in IDS was observed. The sensor shown good selectivity towards  $\text{Hg}^{2+}$  ions and limit of detection was observed 11.52 ppt which is well below than world health organization guidelines. Thus, the trace level detection of toxic  $\text{Hg}^{2+}$  ions can be realized using  $\text{MoS}_2$  functionalized AlGaIn/GaN HEMT.



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*He has received INSA Medal for Young Scientists-2014 by Indian National Science Academy, the MRSI Medal-2016 by Materials Research Society of India, DAE-Young Achiever Award-2016 by BRNS (Department of Atomic Energy), ISSS Young Scientist Award 2017 by the Institute for Smart Structures and Systems, YSAP mission award 2019 by Global Young Academy, JPhysD: Emerging Leader Award 2019 (Runner-up) by Institute of Physics UK, and PHSS Foundation Young Scientist Award 2018-19 by Prof. H. S. Srivastava Foundation. He is founding Member of Indian National Young Academy of Sciences, Member of National Academy of Sciences India, Royal Society of Chemistry & Global Young Academy and IEEE Senior Member from 2016. He has published more than 90 research articles.*

*Activities of Chemistry Division,  
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# Highlights of R&D activities of Chemistry Division, BARC

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Chemistry Division with its basic, directed and applied research activities in materials chemistry carries out important mandates of Bhabha Atomic Research Centre (BARC). Under the mandate, the Division has been contributing to nuclear reactor materials, materials for hydrogen generation and storage, nanotherapeutic and formulation for cancer diagnosis and therapy, ultrapure materials, soft condensed matter, thin films and sensors, atomic/molecular clusters etc. While most of the programs are being executed within this Division, there are some ongoing collaborative projects with different research groups in BARC and other DAE units, Universities/ National Institutes under BRNS schemes. Presently Chemistry Division has 76 scientific members and 09 doctoral students/post-doctoral researchers. This article comprises of inputs from all the members of Chemistry Division.

## 1. Nuclear materials

Chemistry Division, BARC has a dedicated research program on developments material and evaluation of physical, chemical and thermophysical properties materials relevant for nuclear fuel cycles and nuclear reactor safety. Synthesis of materials based on structure property correlations, studies on structural transitions and stability of materials under non-ambient conditions are also being carried out to understand the behavior of materials under extreme conditions of temperature, pressure and chemical environment. The activities on various ceramics materials having alternate technological relevance, like multiferroic, magnetic, dielectric, ferroelectric and ionic conductors are also being pursued. Glimpses of some of the research activities are mentioned as follows.

### 1.1. MSBR activities

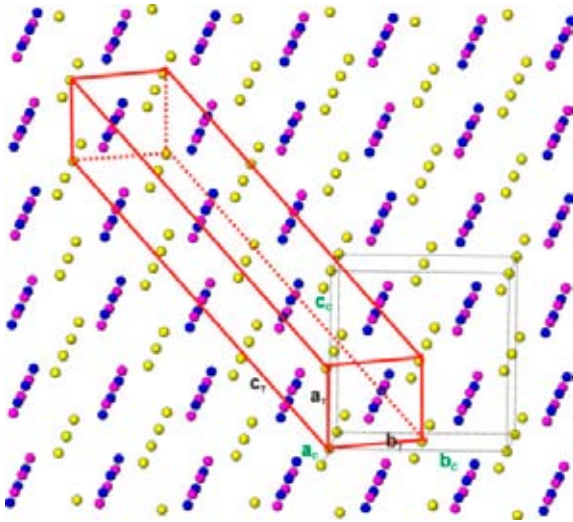
The Molten Salt Breeder Reactor (MSBR) is known as chemist's reactor in view of a considerable chemistry associated with it. This futuristic reactor has fuel in the form of molten salt is circulated through the heat exchangers. These are inherently safe reactors having several distinct advantages like online reprocessing of spent fuel, potentiality to achieve self-sustainable  $^{233}\text{U}/\text{Th}$  cycle, reliability and proliferation resistance. Information on thermo physical properties of the salt systems is important for the design and operation of the MSBR. Chemistry Division is actively engaged in research on high temperature chemistry of Molten Salt Breeder Reactor (MSBR) System. The objective of this activity is to generate relevant data on thermo-physical and thermo chemical properties required for the design and the safe operation of MSBR. Thermo-physical properties of molten salt systems like melting point, enthalpy of fusion, heat capacity, viscosity and density,



thermal conductivity are being measured as a function of temperature. In addition, phase diagram studies of components of MSBR system, measurement of activity of volatile components in the fuel salt, blanket salt and coolant salt, solubility limits of major fission products and oxide tolerance of the fuel salt, calculation of free energy potentials and thermodynamic activities of fission products, studies on interaction of molten salt systems with structural material such as N-hastelloy have been initiated.

## 1.2. R & D Activities for nuclear safety

The R & D activities on nuclear safety are focused to develop materials for sacrificial reactor core catcher applications, immobilization of radioactive elements and radiation detection. Safe management of corium, a complex molten mixture of  $\text{ThO}_2$ ,  $\text{UO}_2$ ,  $\text{PuO}_2$ ,



**Fig.1:** Relation between cubic high carnegieite (black solid thin lines) and the present observed triclinic lattice (solid red lines). (Si, Al and Na are shown as yellow, blue and red spheres, respectively. Oxygen atoms are not shown for clarity).

XRD, and the energetic and mechanisms of hexagonal nepheline to cubic carnegieite type structural transition have been investigated. The cubic carnegieite phase on cooling transforms to triclinic low carnegieite phase having closely similar lattice.

## 1.3. Studies on potential materials relevant for back end of nuclear fuel cycle and radiation detection

The immobilization of radioactive elements in high level nuclear waste relies on suitable matrices to host them without undergoing any degradation due to self-irradiation and heat as well as under the influence of prevailing environment. In this regard phase

Zr-based phases, steel, fission products and other component materials reactor at very high temperatures formed during the unlikely severe accidental condition is an important requirement. The sacrificial materials in general lower the temperature by some physical or chemical processes, and form stable materials by chemical reaction with the radioactive materials. In view of this a wide choice of ceramic materials are being explored to understand their chemical and physical properties. The naturally available minerals and analogous materials are considered as promising for such applications. As an example, the thermophysical and chemical stability of synthetic nepheline ( $\text{NaAlSiO}_4$ ) has been explored in wide range of temperature. Thermal expansion of nepheline has been investigated by high temperature

evolutions with composition and temperature in wide varieties of ceramics are being explored to develop single phase or multiphase ceramics potential hosts matrices for this purpose. Structural stabilities and thermodynamic properties have also been investigated for several pyrochlore, zirconolite and perovskite type zirconates and titanates (Fig. 2). Studies on complex titanates like, calzirtite ( $\text{Ca}_2\text{Zr}_5\text{Ti}_2\text{O}_{16}$ ) and zirconolite ( $\text{CaZrTi}_2\text{O}_7$ ) have been carried to reveal their structural stabilities and high temperature thermodynamic properties and it is inferred that calzirtite phase stable up to about 1820 K. High temperature crystal chemistry and stabilities complex oxides viz.  $\text{K}_2\text{ThP}_2\text{O}_8$ ,  $\text{K}_2\text{CeP}_2\text{O}_8$ ,  $\text{K}_3\text{Gd}_5(\text{PO}_4)_6$ ,  $\text{K}_2\text{Fe}_2\text{Ti}_6\text{O}_{16}$ ,  $\text{Na}_2\text{Fe}_2\text{Ti}_6\text{O}_{16}$  etc. have been investigated. All the materials were found to be stable at higher temperature. Hollandite type  $\text{K}_2\text{Fe}_2\text{Ti}_6\text{O}_{16}$  exhibited significant high stability with temperature as well as pressure.

Similar pressure and temperature dependent structural studies and thermal expansion behavior of  $\text{K}_2\text{Ce}(\text{PO}_4)_2$  and  $\text{K}_2\text{Th}(\text{PO}_4)_2$  have also been investigated to understand their usability as host in phosphate matrices. High structural stability in perovskite-type

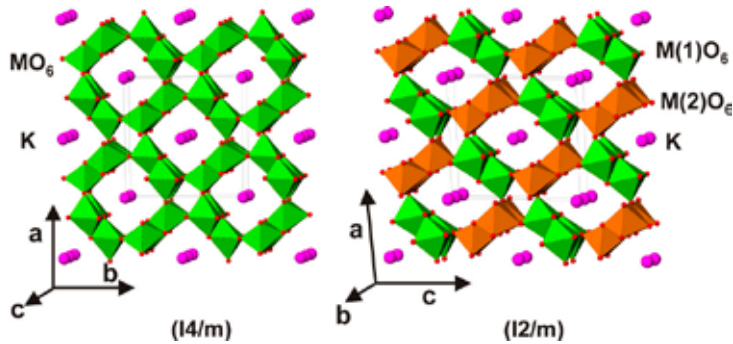


Fig. 2: Crystal structure of tetragonal and monoclinic  $\text{K}_2\text{Fe}_2\text{Ti}_6\text{O}_{16}$

cerium scandate ( $\text{CeScO}_3$ ), up to about 40 GPa, has been observed investigated by in situ high pressure X-ray powder diffraction, using a diamond-anvil cell and high structural stability is observed. In the similar aim to develop glass-ceramics for nuclear waste

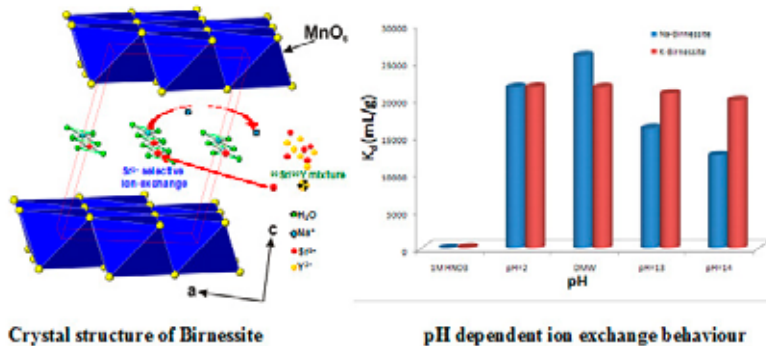


Fig. 3: Crystal structure of  $(\text{Na/K})_x\text{Mn}_2\text{O}_4$  and the distribution coefficient ( $K_d$ ) for separation of  $\text{Sr}^{2+}$  ions in different pH

immobilization, solubility of  $Gd_2O_3$  in barium borosilicate (BBS) glass matrix has been investigated. The solubility limit of  $Gd_2O_3$  in BBS is found to be around 7.0 mol% and increasing trend of glass transition temperature with increasing  $Gd_2O_3$  content has been observed.

R and D activities to develop potential materials for separation of radioactive element are also being pursued. Several materials, like layered complex phosphates, manganates, titanates, etc. and nano-crystalline  $TiO_2$ ,  $MnO_2$  etc. have been investigated for such applications. Efficient exchange of  $Sr^{2+}$  with layered phosphates and birnessite type synthetic phyllomanagates have been revealed in these studies. The birnessite type  $Na_xMn_2O_4$  is found to be a promising material for separation of  $Sr^{2+}$  and  $Y^{3+}$  in radioactive  $^{90}Sr$ - $^{90}Y$  mixture solution (Fig. 3). Potential of nanocrystalline  $MnO_2$  for separation of actinides from low level liquid waste is also revealed in such studies.

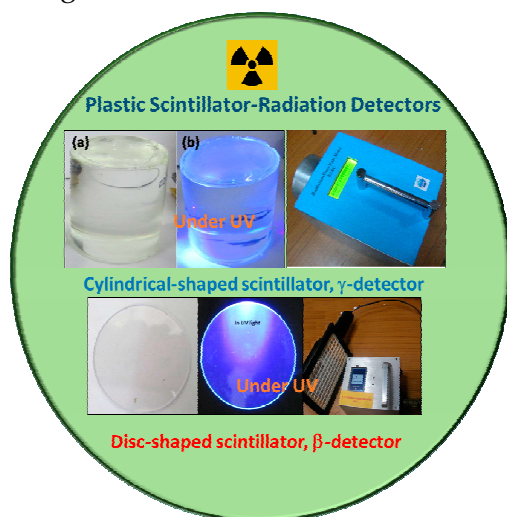


Fig. 4: Various radiation detectors

Development of potential materials for detection of various radiations, like gamma, beta and alpha particles are also being carried out. Organic and polymer based scintillating materials ingeniously developed are being used for in house fabrication and deployment of radiation detectors (Fig. 4). Various

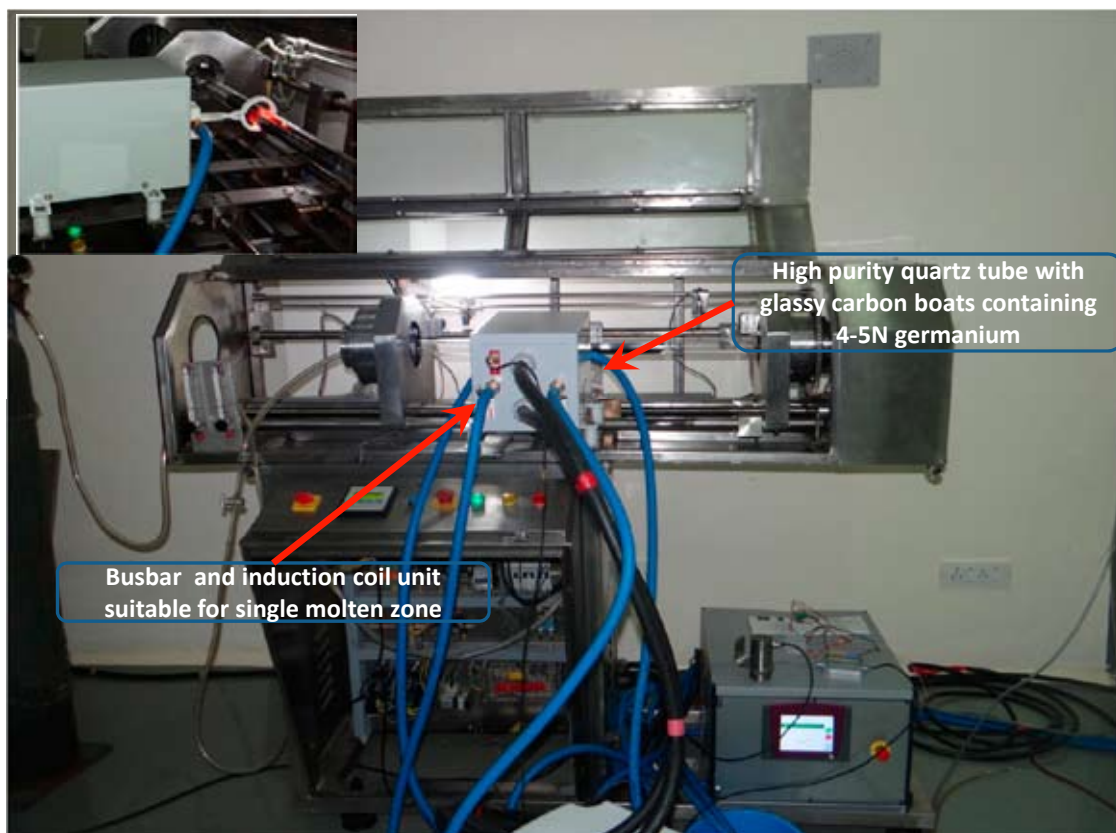
inorganic-polymer composites are being developed for flexible radiation shields.

#### 1.4. High purity materials

High purity materials play a key in high tech industries including electronics, integrated circuits, photovoltaic, optical and chemical applications. The demand for high purity metals has been increasing with the development of technology. Chemistry Division is actively pursuing synthesis of high and ultra-purity materials. Presently purification of germanium for the manufacture of High Purity Ge (HPGe) radiation detectors is under progress. The targeted purity of Ge based on physical measurements is being achieved through zone refining the metal under special conditions. The Division has indigenously developed its own zone refining unit for ultra-purification of Ge (Fig. 5).

Chemistry Division has also formulated and successfully demonstrated methodologies for ultra-purification of Ga, As, In, Sb and CsI which have demand in various sectors. Ultra-purification of Gallium and Indium has been achieved through combination of vacuum heating and electrolytic processes. In contrast to these, arsenic required vacuum sublimation of arsenic trioxide (a highly toxic compound) followed by reduction under hydrogen (fire hazard). CsI required a series of fractional recrystallization steps.

## Zone refining (ZR) unit with induction heating equipment

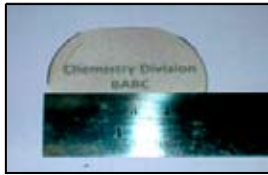


### 1.5. Development of diamond-based $\alpha$ -particle detector

CVD diamond-based alpha particle detector (Fig. 6) has been developed for direct monitoring of actinides in highly acidic and radioactive liquids. The  $\alpha$ -particle detector was comprehensively tested in air using alpha emitters (Pu,  $^{241}\text{Am}$ ) of varying activity ranging from 0.06 nCi (~133 dpm) to 0.09  $\mu\text{Ci}$  (~199800 dpm). All the counting parameters of the detector were optimized during these experiments. The response is linear over the studied concentration range which is reproducible. Having evaluated its performance in air, its suitability in acidic liquid medium (3M  $\text{HNO}_3$ ) was assessed in Fuel Reprocessing Division, BARC. The testing was carried out for different type of solutions namely, 3M  $\text{HNO}_3$  containing 1 to 10000 ppm of Pu in the presence and absence of oxalic acid, 3M  $\text{HNO}_3$  solutions containing 40 to 1500 ppm of  $^{233}\text{U}$ ,  $^{241}\text{Am}$  and Pu.

The results have shown reproducible performance of the detector while measuring individual actinides in the above solutions. Calibration plots have shown linearity for Pu and  $^{233}\text{U}$  in concentration range of 1 to 1000 ppm. Deviation from linearity was observed for concentrations beyond 1000 ppm. Pu content in few process samples was also determined using these calibration plots. The results were in agreement with those





CVD grown diamond film

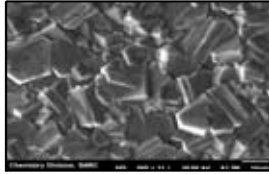
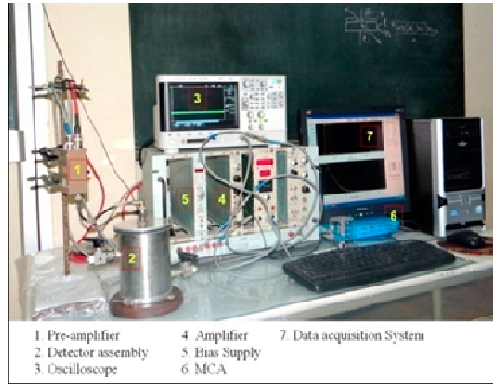
Microstructure  
(CVD diamond)**Alpha Spectrometer setup for diamond detector**

Photo of diamond film based detector

*Fig. 6: diamond-based  $\alpha$ -particle detector*

obtained from the conventional radiometric method presently followed, which is tedious due to multistep involvement. The sensitivity of the detector is lower than that of the conventional solid-state  $\alpha$ -detectors (Si-surface barrier detector, Ag-doped ZnS detector) used at present.

## 1.6. Catalysts for hydrogen mitigation

A large amount of hydrogen is generated in nuclear reactor under loss of coolant accident conditions. Passive catalytic recombination of hydrogen and oxygen is one of the preferred methods of hydrogen mitigation. For the purpose, SS wire gauze supported noble metal (Pt + Pd) catalysts have been developed. After exhaustive evaluation, both at Lab as well as at Hydrogen Recombiner Test Facility (HRTF) Tarapur, these were selected for large scale production and are in process of deployment as passive catalytic recombiner devices (PCRDs) in Indian PHWRs (Fig. 7). Hydrogen removal rates of  $\sim 2.0$  kg/h could be achieved using such PCRD.



(a)



(b)

*Fig. 7: (a) Catalyst Bearing Panel and (b) PCRD*

## 2. Anticancer Therapeutics and Diagnostics

In the prospect of future health security, Chemistry Division, BARC has a dedicated research program on developments material/molecules/formulation for Anticancer Therapeutics and Diagnostics.

### 2.1. Nano formulations for anticancer drugs and nutraceuticals

#### 2.1.1. Self-assembled nanocarriers for drug delivery

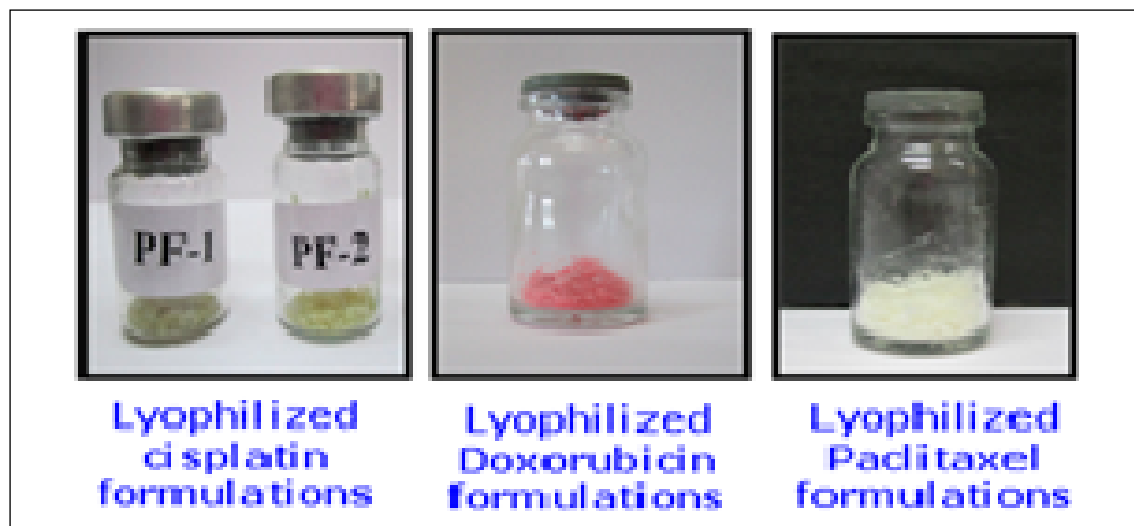


Fig 8: Lyophilized formulations

Novel liposomal nano-formulations for chemotherapy drugs such as doxorubicin and paclitaxel have been developed using cost effective FDA approved ingredients (Fig. 8). PEGylated liposomes comprising egg phosphatidyl choline and triblock copolymers were prepared using self-assembly approach and the drug loading efficiencies were optimised. Drug formulations show time-dependent sustained release at pH 6.5, which is desirable for cancer therapy as mild acidic environment of tumor will specifically stimulate the release of drug. Further, the syngeneic mice model study has shown comparable efficiency in reducing the tumor size with respect to commercially available formulation.

#### 2.1.2. Hydroxyapatite nanoparticles for doxorubicin delivery

Hydroxyapatite is an emerging drug delivery vehicle due to its excellent properties and compositional similarity with natural bones and teeth. Glycine functionalized biocompatible hydroxyapatite nanoparticles were prepared by soft-chemical approach. Doxorubicin hydrochloride (DOX), an anticancer drug was covalently conjugated to these nanoparticles via imine bond. The DOX conjugated nanoparticles showed both time and pH-dependent sustained release of DOX with a higher release rate at acidic pH. *In-vitro*

cell viability experiments showed dose and time dependent cytotoxicity of DOX loaded nanoparticles towards WEHI-164 cells with a significant uptake in the cells (Fig. 9).

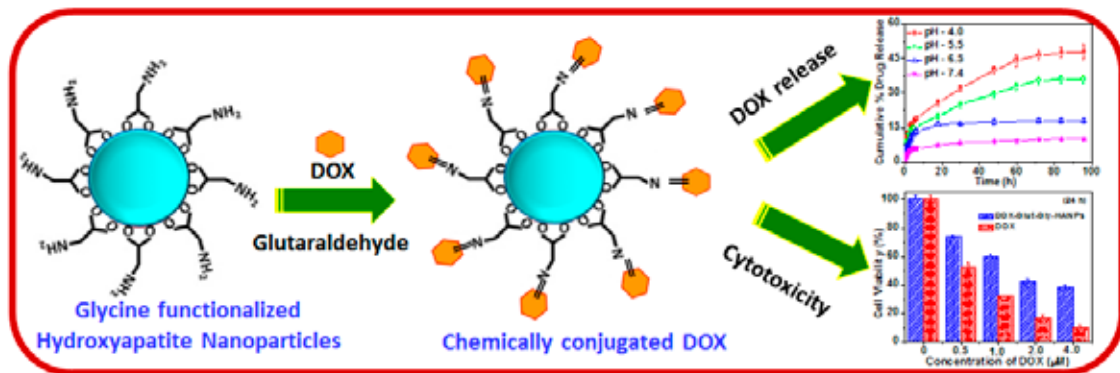


Fig. 9: Glycine functionalized hydroxyapatite nanoparticles for delivery of anticancer drug, DOX

### 2.1.3. Magnetic nanoparticles for hyperthermia and combination therapy

Another area of interest in cancer therapeutics is to employ magnetic nanoparticles for heat activated killing of cancer cells (hyperthermia) and as carriers for other chemotherapy drugs. Magnetic nanoparticles with specific functional groups to impart colloidal stability and drug binding properties were developed and tested in cancer cell lines. Many cancer cell lines such as MCF7, WEHI-164 (Fibro sarcoma), HeLa have been tested and the surface coating ligands includes PEGs and PEG derivatives, peptides and modified oleic acids. In-vitro study shows that 70% cancer cells can be killed using oleic coated MNPs, and in-vivo study shows that reduction of tumour growth is more as compared to control.

### 2.1.4. Nanoformulations for nutraceuticals

A nasal drop concentrate of curcumin was developed using biocompatible amphiphilic liposomes that self-assemble to form micelles. This formulation has capability of encapsulating as high as 50 mg/ml of curcumin and this concentrate can be diluted with water to any extent (Fig. 10). This technology is transferred to an Indian industry for commercialisation

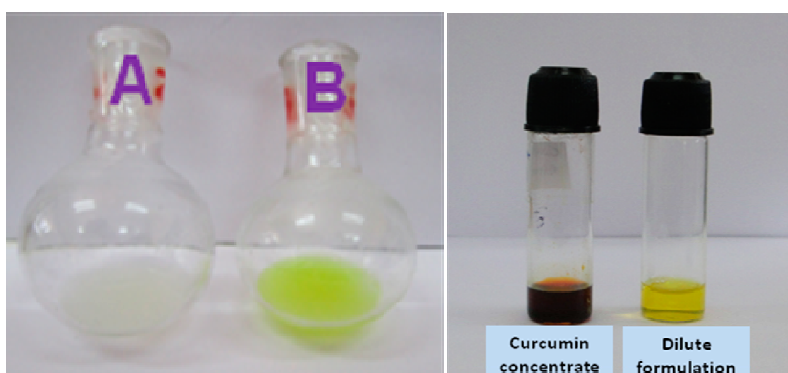


Fig. 10: A. PEGylated liposomes and B Curcumin loaded liposomes (left) Curcumin loaded micelle formulations (right)

Curcumin containing hydrogel patches were also developed for wound healing applications. An optimised hydrogel patch with tensile strength 0.6MPa and elongation at break 42% have been prepared. They are made of biocompatible polysaccharide and contain nano-curcumin solubilized in Pluronic F127 micelles. All ingredients are FDA approved and curcumin has proven wound healing properties. Animal studies are under way to check in-vivo wound healing efficacies of these patches.

## 2.2. Development of bio-sensors for cancer diagnostics

### 2.2.1. Development of portable biosensors for cancer detection

A Portable Extra-Cellular Acidity Analyzer (ECAA) has been developed to differentiate between cancer and normal cells exploiting the difference in their glycolysis rate (Fig. 11). Studies carried out using ECAA on human breast tissue samples obtained from Tata Memorial Hospital revealed increasing current response and high extracellular acidity values for cancerous tissue as compared to normal tissue samples which show a decreasing current with time. This technology has been transferred to four private companies till now.

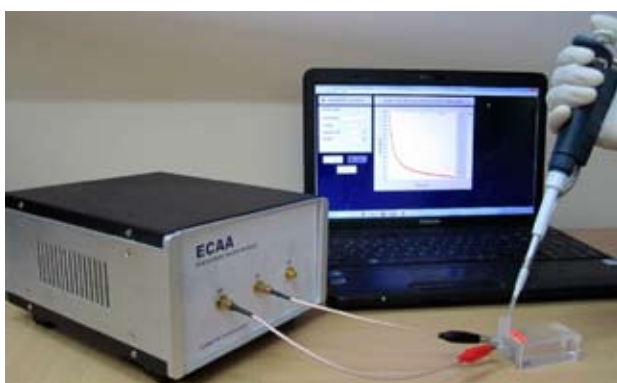


Fig 11: Extra-Cellular Acidity Analyzer (ECAA) setup

### 2.2.2. Biosensor for detection of liver cancer biomarker alpha-fetoprotein

Attempts were also made to develop biosensor for detection of alpha-fetoprotein (AFP), a liver cancer biomarker, using surface plasmon resonance and electrochemical technique. Three different strategies for immobilization of the AFP antibody were explored to obtain best sensitivity. The shift in SPR angle on binding of AFP in the analyte to AFP antibody on the sensor surface was found to be maximum in the case of ethylene diamine - glutaraldehyde chemistry. This can be attributed to proper orientation of AFP antibody on the sensor surface. The sensor displayed good specificity for binding of AFP vs other non-specific protein like BSA. The SPR biosensor was used for estimation of AFP in human serum samples where it gave satisfactory results and no matrix interference was observed. The AFP concentration values obtained using the biosensor were cross checked with the values obtained using ELISA.

### 2.2.3. Biosensors for monitoring specific antigen antibody interactions.

Novel biosensors are fabricated using nanostructured SnO<sub>2</sub> semiconductor thin films. Nanostructured Tin oxide thin films prepared by Langmuir Blodgett technique were deposited on p-type Si substrates (Si/SnO<sub>2</sub>) for using them as working electrodes of electrochemical immunosensor. Immunoglobulin G (IgG) antibody molecules were



covalently immobilized on polyaniline (PANI) functionalized Si/SnO<sub>2</sub> through glutaraldehyde coupler. The structure was able to detect the goat antimouse IgG in few hundreds of picomoles concentration with fast response (10 min.) using impedance measurement. The substrates were found to be reusable.

### 2.3. Development of Radioprotectors

The antioxidant properties of organoselenium compounds have been explored with the aim to develop new drugs showing glutathione peroxidase like activities in human body. Several low molecular weight, water soluble organoselenium compounds were synthesized with the objective as antioxidant and radio-protector properties. Among them 3,3'-diseleno dipropionic acid, DSePA has been identified as a potential radio-protector against thoracic radiotherapy. Several Pt based complexes were developed, showing promising DNA binding and anticancer activities against MCF-7 breast cancer and A549 lung cancer cell lines.

### 2.4. Development of C-C coupling catalyst having implications in drug designing

A new class of supramolecular co-ordination complexes (SCC) of Pd and Pt has been developed as discrete molecules from the commercially available aryl dithiol ligands. The Pd SCCs showed excellent catalytic activity in C–C coupling reactions with high turnover numbers ( $2 \times 10^7$ ). The catalysts are also highly efficient in carbonylation reactions and the synthesis of various active drug molecules (e.g. “betol” as antiseptic agent; “oxybenzone” in sunscreen lotion) has been demonstrated in laboratory in gram scale. These results confirm that sulfur ligands can act as catalyst promoter, rather being treated as catalyst poison for long time.

## 3. Hydrogen energy: Generation and storage

In the prospect of future energy security, Chemistry Division, BARC has a dedicated research program on developments material and evaluation of physical, chemical and thermophysical properties materials relevant for hydrogen Energy: Generation, and Storage.

### 3.1. Hydrogen production from water

For large scale hydrogen production by thermochemical splitting of water, research has been carried out on iodine-sulfur (I-S), hybrid sulfur (Hy-S) and copper-chlorine (Cu-Cl) thermochemical cycles to complement and support the engineering scale efforts at BARC. The following are some of the contributions towards these areas of research:

#### 3.1.1. Thermochemical and photocatalytic hydrogen generation

##### 3.1.1.1. Iodine-Sulfur Cycle

Among the three steps involved in Iodine-Sulfur (I-S) thermochemical cycle, namely, Bunsen reaction, hydriodic acid decomposition and sulphuric acid decomposition, investigations were carried out to develop catalyst for the sulfuric acid decomposition – the most endothermic step ( $\sim 800\text{-}900^\circ\text{C}$ ) and also for hydroiodic acid decomposition.

Several iron oxide based catalysts for sulfuric acid decomposition were developed and the catalyst  $\text{Fe}_{1.8}\text{Cr}_{0.2}\text{O}_3$ , found to be the most efficient, chemically stable and resistant to poisons was deployed in a glass closed-loop operation of sulfur-iodine cycle to generate hydrogen at the rate of 30 NLPH for 20 h.

### 3.1.1.2. DFT designing of new single atom alloy catalyst for $\text{SO}_3$ decomposition

DFT calculation predicted that alloying the alumina supported platinum nanocluster with single Ag atom drastically improve its catalytic potential for  $\text{SO}_3$  decomposition (Fig. 12). Inclusion of single Ag atom, lowers the activation barrier for S-O bond breaking by more than 50% in comparison to pristine platinum counterpart, strengthens sintering resistance, weakens the binding of reaction product  $\text{SO}_2$  with catalyst rendering better recyclability. Activation barrier for  $\text{AgPt}_9@ \text{Al}_2\text{O}_3$  catalyst is 0.52 eV which is the lowest for any platinum based catalyst reported so far. The catalytic feature of single atom alloying in Pt surface retains even at larger length scale.

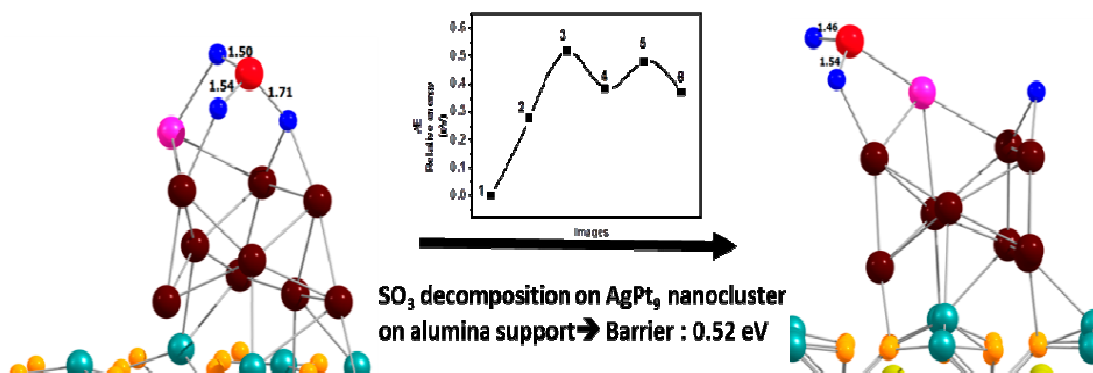


Fig. 12: Activation barrier calculation under DFT formalism

### 3.1.1.3. Hybrid-Sulfur Cycle

In hybrid sulfur thermochemical cycle, the Bunsen reaction and hydriodic acid decomposition steps of I-S cycle are replaced by aqueous  $\text{SO}_2$  electrolysis to produce sulfuric acid and hydrogen, while sulphuric acid decomposition step is similar. A single cell proton exchange membrane (PEM) based aqueous  $\text{SO}_2$  electrolyzers comprising of indigenously developed Pt/C electrocatalyst coated membrane electrode assembly (2cm x cm and 16 cm x 16 cm) hastalloy flow field plates were fabricated, tested and used for closed loop hybrid-sulfur cycle demonstration producing hydrogen at the rate of 2 NLPH for 25 h at Chemical Technology Division, BARC.

### 3.1.1.4. Copper-Chlorine Cycle

Work is underway on different steps of Cu-Cl thermochemical cycle, namely,  $\text{CuCl}/\text{HCl}$  electrolysis,  $\text{CuCl}_2$  hydrolysis and  $\text{Cu}_2\text{OCl}_2$  decomposition (Fig. 13). Effect of various parameters viz., GHSV, temperature and Steam/ $\text{CuCl}_2$  (Steam/Cu) ratio, was evaluated

in a fixed bed glass reactor on the product ( $\text{Cu}_2\text{OCl}_2$ ) yield of  $\text{CuCl}_2$  hydrolysis step. Also, phase-pure  $\text{Cu}_2\text{OCl}_2$ , not available commercially, was synthesized to generate the kinetic data for decomposition step.

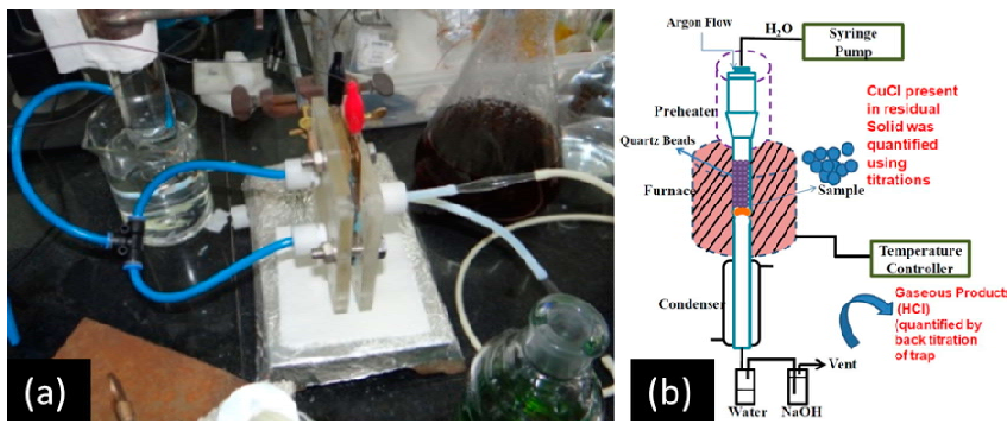


Fig.13: (a) PEM based electrolyser developed for Cu-Cl/HCl electrolysis, (b) Schematic of lab scale fixed bed reactor developed for  $\text{CuCl}_2$  hydrolysis step of Cu-Cl thermochemical cycle.

### 3.1.2. Photocatalytic hydrogen generation

Visible light active photocatalysts are being developed for hydrogen generation by photocatalytic water splitting using solar radiation. Several modified/doped titania, CdS and  $\text{g-C}_3\text{N}_4$  based photocatalysts active in sunlight were developed for photocatalytic splitting water. Notable among these are Cu modified titania photocatalyst ( $\text{Cu}_{0.02}\text{Ti}_{0.98}\text{O}_2$ ) and Pt-CdS-ZnS- $\text{Cd}_{0.8}\text{Zn}_{0.2}\text{S}$  and Pt-Cd $_{0.95}$ Pd $_{0.05}$ S composite photocatalysts where hydrogen generation rates of 1.4 - 1.72 L/h/m<sup>2</sup> were achieved using methanol, sodium sulfide and sodium sulfite as sacrificial agent under sunlight irradiation.

## 3.2. Hydrogen utilization in fuel cell

Proton conductor electro-ceramic based materials, electrolyte, anode and cathode, were developed and evaluated for their chemical compatibility, thermo-physical properties like thermal expansion behaviour and for conductivity employing four probe and AC impedance measurements. Based on stringent material selection, a button cell employing a unique combination of  $\text{BaCe}_{0.8}\text{Y}_{0.2}\text{O}_3$  (electrolyte), Ni (35%) -  $\text{BaCeO}_3$  (anode) and  $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Fe}_{0.8}\text{Co}_{0.2}\text{O}_3$  (cathode) was fabricated by co-sintering and co-firing technique

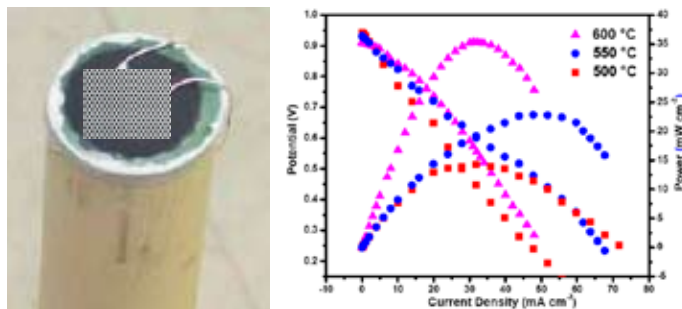


Fig. 14: Fabricated button cell and the I-V characteristics of the button cell.

(Fig. 14). The cell fabricated generated an OCV of 0.91 V at 873 K and a maximum power density of 35 mWcm<sup>-2</sup> was achieved (Fig. 14).

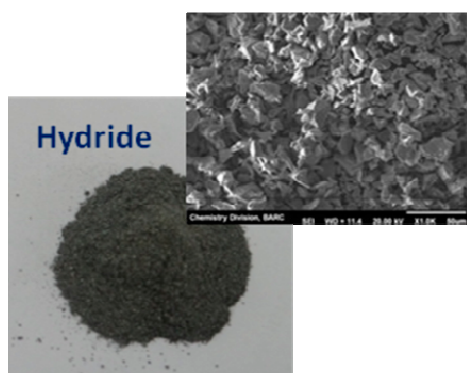
### 3.3. Hydrogen storage

For efficient utilization of hydrogen for energy purpose, suitable strategies need to be developed. Besides pressurization or liquefaction (an energy intensive process), several other hydrogen storage strategies such as metal hydride, chemical hydrides or adsorption on solid support (e.g. activated carbon, nano-structured carbon, MOFs, etc.) are being pursued globally. Chemistry Division has been actively involved for the development of alloys and carbon based materials for hydrogen storage application. In this direction hydriding behavior of a wide range of alloys/ inter-metallic compounds and metals has been investigated in detail

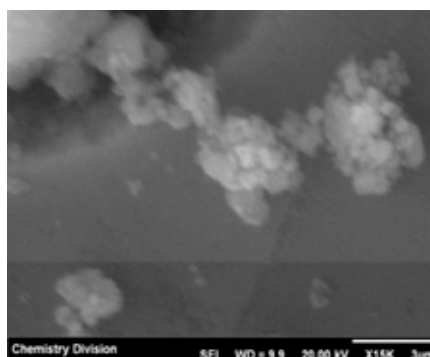
#### 3.3.1. Hydrogen absorption studies on Ti<sub>2</sub>CrV and Mg based systems

Hydrogen absorption studies on alloys and metals was carried out after absorption-desorption cycle at room temperature and 20 bar hydrogen pressure (Fig. 15). The results showed hydrogen absorption is fast for all the alloy samples. It is evident from the qualitative behavior of the kinetic plots that for the alloy Ti<sub>2</sub>CrV, the reaction starts immediately without any incubation time. Reacted fraction,  $\xi$ , increases with time and reaches a saturation value after certain time depending on the rate of the hydriding reaction.

To understand hydrogen absorption mechanism of the alloy, the kinetic data has been fitted with different equations and the mechanism has been predicted accordingly. The initial part of the hydrogen absorption reaction was fitted successfully with the equation for chemical reaction ( $kt = 1 - (1 - \zeta)^4$ ), where chemical reaction occurs between hydrogen and



Photo(left) and SEM image (right) of Ti<sub>2</sub>CrV alloy hydride. Hydrogen storage capacity is around 4 wt % (at room temperature and 20 bar pressure).



Ball milled Mg nanoparticles (80-100 nm)  
Hydrogen storage capacity: ~ 6wt % (at 275°C and 20 bar pressure)

Fig. 15: Hydrogen storage materials

the alloy. The later part of absorption reaction path can be fitted with the 3-dimensional diffusion mechanism ( $kt = 1-2\zeta/3-(1-\zeta)^{2/3}$ ), where hydrogen diffuses through the solid matrix. From the rate constant value it can be seen that the chemical reaction occurs at a much faster rate in the alloy compared to Mg. For alloy samples with multiple phases, the rate constant for the chemical reaction stage increases due to the presence of more interfaces. In multi component alloys due to the formation of mixed phase structure the crack formation and initial penetration of hydrogen through the phase boundary is faster so the initial hydrogen adsorption rate increases. For magnesium based system the hydrogen storage capacity is found to be remarkable with a value of around 6 wt.%. However the absorption and desorption temperatures are quite higher (above 250°C)

#### 4. Material and Methodology for Energy application

Chemistry Division, BARC also has a dedicated research program on developments material for energy application (energy storage, energy saving).

##### 4.1. Lithium and sodium ion batteries

Upcoming energy storage is primarily focused on the solid state battery and supercapacitors. Among them, lithium ion battery is one of the most promising energy-storage devices. In this regard R & D activities to develop newer materials or develop cost effective methods for production of desired materials are being carried out in the section. Attempts to increase the energy density of lithium ion batteries are being carried out by using modified electrodes.  $\text{LiFePO}_4$  and carbon coated  $\text{LiFePO}_4$  have been prepared, and the effect of Li concentration in  $\text{Li}_x\text{FePO}_4$  on the electrochemical performance such electrodes have been evaluated.

High energy density ( $\sim 107 \text{ mAh/g}$ ) is achieved in the cell based on electrodes made from  $\text{Li}_{1.05}\text{FePO}_4$ . Two-dimensional (2D-) carbon nanosheets derived from agricultural waste has been fabricated by heat treatment under controlled oxygen atmosphere. A full-cell lab prototype for sodium-ion batteries (SIBs) with discharge capacity of

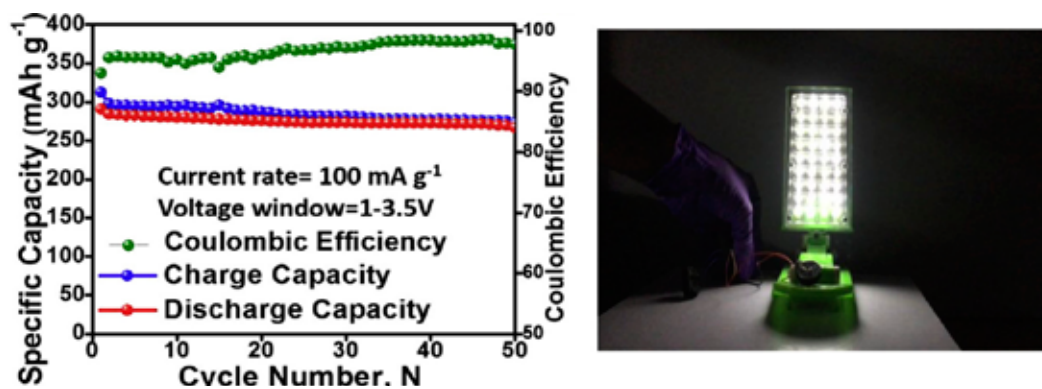
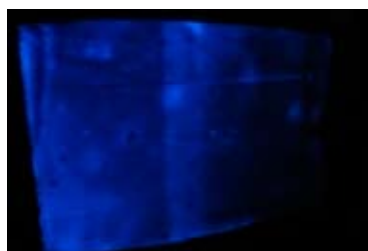


Fig. 16: Cycling rate performance with coulombic efficiency for indigenously developed Na ion coin cell prototype and LED lantern powered by it.

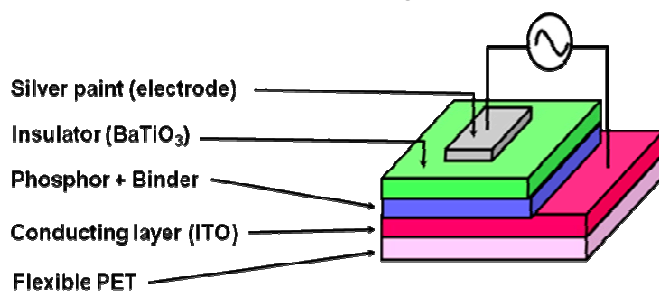
$\sim 266 \text{ mAh g}^{-1}$  was developed in collaboration with IIT Bombay using indigenously synthesized disordered mesoporous carbon anode from biowaste and NVP (sodium vanadium phosphate) cathode. A considerable energy density of  $\sim 380 \text{ Wh kg}^{-1}$  at  $\sim 2 \text{ V}$  region confirmed the efficient charge-discharge reaction of the full cell and its feasibility for practical applications was demonstrated by lighting a LED panel using a single Nacion coin cell (Fig. 16).

## 4.2. Electro-luminescence from inorganic materials in the powder form for solid state lighting applications

Many inorganic oxides in bulk and nano-size dimensions are potential candidates for the development of cost effective display devices. Such devices can be made by powder coating method and can be activated by applying AC and/or DC voltages. Powder electroluminescent devices are cost effective alternative to thin film electro-luminescent devices since the former devices can be made based on powder coating or screen printing techniques rather than the costlier vapour phase deposition processes. Using a substrate based on organic polymer (like for example ITO coated PTFE) for powder coating, additional advantage of mechanical flexibility for the devices can be achieved. Electro-luminescent devices based on ZnS:Cu which emit blue light has been fabricated and characterized (Fig. 17).



Blue light emitting display with size around 3" x 6" fabricated at Chemistry Division,



Schematic configuration of AC powder electro luminescence device

Fig. 17: Display devices

## 4.3. Search for rare earth phosphor for UV-pcLED

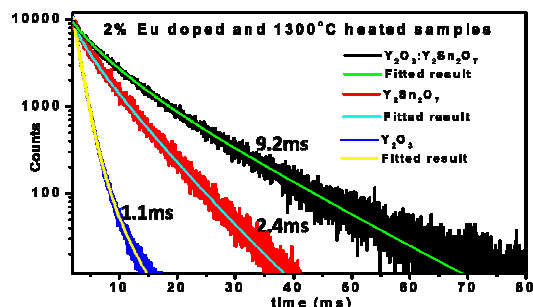


Fig. 18: Decay profile for  $^5D_0$  level of  $\text{Eu}^{3+}$  ion in different hosts

Energy loss in a phosphor coated LED (pcLED) originates from two sources after photons leave the LED chip: quantum efficiency (photoluminescent quantum yield) for the phosphor ( $\eta_q$  or  $f$ ), efficiency by package design ( $\eta_p$ ). In order to get phosphor with high internal quantum efficiency, joint experiment and theoretical investigation on various rare earth doped inorganic oxide matrices has been carried out (Fig. 18). Eu-



doped  $Y_2Sn_2O_7$  nanoparticle dispersed in  $Y_2O_3$  matrix has been found to be give very high Eu-life time and good internal quantum efficiency.

#### 4.4. Organometallic Chemistry

Organometallic chemistry of platinum and main group elements has been pursued with reference to their utility for the preparation of semiconductor materials, homogeneous catalysts and anticancer agents (Fig 19). The growing miniaturization and integration of electronic devices has evolved new growth processes. Success of these processes relies on the availability of suitable precursors of high purity. The Division has developed synthesis and purification methods for Groups III and V organometallic compounds. A facile preparative method based on gallium/-indium-magnesium alloy, rather than expensive and moisture-sensitive metal trichlorides was developed for the synthesis of trialkyl gallium/indium compounds (Fig. 20). The indigenous method of purification of these precursors has been developed.

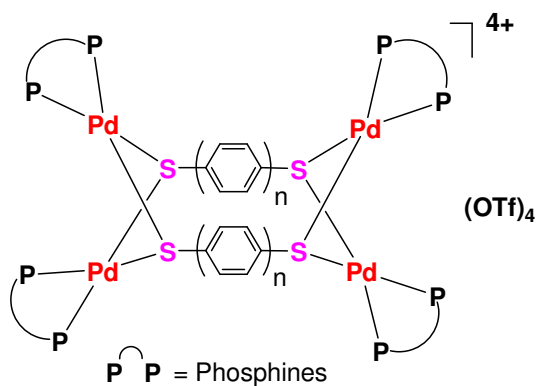


Fig.19: Supramolecular Pd complexes developed as excellent homogeneous catalysts for C-C and carbonylation reactions



Fig. 20: High purity tri-methyl gallium for CVD applications

The designed and synthesized several single source molecular precursors for meta I chalcogenides, e.g.  $ME$  ( $M = Zn, Cd, Hg; E = S, Se, Te$ ),  $Pd_4E$ ,  $Pd_7Se_4$ ,  $M_2E_3$  ( $M = In, Sb, Bi$ ),  $CuInE_2$  have been carried out. These precursors have been used for the synthesis of mono-dispersed metal chalcogenide nano-crystals and for deposition of thin films at moderately low temperatures.

#### 5. Environmental and Separation Science

Chemistry Division, has a research program on developments material for environmental and sensing application.

##### 5.1. Ionisation study of atmospherically important $CS_2$ molecules and clusters

Carbon disulfide ( $CS_2$ ) is one of the important species to contribute to global sulphur cycle along with  $SO_2$  and  $OCS$ . Volcanic eruptions and bushfires are responsible for

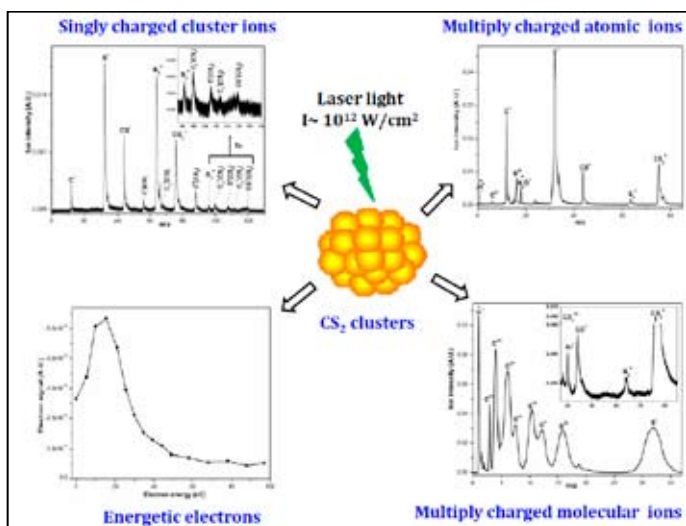


Fig. 21: Studies of interaction of light with  $\text{CS}_2$  clusters

ions were observed in the mass spectra. Based on electron energy measurement, generation of multiply charged atomic and molecular ion formation at  $10^{12}$  W/cm<sup>2</sup> laser intensity has been explained.

## 5.2. Thin film-based hydrogen sulfide sensor

Tin oxide thin films deposited on quartz substrates were used as  $\text{H}_2\text{S}/\text{SO}_2$  gas sensors by depositing gold interdigitated electrodes on top of the  $\text{SnO}_2$  thin film (Fig. 22). These sensors operate room temperature with sensitivity in the range of 1-80 ppm. The sensor was tested with Uran, ONGC plant gas samples (containing 98% hydrocarbons and  $\text{H}_2\text{S}$  in ppm range) and was found to be performing satisfactorily.



Fig. 22:  $\text{SnO}_2$  film-based sensor

Hydrogen Sulfide ( $\text{H}_2\text{S}$ ) is a toxic and flammable gas, usually generated in sewages, swamps, mines etc. It is also used in laboratories, industries and in heavy water plants as a process gas for producing heavy water ( $\text{D}_2\text{O}$ ). Hydrogen sulfide reacts strongly with living tissues and attacks the central nervous system. According to the Occupational Safety & Health Administration (OSHA, USA), the acceptable concentration limit for exposure to  $\text{H}_2\text{S}$  is 10 ppm for an 8-hour period. Chemistry Division has developed synthetic diamond based gas sensor to detect sub ppm levels of hydrogen sulfide at room temperature. Diamond is a unique material with a wide range of mechanical, optical, electrical, thermal and chemical properties. Though undoped diamond is an excellent insulator, hydrogen terminated diamond shows p-type surface conductivity, which has been exploited to detect trace levels (<1ppm) of hydrogen sulfide. The sensor operates at room temperature hence requires low thermal



budget and power, has stable and long life (> 3 years) and suitable for operation in corrosive and radiation environment.

## 6. Instrument Development

Chemistry Division is also involved in developing the scientific instruments for various in-house applications.

### 6.1. Indigenous development of a fully automated low temperature (10-310 K) calorimeter

Specific heat at low temperatures is an important material property to obtain fundamental understanding of material behaviour and also to qualify the material for high-end applications (cryogenics, refrigeration, superconductivity research, particle accelerators, vacuum science, biology, etc) where sub-ambient (cryogenic) temperatures are encountered. Techniques enabling indirect measurement of specific heat are enormously expensive. To cater the in-house requirement of low temperature calorimetric characterization of solids, a technology for a fully automated low temperature calorimeter (10 - 310 K) for measurement of specific heat of small solid samples (sample mass ~ 500 mg to 2 g) has been indigenously developed in Chemistry Group, BARC (Fig. 23). Unique attributes of this system are good accuracy ( $\pm 2-3\%$ ) and reliable, simple operation, easy maintenance, and cost effectiveness. This



Fig. 23: fully automated low temperature (10-310 K) calorimeter

equipment is an excellent import substitute to commercial cryogenic calorimeters, which are comparatively very costly and delicate to operate and maintain. Complete design, fabrication, testing and performance assessment of the calorimeter has been established, documented and is available in BARC website.

equipment is an excellent import substitute to commercial cryogenic calorimeters, which are comparatively very costly and delicate to operate and maintain. Complete design, fabrication, testing and performance assessment of the calorimeter has been established, documented and is available in BARC website.

### 6.2. Indigenously Developed High Temperature Dilatometer (RT - 1373 K)

Technology for an LVDT-based high temperature vertical dilatometer has been indigenously developed. A system capable of measuring the linear dilation behavior of solid samples over the temperature range from RT to 1373 K has been setup in Chemistry Division, BARC (Fig. 24). Developed system has excellent performance with  $\pm 3\%$  accuracy,  $\pm 1$  mm dilation measurement range and  $\pm 1$   $\mu\text{m}$  resolution. Developed equipment has very useful attributes such as complete indigenization with all locally manufactured components and accuracy at par with commercial dilatometer, minimum maintenance and nearly 5 times cost effective than equivalent commercial systems. This technology is presently available for commercialization through BARC website.



Fig. 24: High Temperature Dilato-meter (RT - 1373 K)

## 7. HRD Activities:

Other than the above mentioned scientific activities, Chemistry Division, BARC is also involved in various human resource development activities.

- (1) BARC-outreach program
- (2) Teaching in BARC Training School
- (3) Teaching in HBNI PhD Programme
- (4) Teaching in UM-DAE-CEBS
- (5) Member selection committee/promotion committees of Scientific officers.
- (6) Mentoring Research Scholars/ project trainees/ summer students of Chemistry Division
- (7) Organizing ISMC series of conferences and NWMC series of workshops
- (8) Invited talk/lectures at various national/international events

In summary, the above mentioned research activities carried out in Chemistry Division indicate that Division strives to strike a perfect balance between fundamental and technology oriented research. The efforts made by our scientists have resulted good number of publications in international peer reviewed journals and in various technologies. The work has been appreciated and recognized at various forums in form of awards to our scientists by different scientific bodies.



**Dr. A. K. Tyagi** is presently heading the Chemistry Division of Bhabha Atomic Research Centre, Mumbai, and is also a Senior Professor (Chemistry) and Dean-Academic (Chemical Sciences) at Homi Bhabha National Institute (HBNI), Mumbai. His research interests are in the field of nanomaterials, functional materials, nuclear materials and Hybrid materials. He has published more than 600 papers in international journals, five books and several review articles. He has supervised / co-supervised 28 students for their PhD and another 10 students are presently pursuing PhD under his supervision / co-supervision.

He has been conferred with a number of prestigious awards such as DAE-Homi Bhabha Science and Technology Award, DAE-SRC Outstanding Researcher Award, DAE-Group Achievement Award; MRSI Medal; MRSI-ICSC Materials Science Senior Award; MRSI-CNR Rao Prize in Advanced Materials; CRSI Bronze Medal; CRSI-CNR Rao National Prize in Chemical Sciences; CRSI-Silver Medal; Medal of Indian Nuclear Society; Rheometric-ITAS Award; ISCAS-Dr. Lakshmi Award; IANCAS-Dr. Tarun Datta Memorial Award; R. D. Desai Memorial Award of Indian Chemical Society; Rajib Goyal Prize in Chemical Sciences; ISCB Excellence Award in Chemical Sciences; CCRS Award in Chemical Sciences; ISCA Platinum Jubilee Lecture Award in Materials Science; Metallurgist of the year award from Ministry of steel, GOI; and National Prize in Solid State and Materials Chemistry.

He is a Fellow of the Maharashtra Academy of Sciences; Royal Society of Chemistry; National Academy of Sciences, India; Indian Academy of Sciences and Asia Pacific Academy of Materials.

He is a Member of INSA National Committee on Crystallography, Member DST-Project Assessment Committee (Inorganic and Physical Chemistry), Member Board of Studies (Chemical Sciences), Homi Bhabha National Institute, and Member Academic Council of Jawaharlal Nehru University, Delhi (2016-18).

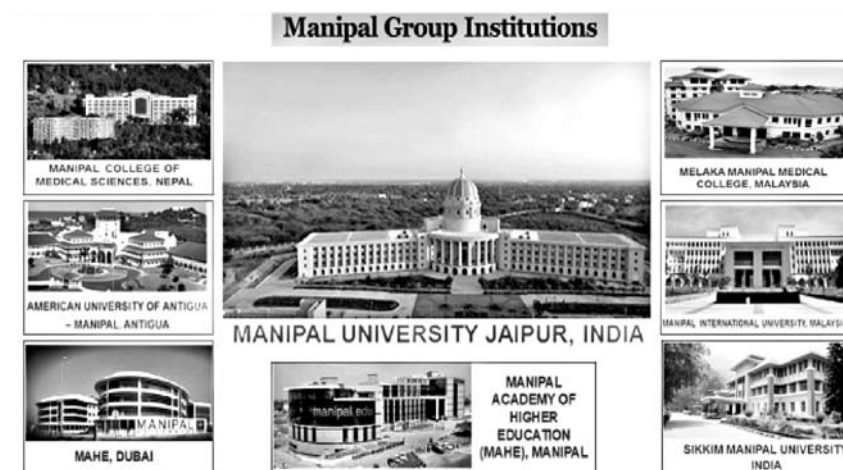
He did postdoctoral research at Max-Planck Institute, Stuttgart, Germany (1995-96) and subsequently has been a visiting scientist to several countries like USA, France, Canada, Japan, Russia, Germany, China, Portugal, Singapore, Australia, Sweden, Italy, Spain, Israel, Malaysia and South Africa.

## The School of Basic Sciences @ MUJ

**Lalita Ledwani**

*School of Basic Sciences, Manipal University Jaipur, Rajasthan*

The Manipal Education Group, with its heritage of excellence in higher education for over 60 years, launched Manipal University Jaipur (MUJ) in 2011 with the vision “*Global Leadership in Higher Education and Human Development*”.

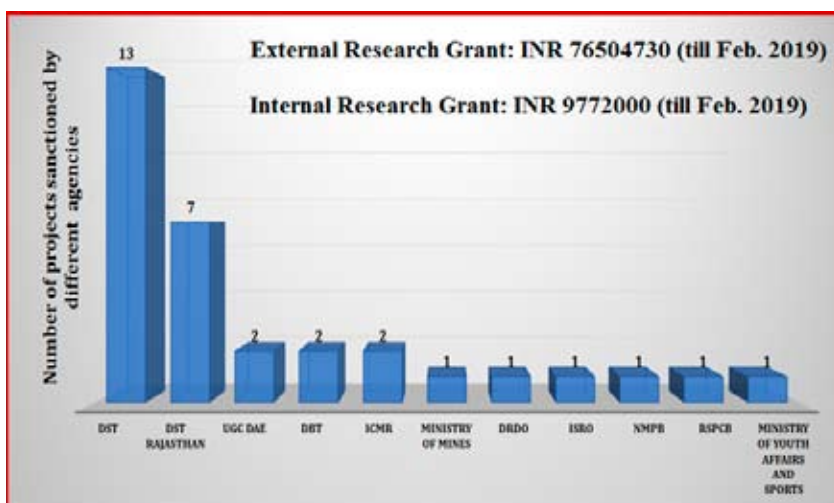


MUJ was established on an invitation from the Government of Rajasthan and has been established by an Act (No. 21 of 2011) of State Legislature of Rajasthan as a State Private University as specified by UGC under section 22 of the UGC Act 1956. MUJ is driven by the mission of “*Be the most preferred University for Innovation and Interdisciplinary learning*”

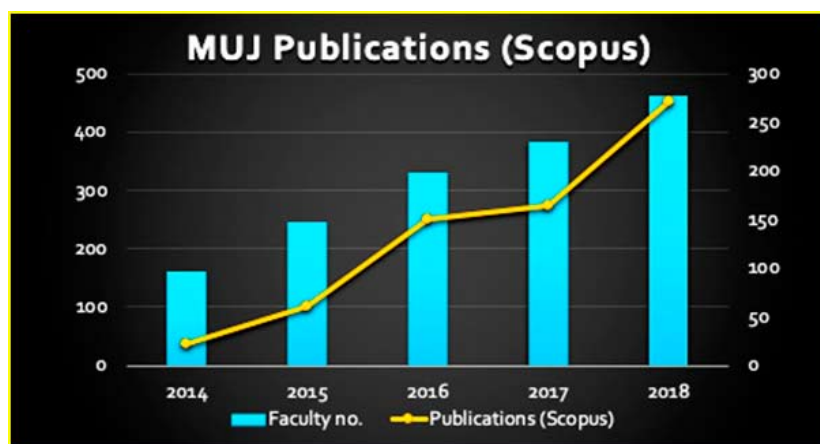
*Foster academic research and professional excellence in all domains. Transferring young minds into competent professionals with good human values*”. The university has a total land area of 122 acres, with constructed area of 2.0 million sq. ft. located at Dehmi Kalan village 30kms from Jaipur off Jaipur-Ajmer Expressway. MUJ has best in-class infrastructure, including the state-of-the-art research facilities and a modern digital library. As a multi-disciplinary University, MUJ offers career-oriented courses at UG, PG and Doctoral levels, across diverse streams. Currently more than 7000 students are enrolled across all programs. A well-qualified team of 463 faculty members is the asset of the University. MUJ has won many Awards and Recognitions in a short span of time, like 2<sup>nd</sup> in 2017-18 and 5<sup>th</sup> in 2018-19 Swachhta Ranking awarded by MHRD, NIRF TOP 200 Universities GRIHA Five Star Award conferred by MNRE, Govt. of India, Digital India - Smart Campus Award given by NDTV-CISCO, Best University Campus Award conferred by ASSOCHAM, Outstanding Contribution to Digital India Award given by The Economics Times, Indo Global Architecture Education Excellence Award for

promoting quality education in the field of Architecture by Indo Global Chamber of Commerce, Week Ranking, Outlook ICARE Ranking, Industries and Agriculture Pune and Dewang Mehta National Education Award for Best B School 2015 awarded to TAPMI School of Business. MUJ has signed over 89 MOUs Academic Institutions & Industries to provide its students international exposure and job opportunities at global level.

MUJ, a new generation University, is committed to nurturing talent and strengthening academics & research by adopting unique & innovative practices to continue to redefine academic excellence. MUJ envisages process of convergence of traditional disciplines as key to accomplish previously unimaginable. With this foresight, MUJ has been promoting multidisciplinary research programme, focusing on basic and applied research, technology development and innovation. It is this vision that has helped the



*External Research Grants*



*Last five years publications (Scopus Indexed)*

institute to do very well in all spheres of science, engineering and humanities and social sciences. MUJ provides excellent environment for fostering research among faculty and students through a dedicated Directorate.

MUJ provides strong support for research projects and consultancies with the state-of-the-art central analytical facilities, industry sponsored labs, internal and external fund provisions. Research has always been an area of paramount importance to University. To this end, mentioned policies have been put in place to nurture, promote and elevate research activities and to create an enabling environment within MUJ in order to foster research culture.

Central Analytical Facility has been established at the university premise, which provides several sophisticated instrumentation facility including Atomic Absorption Spectroscopy (AAS), Gas Chromatography–Mass Spectrometry (GC-MS), High Performance Liquid Chromatography (HPLC), Thermo-Gravimetric Analyser (TGA), UV-Vis Spectrophotometer and Fourier-Transform Infrared Spectroscopy (FTIR) etc.

MUJ also has Teacher Empowerment Centre to equip, synergize and foster them as active learners. MUJ follows proactive and transparent system of governance with efficient and effective holistic human development programs in line with Manipal Group legacy. The University has faculty to student ratio of 1:16. MUJ has distributed more than 7000 computers/ laptops. There is central media centre with recording facility for lecture capturing at MUJ. E-governance based on ERP is used by MUJ for academic/ administrative/ financial functions. University has more than 200 Wi-Fi network points with 1Gbps total bandwidth.

Manipal group believes in giving back to society, following this ideology scholarship worth Rs. 6.40 Crores is given to students. Directorate of Student Welfare provides 360-degree student support. Standing committees for anti-ragging, women's grievances redressal are being constituted by MUJ. University has 31 active professional associations, student chapters and student clubs.

### **School of Basic Sciences**

The School of Basic Sciences (SBS) under Faculty of Science (FOS) aims to foster creativity and innovation for an intellectually satisfying learning environment as well as to establish MUJ as a globally preferred destination for students, faculty, researchers and other stakeholders. The School of Basic Sciences (SBS) which was entrusted with the responsibility of developing and executing academic programs in different discipline of Basic Sciences at undergraduate, postgraduate and research levels. The School operates through five departments: Physics, Chemistry, Mathematics & Statistics Biosciences, and Department of Computer Applications. It also supports the teaching of Science courses in other Schools of the University to promote interdisciplinary studies. The SBS has developed syllabi for various core courses blending basic science with interdisciplinary topics. Experimental learning, study visits to industries and research institutes are integral

parts of all programs. These enable students to excel in the areas of basic as well as applied sciences. In addition, they serve as launching pads for attractive carrier opportunities in the academia and industry. The school has unique synergy of teaching and research with many national as well as international interactions and collaborations.

More than 100 research scholars are pursuing their research degree under the School. SBS is also receiving the funds from various government agency in the form of research projects. SBS organizes regular workshops, seminars and expert lectures to facilitate the scientific activity in the university campus. Beside such international and national level conferences, DST- inspire camps have been organized in the campus.

Along with academics and research, SBS is routinely organizing various events and outsourcing activities. Glimpses of some important events are given below:

### **Major Events Conducted by School of Basic Sciences (2018-19)**



### **Fourth Inspire Camp (January 02 to January 06, 2018)**



*Outreach activity (School-connect) on January 18, 2019*





*National Workshop on “Statistical and Optimization Learning in Multidisciplinary Arena in Conjunction with National Statistics Day from June 25-29, 2018*



*24th ISCB International Conference from January 11-13, 2018*



*National Conference on Advancement in Materials Science & Physics (November 19, 2018)*





*National Workshop on FOLDSCOPE & Symposium on Applied Microbiology (November 23-24, 2018)*



*Nukkad Natak on Hygiene in Govt. School, Dehmi Kalan on January 24, 2019*



*National Science Day (February 28, 2019)*



*Science Colloquium (2018-19)*



*Poster Exhibition and Competition (October 03, 2019)*

### **Department of Chemistry:**

Department of Chemistry has started its functioning since the inception of the University. Department of Chemistry, MUJ, has a vibrant research program which includes all frontier areas of research. There are 16 faculty members who are actively involved in state of art research on all major domains of chemistry like Organic synthesis, Heterocyclic chemistry, Plasma Chemistry, Sensitized solar cells, Photocatalysis, Homogeneous catalysis, Polymer Nano-composites, Computational & Quantum Chemistry, Supra-Molecular Chemistry, Waste water Treatment, Blue Carbon Sequestration, Electrochemistry, Heavy metal pollution & Remediation. The department has adequate equipment for carrying out cutting edge research and the research is showcased in major journals of repute. Department has received research grants from major funding agencies like DST, GoI, DST Rajasthan, DAE, DBT, KWEF Japan.

## Faculty members &amp; their specializations @ Chemistry Department

S. NO.	Name of Faculty	Designation	Specialization
1.	Dr. Lalita Ledwani	Professor/ Director SBS	Natural Products, Surface modification of polymers, Bioremediation, Medicinal Plants.
2.	Dr. Babita Malik	Professor	Synthetic organic chemistry, Heterocyclic chemistry, Green Chemistry, Engineering Chemistry
3.	Dr. Rahul Shrivastava	Head Department of Chemistry and Associate Professor	Host-Guest chemistry, Molecular recognition and Supramolecular chemistry, Dye Synthesized Solar Cell
4.	Dr. Nitu Bhatnagar	Associate Professor	Polymeric composites & Nanotechnology, Plasma Chemistry, Adhesion science, Biomaterials, Pesticide Analysis
5.	Dr. Veena Dhayal	Associate Professor	Coordination chemistry, Organometallic chemistry and nanomaterials
6.	Dr. Arunava Agarwala	Associate Professor	Inorganic Chemistry
7.	Dr. Praveen Kumar Surolia	Associate Professor	Solar Energy and Photocatalysis, Energy storage, Material science
8.	Dr. Debasis Behera	Assistant Professor	Corrosion Inhibitors, corrosion monitoring, electrochemistry, molecular modelling
9.	Dr. Naveen Kumar Singh	Assistant Professor	Ecotoxicology & Bioremediation, Pollution monitoring and Assessment, Risk Assessment and mitigation, Heavy metal pollution.
10.	Dr. Meenakshi Pilia	Assistant Professor	Organic Synthesis, Heterocyclic chemistry, C-H activation, Organoiodine chemistry

11.	Dr. Sriparna Ray	Assistant Professor	Organometallic Chemistry, Organometallic Chemistry, Homogeneous catalysis, Biocatalysis, Bioelectrocatalysis
12.	Dr. Susruta Samanta	Assistant Professor	Computational Chemistry, Molecular dynamics simulations, Free energy calculations, Antibiotic translocation, drug-polymer interactions, polymer-biomembrane interactions, computer aided drug designing.
13.	Dr. Sarika Singh	Assistant Professor	Shape controlled synthesis of oxide, Mixed-oxide nanomaterials, Nanocomposites, Core shell nanosphere, Functional nanomaterials, Nanomaterials for waste water purification, Antibacterials activity, Dry reforming of methane
14.	Dr. Abhiroop Chowdhury	Assistant Professor	Heavy metal mobilization, Remediation of metal pollutants, Blue-Carbon sequestration, Climate change Ecology, Mangrove regeneration.
15.	Dr. M. Prabhu Inbaraj	Assistant Professor	Wastewater Treatment, Adsorption technology, Stress physiology, Chlorophyll fluorescence, SEM/TEM, Phytoremediation, Mine Rehabilitation,



**Dr. Lalita Ledwani** is working as Professor of Chemistry and Director, School of Basic Sciences at Manipal University Jaipur, Rajasthan, India. Her areas of research interest are natural products, polymer surface modification techniques, green nano-materials, wastewater treatment. She is recipient of Research Grant Award 2015 from KWEF, Japan and also received financial support for research projects from different funding agencies namely DST, Govt of India; DST, Govt. of Rajasthan; DBT, Govt of India and UGC, Govt. of India. Dr. Ledwani has more than thirty research manuscripts published in reputed peer reviewed journals and books, delivered around two dozen invited/expert lectures besides over forty five research papers in conferences and edited two books. She is guiding UG, PG, Ph.D and post-doctoral students. Dr. Ledwani is associated with various national and international professional bodies as fellow, life member, or member. Dr. Ledwani has also organized various national and international academic events in a lead role.

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**List of Participant – NWMC 2019**

<b>Sr. No.</b>	<b>Name</b>	<b>Institute</b>
1	A Samson Nesaraj	Karunya Institute of Technology and Sciences, Coimbatore
2	A. K. Chauhan	BARC, Mumbai
3	A. K. Satpati	BARC, Mumbai
4	Abdul Kaium Mia	IIT-Guwahati, Guwahati
5	Abhijeet Singh	Manipal University Jaipur, Rajasthan
6	Abhilasha Jain	Visvesvaraya National Institute of Tech., Nagpur
7	Abhiram Senapati	IGCAR, Kalpakkam
8	Abhishek Sharma	Manipal University Jaipur, Rajasthan
9	Abhishek Sharma	HBNI, Mumbai
10	Abiroop Chowdhury	Manipal University Jaipur, Rajasthan
11	Adish Tyagi	BARC, Mumbai
12	Ajay Kumar	Manipal University Jaipur, Rajasthan
13	Ajay Saini	Manipal University Jaipur, Rajasthan
14	Akshay Narayan Gaikwad	Bits Pilani K K Birla Goa Campus, Goa
15	Amit K. Sharma	HBNI, Mumbai
16	Anees Y. Khan	Manipal University Jaipur, Rajasthan
17	Ankit Kumar	SLIET, Longowal
18	Ankit Yadav	IISc, Bangalore
19	Annu Dahiya	University of Delhi, Delhi
20	Anoop Mukhopadhyay	Manipal University Jaipur, Rajasthan
21	Anupam Agarwal	Manipal University Jaipur, Rajasthan
22	Anupam Sharma	Manipal University Jaipur, Rajasthan
23	Anushree P Khandale	IIITDM, Kancheepuram
24	Arjun Singh	CSIR-NPL, New Delhi
25	Aruna	Manipal University Jaipur, Rajasthan
26	Arunava Agarwala	Manipal University Jaipur, Rajasthan

<b>Sr. No.</b>	<b>Name</b>	<b>Institute</b>
27	Ashima Bagaria	Manipal University Jaipur, Rajasthan
28	Ashok Kumar Kakodia	ShriGovind Guru Govt. College, Banswara, Rajasthan
29	Babita Malik	Manipal University Jaipur, Rajasthan
30	Bhumika	J.C.BoseUniversity, YMCA, Faridabad
31	Bhupender Singh	Panjab University, Chandigarh
32	C. A. Amarnath	BARC, Mumbai
33	Chandrani Deep Niranjana	RK University, Rajkot
34	D. K Aswal	CSIR-NPL, New Delhi
35	Dachepalli Ravinder	Osmania University, Hyderabad
36	Dalip. S. Shekhawat	Manipal University Jaipur, Rajasthan
37	Darshanan Ghonge	BARC, Mumbai
38	Dasarath Maji	IGCAR, kalpakkam
39	Debasis Behera	Manipal University Jaipur, Rajasthan
40	Deepak Tyagi	BARC, Mumbai
41	Deepali Shrivastava	Pillai College of Engineering, Panvel, Navi Mumbai
42	Deepti Jain	Manipal University Jaipur, Rajasthan
43	Deepti Sharma	Manipal University Jaipur, Rajasthan
44	Dheeraj Jain	BARC, Mumbai
45	Dileep Kumar Yadav	University of Delhi, Delhi
46	Garima	Manipal University Jaipur, Rajasthan
47	Harshavardhan Thodupunoori	Bits Pilani K K Birla Goa Campus, Goa
48	Harshita Sachdeva	University of Rajasthan, Jaipur
49	Indeewar	Manipal University Jaipur, Rajasthan
50	Ishant Chauhan	Sri Guru Granth Sahib World University, Fatehgarh Sahib
51	J. P. Mittal	DAE, Mumbai

<b>Sr. No.</b>	<b>Name</b>	<b>Institute</b>
52	Jagannath Korody	Manipal University Jaipur, Rajasthan
53	Jamil Akhtar	Manipal University Jaipur, Rajasthan
54	Jaspreet Singh Aulakh	G. B. Pant University of Agri. & Tech., Pantnagar
55	Jayesh Rajendra Pawar	Swami RamanandTeerthMarathwada University, Nanded
56	Jyoti	IIT-DELHI, New Delhi
57	JyotiLaxmi Sharma	Manipal University Jaipur, Rajasthan
58	K. C. Barick	BARC, Mumbai
59	K. P. Mishra	Manipal University Jaipur, Rajasthan
60	K. Sandeep Rao	BARC, Mumbai
61	Kalisadhan Mukherjee	PanditDeendayal Petroleum University, Gandhinagar
62	Kanchan	Manipal University Jaipur, Rajasthan
63	Kruti Krishna Halankar	BARC, Mumbai
64	Kulwinder Singh	Sri Guru Granth Sahib World University, Fatehgarh Sahib
65	Kuntal Kumar Pal	IGCAR, kalpakkam
66	Lalita Ledwani	Manipal University Jaipur, Rajasthan
67	Linesh Raja	Manipal University Jaipur, Rajasthan
68	M. Riswan Ahamed	SRM Institute of Sci. & Tech., Chennai
69	M. Shankar	Yogi Vemana University, Kadapa
70	Mahesh G. Bansod	RTM Nagpur University, Nagpur
71	Mahesh Kumar	IIT Jhodhpur, Jhodupur
72	Mahesh Kumar Paliwal	Govt. Girls College, Chomu, Jaipur
73	Mahesh Kumar Yadav	Central University of Rajasthan, Kishangarh
74	Manpreet Kaur	Punjab Agricultural University, Ludhiana
75	Manpreet Singh	CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar



<b>Sr. No.</b>	<b>Name</b>	<b>Institute</b>
76	Meenakshi Pilia	Manipal University Jaipur, Rajasthan
77	Michel P. Inbaraj	Manipal University Jaipur, Rajasthan
78	Mona Vajpayee	Manipal University Jaipur, Rajasthan
79	Mousumi Debnath	Manipal University Jaipur, Rajasthan
80	Mumal Singh	Manipal University Jaipur, Rajasthan
81	Muthukumar V R	SRM Institute of Sci. & Tech., Chennai
82	Naveen Kumar	Manipal University Jaipur, Rajasthan
83	Neelamsharma	Manipal University Jaipur, Rajasthan
84	Neeraj Kumar Mishra	IIT(ISM), Dhanbad
85	Nidhi Deveshbhai Ruparelia	P.D.Patel Institute of Applied Sciences, Changa, Anand
86	Niharika	CSIR-IMMT, Bhubaneswar
87	Nitin Kumar Khandelwal	IISER Kolkata, Mohanpur
88	Nitu Bhatnagar	Manipal University Jaipur, Rajasthan
89	Nobel Tomar	J.C.Bose University, YMCA, Faridabad
90	Nowduri Annapurna	Andhra University College of Engineering, Visakhapatnam
91	Oinam Bedajit Meitei	Manipal University Jaipur, Rajasthan
92	P. A. Hassan	BARC, Mumbai
93	Pallavi Saxena	Mohanlal Sukhadia University, Udaipur
94	Paramesh Chandra	Visva-Bharati, Bolpur
95	Parveen Kumar	University of Delhi, Delhi
96	Pawan Sharma	Guru Jambheshwar University of Sci. & Tech., Hisar
97	Pooja Singh	Manipal University Jaipur, Rajasthan
98	Prabhat Ranjan	Manipal University Jaipur, Rajasthan
99	Pragati Shukla	BARC, Mumbai
100	Prashant Kumar	CSIR-NPL, New Delhi

<b>Sr. No.</b>	<b>Name</b>	<b>Institute</b>
101	Pratibha Sunil Agrawal	Laxminarayan Institute of Technology, Nagpur
102	Pratiksha Joshi	CSIR-Indian Institute of Petroleum, Dehradun
103	Praveen K. Surolia	Manipal University Jaipur, Rajasthan
104	Preeti Chaudhary	IIT-DELHI, New Delhi
105	Priyanka Hanumant Kamble	HBNI, Mumbai
106	PriyankaPareek	Manipal University Jaipur, Rajasthan
107	PriyankaYadav	University of Delhi, Delhi
108	Pruthivi G	Bits Pilani K K Birla Goa Campus, Goa
109	Puruman Singh Rathore	HBNI, Mumbai
110	Pushpal Ghosh	HS Gour Central University, Sagar
111	Pushpendra Kumar	Manipal University Jaipur, Rajasthan
112	R Srinivasan	SRM University, Sonapat
113	R. Azarudeen	Coimbatore Institute of Tech., Coimbatore
114	R. Dhaka	IIT-DELHI, New Delhi
115	R. N. Ambade	BARC, Mumbai
116	Rahul Shrivastava	Manipal University Jaipur, Rajasthan
117	Rajeev Mishra	Manipal University Jaipur, Rajasthan
118	Rakesh Sharma	Manipal University Jaipur, Rajasthan
119	Ramesh Nath Goswami	CSIR-Indian Institute of Petroleum, Dehradun
120	Randeep Kaur	Panjab University, Chandigarh
121	Rashi Nathawat	Manipal University Jaipur, Rajasthan
122	Rasmita Barik	IIT-DELHI, New Delhi
123	Ravinder	IIT-Guwahati, Guwahati
124	Renu Bist	University of Rajasthan, Jaipur
125	Renuka	Manipal University Jaipur, Rajasthan
126	Rohit Jain	Manipal University Jaipur, Rajasthan
127	Rubel Chakravaty	BARC, Mumbai

<b>Sr. No.</b>	<b>Name</b>	<b>Institute</b>
128	Rupesh Hiranman Gaikwad	MaharshiDayanand College, Parel ,Mumbai
129	S. A. Ansari	BARC, Mumbai
130	S. K. Samanta	BARC, Mumbai
131	Sabina Gurung	Raja Ramanna Centre for Advanced Technology, Indore
132	Sachin Pal	University of Delhi, Delhi
133	SaiKiran M	Sri SathyaSai Institute of Higher Learning, Anantapur
134	Saikat Chattopadhyay	Manipal University Jaipur, Rajasthan
135	Sama Jain	Poornima Institute of Engineering and Technology, Jaipur
136	Sameer Sapra	IIT-DELHI, New Delhi
137	Sandeep Nigam	BARC, Mumbai
138	SandeepYadav	Guru JambheshwarUnviersity of Sci. & Tech., Hisar
139	Sandip Dhara	IGCAR, Kalpakkam
140	Sangeeta Tantubay	IIT-Kharagpur, Kharagpur
141	Sanjay Soni	Manipal University Jaipur, Rajasthan
142	Santosh Patil	Manipal University Jaipur, Rajasthan
143	Sanyukta	IIT-DELHI, New Delhi
144	Saraswathi G	SRM Institute of Sci. & Tech., Chennai
145	Saroj Saha	Visva-Bharati, Bolpur
146	Sayan Bhattacharya	IISER Kolkata, Mohanpur
147	Shahla Imteyaz	IIT-DELHI, New Delhi
148	Shreya	University of Delhi, Delhi
149	Shubhra Pareek	Manipal University Jaipur, Rajasthan
150	Shwetambara Jha	IIT-DELHI, New Delhi
151	Somak Chatterjee	BITS Pilani, Pilani, Rajasthan
152	Sonal Maroo	BARC facility, Kalpakkam

Sr. No.	Name	Institute
153	Sonali Mehra	CSIR-NPL, New Delhi
154	Sriparna Ray	Manipal University Jaipur, Rajasthan
155	Sumit Kumar	University of Delhi, Delhi
156	Sunil Duhan	IIT Jhoshpur, Jhoshpur
157	Suraj Tamta	University of Delhi, Delhi
158	Susruta Samanta	Manipal University Jaipur, Rajasthan
159	Suvendu Kumar Barik	IGCAR, Kalpakkam
160	Tadasha Jena	IIT-Guwahati, Guwahati
161	Tarunbhai Fulaji Parangi	Sardar Patel University, Vallabh Vidyanagar
162	V. K. Jain	CEBS, DAE, Mumbai
163	V. Sudarsan	BARC, Mumbai
164	Vaishali Anandrao Sawant	Shivaji University, Kolhapur
165	Veena Dhayal	Manipal University Jaipur, Rajasthan
166	Vinita Sharma	BBD Govt. College, Chimanpura
167	Y. K. Bhardwaj	BARC, Mumbai
168	Yogendra Nath Chouryal	HS Gour Central University, Sagar

**List of Volunteers from Manipal University Jaipur, Rajasthan**

Sr. No.	Name
1	Ashish Sharma
2	Bhanupratap
3	Devanshi Ledwani
4	Divyansh Choudhary
5	Hitlesh Ajmera
6	Khushal
7	Khyati Malik
8	Manan
9	Nandita

Sr. No.	Name
10	Neeraj Gaur
11	Pranjal
12	Ram Prawesh
13	Sandeep Rana
14	Shivangi Tripathi
15	Shruti Sujit
16	Subhanushi
17	Suman Yadav
18	Tarun B. Kriplani
19	Tushar

**List of Institutes:**

<b>Sr. No.</b>	<b>Institute Name</b>
1	Andhra University College of Engineering, Visakhapatnam
2	BARC facility, Kalpakkam
3	BARC, Mumbai
4	BBD Govt. College, Chimanpura
5	Bits Pilani K K Birla Goa Campus, Goa
6	BITS Pilani, Pilani, Rajasthan
7	CEBS, DAE, Mumbai
8	Central University of Rajasthan, Kishangarh
9	Coimbatore Institute of Tech., Coimbatore
10	CSIR-Central Salt and Marine Chemicals Research Institute, Bhavnagar
11	CSIR-IMMT, Bhubaneswar
12	CSIR-Indian Institute of Petroleum, Dehradun
13	CSIR-NPL, New Delhi
14	G. B. Pant University of Agri. & Tech., Pantnagar
15	Govt. Girls College, Chomu, Jaipur
16	Guru Jambheshwar University of Sci. & Tech., Hisar
17	HBNI, Mumbai
18	HS Gour Central University, Sagar
19	IGCAR, Kalpakkam
20	IIITDM, Kancheepuram
21	IISc, Bangalore
22	IISER Kolkata, Mohanpur
23	IIT Jhoshpur, Jhoshpur
24	IIT(ISM), Dhanbad
25	IIT-DELHI, New Delhi
26	IIT-Guwahati, Guwahati
27	IIT-Kharagpur, Kharagpur
28	J.C.Bose University, YMCA, Faridabad
29	Karunya Institute of Technology and Sciences, Coimbatore

<b>Sr. No.</b>	<b>Institute Name</b>
30	Laxminarayan Institute of Technology, Nagpur
31	Maharshi Dayanand College, Parel ,Mumbai
32	Manipal University Jaipur, Rajasthan
33	Mohanlal Sukhadia University, Udaipur
34	Osmania University, Hyderabad
35	P.D.Patel Institute of Applied Sciences, Changa, Anand
36	Pandit Deendayal Petroleum University, Gandhinagar
37	Panjab University, Chandigarh
38	Pillai College of Engineering, Panvel, Navi Mumbai
39	Poornima Institute of Engineering and Technology, Jaipur
40	Punjab Agricultural University, Ludhiana
41	Raja Ramanna Centre for Advanced Technology, Indore
42	RK University, Rajkot
43	RTM Nagpur University, Nagpur
44	Sardar Patel University, VallabhVidyanagar
45	Shivaji University, Kolhapur
46	Shri Govind Guru Govt. College, Banswara, Rajasthan
47	SLIET, Longowal
48	Sri Guru Granth Sahib World University, Fatehgarh Sahib
49	Sri Sathya Sai Institute of Higher Learning, Anantapur
50	SRM Institute of Sci. & Tech., Chennai
51	SRM University, Sonapat
52	Swami Ramanand Teerth Marathwada University, Nanded
53	University of Delhi, Delhi
54	University of Rajasthan, Jaipur
55	Visva-Bharati, Bolpur
56	Visvesvaraya National Institute of Tech., Nagpur
57	Yogi Vemana University, Kadapa

Researcher from different institutes taking part in NWMC 2019.

Institutes are marked in map of India









